Electronic Supplementary Information for Dalton Transactions

μ-Chlorido,μ-Hydroxo-bridged Dicarbonyl Ruthenacycles: Synthesis, Structure and Catalytic Properties in Hydrogen Atom Transfer.

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Electronic Supporting Information.

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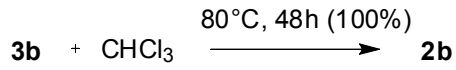
A. Experimental Details

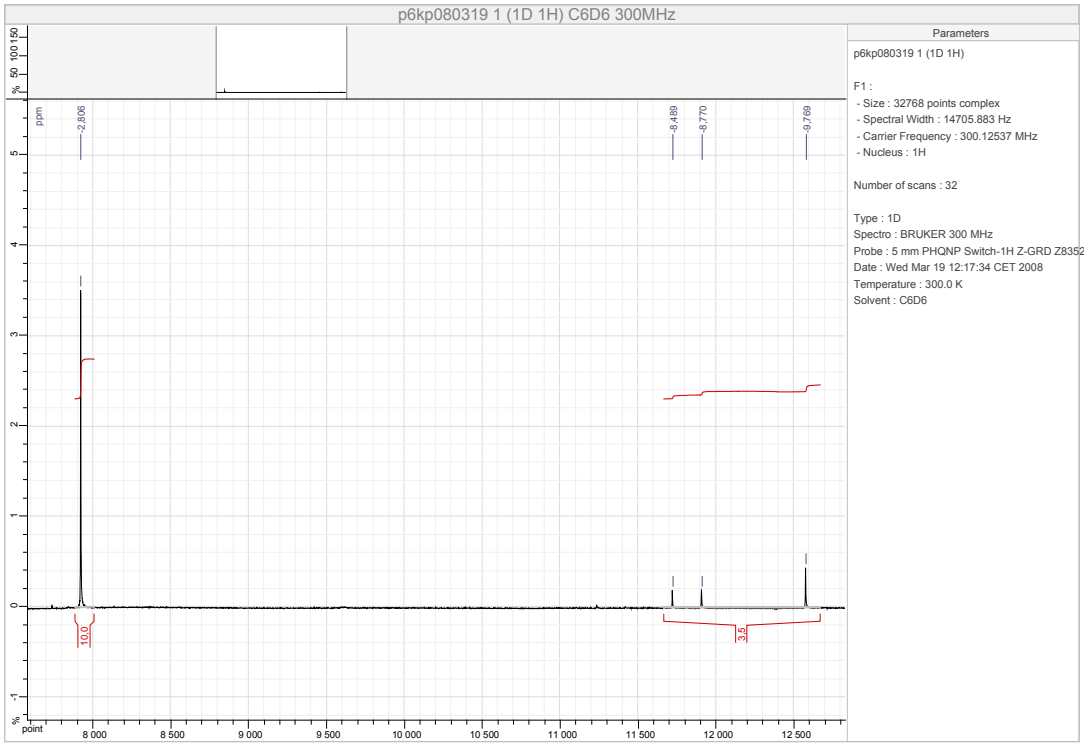
1. Reaction of hydroxo,chloro-bridged dimers with chloroform



Under argon atmosphere, a 100-mL *Schlenk* tube containing a magnetic stirring bar was loaded with 90 mg of **3b** (0.104 mmol) and 15 mL oxygen-free freshly distilled chloroform was added. The solution was brought to 80 °C on the oil bath and after 48 h refluxing it gave **2b** in 100 % yield (determined by ^{1}H NMR – no residual signal of Ru-O*H* at –3 ppm).

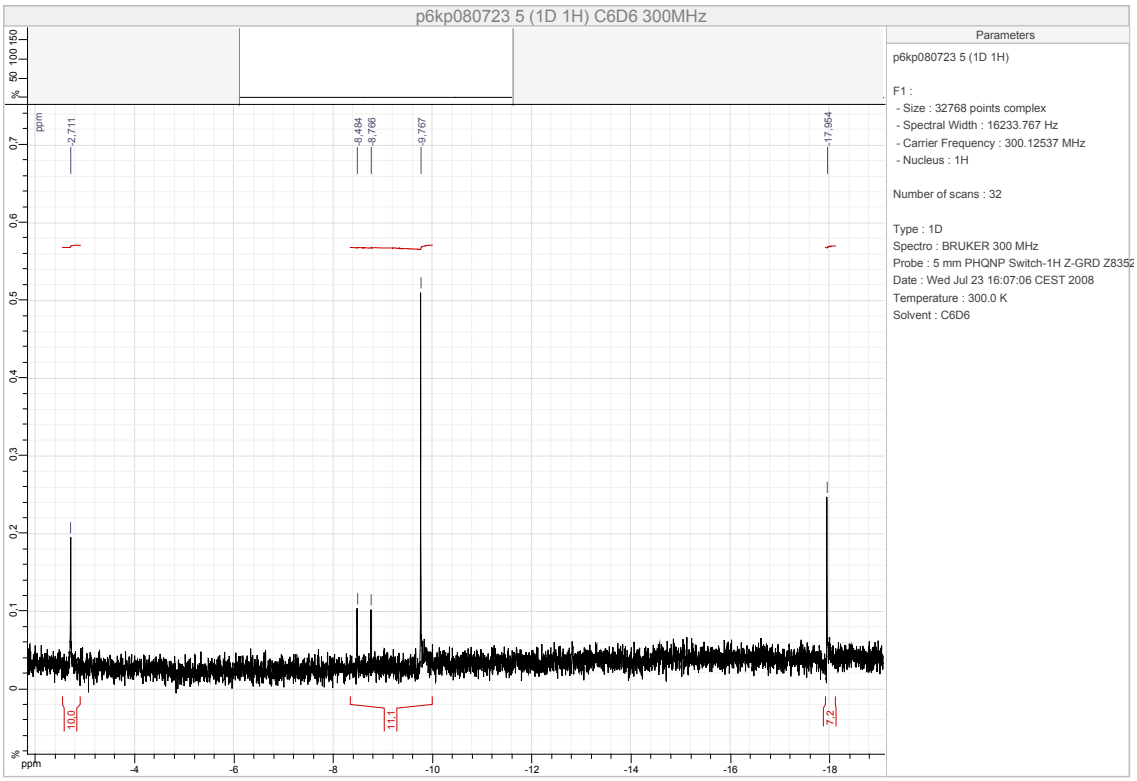
2. Reaction of hydroxo,chloro-bridged dimers with isopropanol

3a (110 mg, 0.135 mmol) reacted with a mixture of toluene (5 mL) and *i*-PrOH (15 mL) in the presence of Na_2CO_3 (110 mg, 1.1 mmol) at 90 °C during 1 h. The suspension was filtered through a mixture of celite and $MgSO_4$, washed with toluene and pentane, evaporated under vacuum to yield brownish-red powder, yield 25 % (determined by ^{1}H NMR).

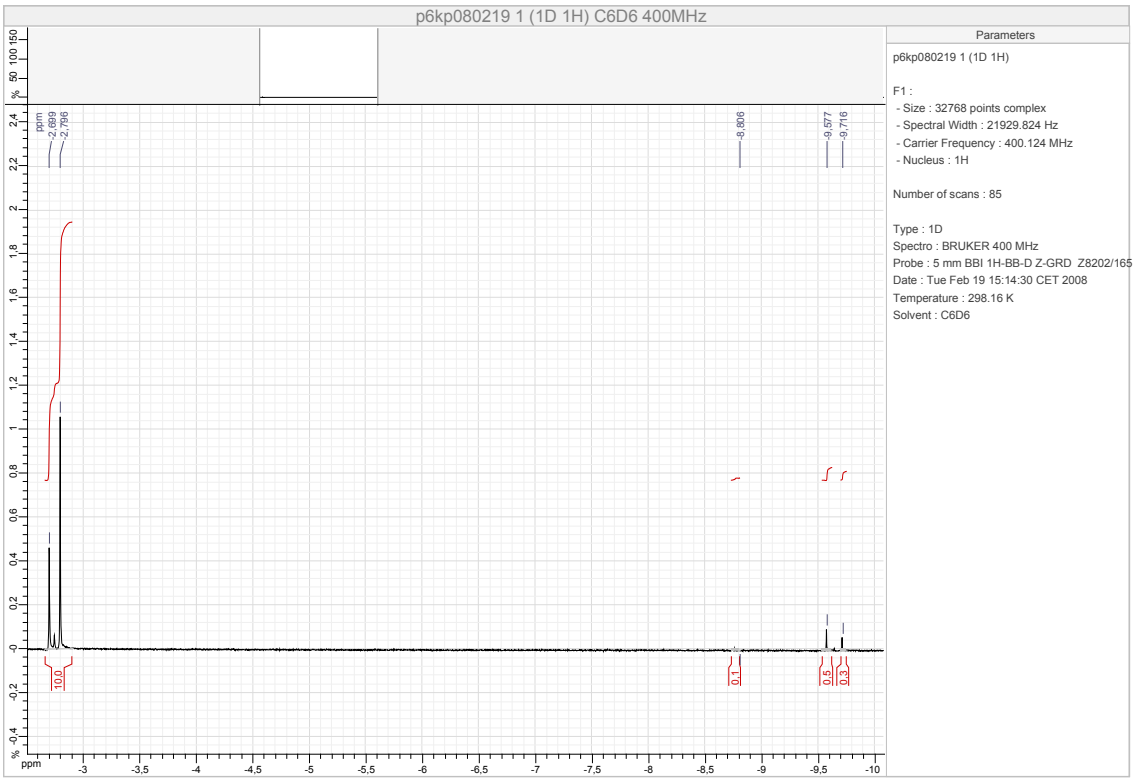


3. Reaction of hydroxo,chloro-bridged dimers with indanol

3a (30 mg, 0.04 mmol) was mixed with indanol (214 mg, 1.6 mmol, 40 eq) in d_6-benzene in NMR-tube, the tube was kept 1 h at 90 °C and analysed subsequently; the yield in ruthenium hydride species is 42 %.



3b (30 mg, 0.035 mmol) reacted with indanol (5 mg, 0.035 mmol) in d_6-benzene (4 mL) at 90 °C during 6 h. The solution was taken for NMR-analysis without any preparations, the yield of ruthenium hydride systems 10% (determined by ^{1}H NMR).



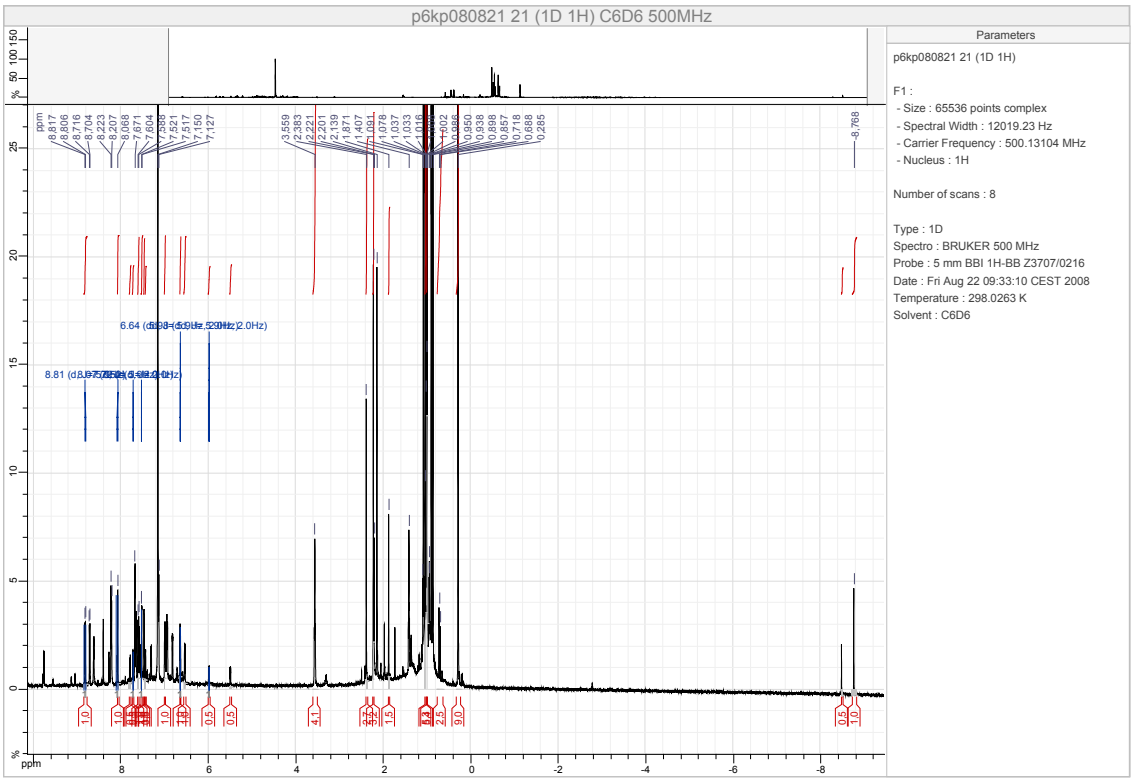
6a

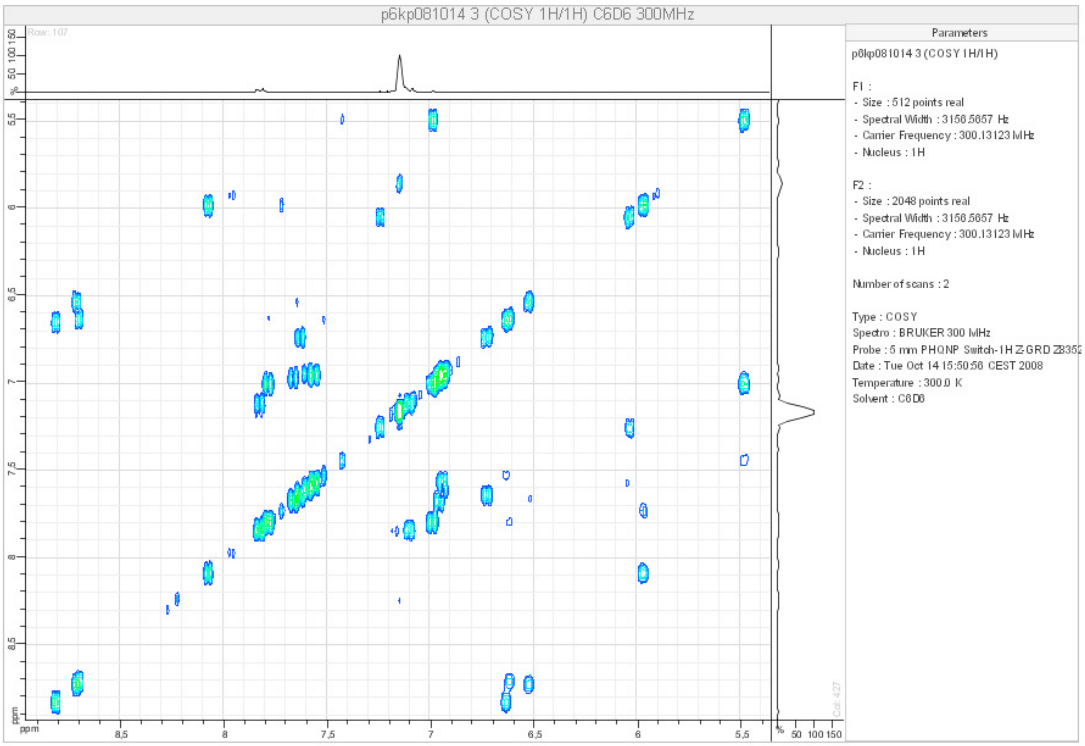
Major compound:

^{1}H NMR (500 MHz, C_6D_6, 298K): δ 8.81 (d, 2 H, $J_{H\text{-}H}$= 5.9), 8.07 (d, 2 H, $J_{H\text{-}H}$= 5.9), 7.72 (m, 2 H), 7.52 (d, 2 H, $J_{H\text{-}H}$= 2.0), 6.64 (dd, 2H, $J_{H\text{-}H}$= 5.9, $J_{H\text{-}H}$= 2.0), 5.98 (dd, 2 H, $J_{H\text{-}H}$= 5.9, $J_{H\text{-}H}$= 2.0), 2.22 (s, 6 H), 1.00 (m, 18 H), -8.77 (s, 1H).

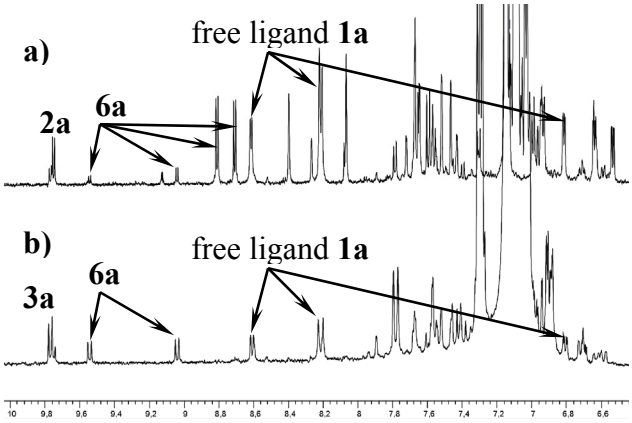
Minor compound:

^{1}H NMR (500 MHz, C_6D_6, 298K): δ 8.71 (d, 2 H, $J_{H\text{-}H}$= 5.9), 7.65 (d, 2 H, $J_{H\text{-}H}$= 2.0), 7.43 (d, 2 H, $J_{H\text{-}H}$= 2.0), 6.99 (d, 2 H, $J_{H\text{-}H}$= 5.9), 6.53 (dd, 2H, $J_{H\text{-}H}$= 5.9, $J_{H\text{-}H}$= 2.0), 5.49 (dd, 2 H, $J_{H\text{-}H}$= 5.9, $J_{H\text{-}H}$= 2.0), 2.38 (s, 6 H), 0.90 (m, 18 H), -8.49 (s, 1H).


p6kp080821 21 (1D 1H) C6D6 500MHz
Parameters
p6kp080821 21 (1D 1H)
F1 :
- Size : 65536 points complex
- Spectral Width : 12019.23 Hz
- Carrier Frequency : 500.13104 MHz
- Nucleus : 1H
Number of scans : 8
Type : 1D
Spectro : BRUKER 500 MHz
Probe : 5 mm BBI 1H-BB Z3707/0216
Date : Fri Aug 22 09:33:10 CEST 2008
Temperature : 298.0263 K
Solvent : C6D6


p6kp081014 3 (COSY 1H/1H) C6D6 300MHz
Parameters
p6kp081014 3 (COSY 1H/1H)
F1 :
- Size : 512 points real
- Spectral Width : 3156.5657 Hz
- Carrier Frequency : 300.13123 MHz
- Nucleus : 1H
F2 :
- Size : 2048 points real
- Spectral Width : 3156.5657 Hz
- Carrier Frequency : 300.13123 MHz
- Nucleus : 1H
Number of scans : 2
Type : COSY
Spectro : BRUKER 300 MHz
Date : Tue Oct 14 15:50:56 CEST 2008
Temperature : 300.0 K
Solvent : C6D6

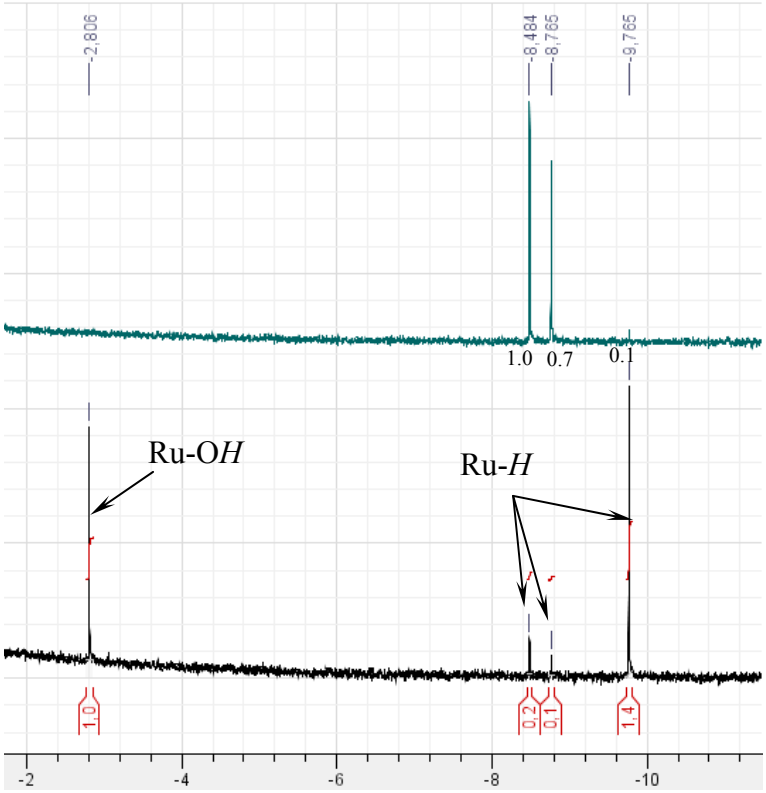
4. Evidence for the spontaneous decomposition of hydrido species 6a and the formation of ligand 1a.



a) **2a** – 20 %, **6a** – 64 %, **1a** – 16 % (Scheme 3)
b) **3a** – 20 %, **6a** – 64 %, **1a** – 16 % (Scheme 3)

5. Isomerisation of 6a in C_6D_6

All the manipulations were carried out in argon atmosphere. Compound **6a** (7 mg, 0.01 mmol) produced by reaction of **2a** with Li[Et_3BH] was dissolved in moist deuterated benzene (~0.5 mL) and placed in a NMR-tube; the tube was sealed and heated for 1 h at 90 °C in a silicone oil bath. ^{1}H NMR spectra of the content of the tube before and after heating is displayed in the pictures below.



6a before treatment

6a after 1 h at 90 °C in C_6D_6, a part of **6a** converted into **3a**

6. Catalytic reduction of diphenylacetylene with indanol

The reaction was typically carried out using 2.5 molar % of the catalysts **2a**, **2b** or **3b**-**b'** versus substrate in a 100 mL Schlenk tube. Flushing the Schlenk with argon, loading calculated amount of catalyst, diphenylacetylene (200 mg, 1.122 mmol), indanol (150.5 mg, 1.122 mmol), 1,3,5-tri-*tert*-butylbenzene as internal standard (30.7 mg, 0.125 mmol) and excess of a base, add 10 mL of toluene under argon atmosphere and bring the solution slowly to 90°C. Take 1 mL samples in a different Schlenk tube before heating and at 4, 16 or 24 h, evaporating the solvent and adding deuterated chloroform for NMR analysis. Only *cis*-stilbene and *trans*-stilbene were found as the products.

7. Catalytic reduction of diphenylacetylene with i-PrOH

Flushing the Schlenk with argon, loading calculated amount of the catalyst **2a** (2.5 %mol, 21 mg), diphenylacetylene (178 mg, 1 mmol), Na_2CO_3 (60 mg, 0.57 mmol), 1,3,5-tri-tert-butylbenzene as internal standard (30.7 mg, 0.125 mmol), add 10 mL of i-PrOH under argon atmosphere and 0.5 mL of distilled water, bringing the solution slowly to 90°C. Take 1 mL samples in another Schlenk tube before heating and at 4, 24 and 48 h, evaporate the solvent and add deuterated chloroform for NMR analysis.

8. Catalytic reduction of 1-(3-fluoromethylphenyl)-2-phenylacetylene with indanol

The initial compound was synthesized according to known procedures.[1] Reaction was typically carried out using 2.5 molar % versus substrate of the catalysts **2a** or **3b**-**b'** in a 100 mL Schlenk tube. Flush the Schlenk with argon, load calculated amount of the catalyst, 1-(3-fluoromethylphenyl)-2-phenylacetylene (200 mg, 0.813 mmol), indanol (109.1 mg, 0.813 mmol), 1,3,5-tri-tert-butylbenzene as internal standard (30.7 mg, 0.125 mmol), add 10 mL of toluene under argon atmosphere and bring the solution slowly to 90°C. Withdraw 1 mL samples in another Schlenk tube before heating and at 4 or 24 h, evaporate the solvent and add deuterated chloroform for NMR analysis. Only cis[2] and trans[3] monosubstituted stilbenes were found as the products.

9. Catalytic reduction of 1-(3-fluoromethylphenyl)-2-phenylacetylene with i-PrOH

Flush the Schlenk with argon, load calculated amount of the catalyst **2a** (2.5 %mol, 21 mg), 1-(3-fluoromethylphenyl)-2-phenylacetylene (246 mg, 1 mmol), Na_2CO_3 (60 mg, 0.57 mmol), 1,3,5-tri-tert-butylbenzene as internal standard (30.7 mg, 0.125 mmol), add 10 mL of i-PrOH under argon atmosphere and 0.5 mL of distilled water, bring the solution slowly to 90°C. Withdraw 1 mL samples in another Schlenk tube before heating and at 4, 24 and 48 h, evaporate the solvent and add deuterated chloroform for NMR analysis.

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[1] A. Koellhofer and H. Plenio. *Adv. Synth. & Cat.* **2005**, *347*, 1295-1300.
[2] M.-F. Ruasse, G. Lo Moro, B. Galland, R. Bianchini, C. Chiappe, and G.Bellucci. *J. Am. Chem. Soc.,* **1997**, *119*, 12492-12502.
[3] Xin Cui, Juan Li, Zhi-Ping Zhang, Yao Fu, Lei Liu and Qing-Xiang Guo. *J. Org. Chem.,* **2007**, *72*, 9342 - 9345,

10. Catalytic reduction of 1-(4-nitrophenyl)-2-phenylacetylene with indanol

The initial compound was synthesized according to known procedures.[4] Reaction was typically carried out using 2.5 molar % versus substrate of the catalysts **2a** or **3b**-**b'** in a 100 mL Schlenk tube. Flash the Schlenk with argon, load calculated amount of the catalyst, 1-(4-nitrophenyl)-2-phenylacetylene (200 mg, 0.881 mmol), indanol (118.2 mg, 0.881mmol), 1,3,5-tri-tert-butylbenzene as internal standard (30.7 mg, 0.125 mmol), add 10 mL of toluene under argon atmosphere and bring the solution slowly to 90°C. Withdraw 1 mL samples in another Schlenk tube before heating and at 4 or 24 h, evaporate the solvent and add deuterated chloroform for NMR analysis. Only cis[5] and trans[6] monosubstituted stilbenes were found as the products.

11. Catalytic reduction of 1-(4-nitrophenyl)-2-phenylacetylene with i-PrOH

Flush the Schlenk with argon, load calculated amount of the catalyst **2a** (2.5 %mol, 21 mg), 1-(4-nitrophenyl)-2-phenylacetylene (223 mg, 1 mmol), Na_2CO_3 (60 mg, 0.57 mmol), 1,3,5-tri-tert-butylbenzene as internal standard (30.7 mg, 0.125 mmol), add 10 mL of i-PrOH under argon atmosphere and 0.5 mL of distilled water, bring the solution slowly to 90°C. Withdraw 1 mL samples in another Schlenk tube before heating, evaporate the solvent and add deuterated chloroform for NMR analysis.

12. Catalytic reduction of 1,4-diphenylbutadiyne with indanol

A Schlenk tube was charged with 1,4-diphenylbutadiyne (227 mg, 1.122 mmol), catalyst **3b-b'** (2.5 %mol, 24 mg), indanol (150.5 mg, 1.122 mmol), 1,3,5-tri-tert-butylbenzene as internal standard (30.7 mg, 0.125 mmol), and 10 mL of toluene under argon atmosphere. The reaction mixture was stirred at 90°C. The course of the reactions was followed by NMR, samples were withdrawn at 0, 2, 4, 6, 24, 30 and 72 h.

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[4] N.Sakai, K. Annaka, T. Konakahara. *Org. Lett.* **2004**, *6*, 1527-1530.
[5] H. Zhao, Y. Wang, J. Sha, S. Sheng and M. Cai, *Tetrahedron* **2008**, *64*, 7517-7523.
[6] B. Ludolph, M. Klein, L. Erdinger and G. Boche**.** *Mutation Research,* **2001**, *491*, 195–209.

13. Catalytic reduction of 1,4-diphenylbutadiyne with i-PrOH

A Schlenk tube was charged with 1,4-diphenylbutadiyne (227 mg, 1.122 mmol), catalyst **3b-b'** (2.5 %mol, 24 mg), 1,3,5-tri-tert-butylbenzene as internal standard (30.7 mg, 0.125 mmol), and 10 mL of i-PrOH under argon atmosphere. The reaction mixture was stirred at 90°C. The course of the reactions was followed by NMR, samples were withdrawn at 0, 4, 24 and 72 h.

14. Kinetic study of the catalytic reduction of diphenylacetylene with indanol

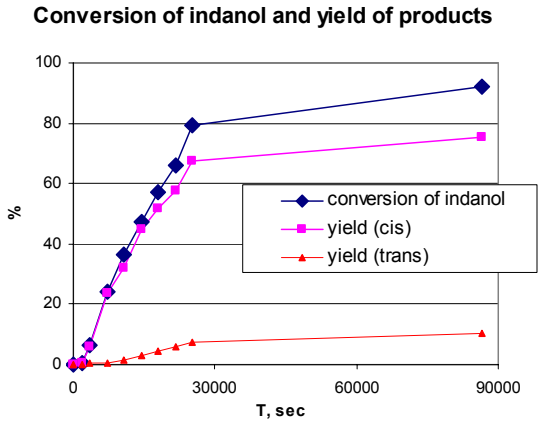
In a typical reaction a 100 mL Schlenk-tube flashed with argon was charged with the catalyst **3b-b'** (2.5 %mol, 48.4 mg), diphenylacetylene (400 mg, 2.244 mmol), indanol (1 eq: 301 mg, 2.244 mmol), 1,3,5-tri-tert-butylbenzene as internal standard (61.4 mg, 0.25 mmol), add 20 mL of toluene under argon atmosphere, the solution was brought slowly to 90°C. Withdraw 1 mL samples in another smaller Schlenk tube before heating and every hour during 6-7 h, 24 and 100 h, evaporate the solvent and add deuterated chloroform for NMR analysis.

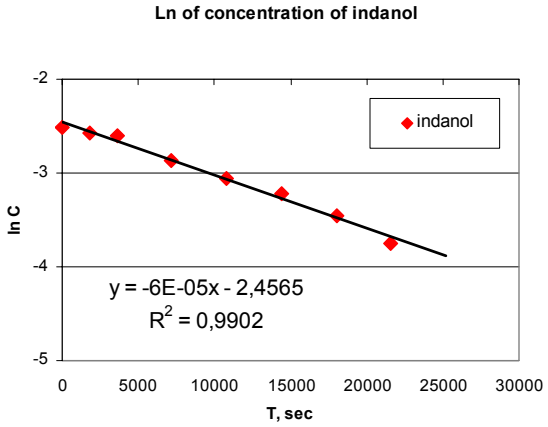
Kinetic study was carried out varying the ratio of the substrates, the amount of the catalyst and at lower temperature. All the information is listed in the table below.

n° of the experiment	Diphenyl-acetylene, mM	Indanol, mM	Ratio, diphenyl-acetylene:indanol	**3b-b'**, mM	T, °C
1	0.11	0.11	1:1	2.8	90
2	0.11	0.22	1:2	2.8	90
3	0.06	0.60	1:10	2.8	90
4	0.22	0.11	2:1	2.8	90
5	0.11	0.11	1:1	1.12	90
6	0.11	0.11	1:1	0.56	90
7	0.11	0.11	1:1	2.8	70
8	0.11	0.11 (indanol-d_1)	1:1	2.8	90

[a] Selectivity determined after 24 h reaction

Graphics for experiment 1.





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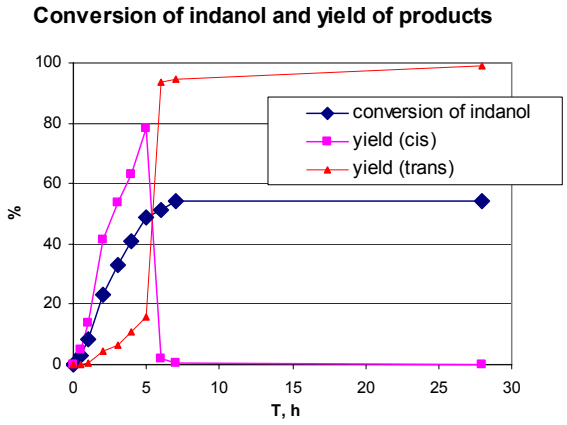

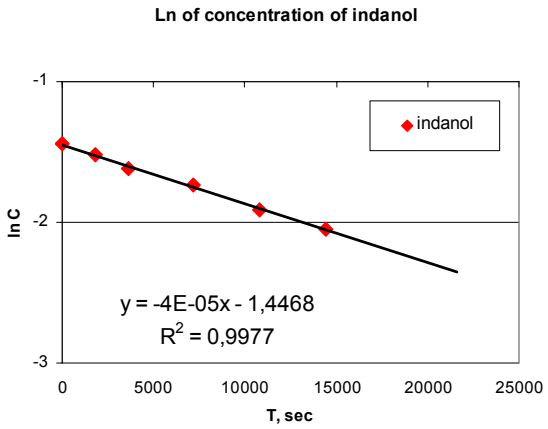

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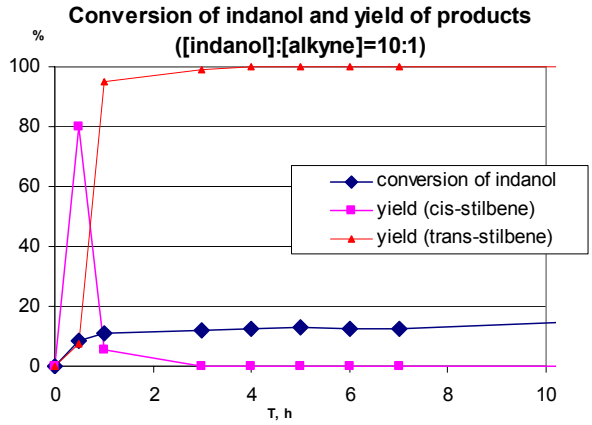

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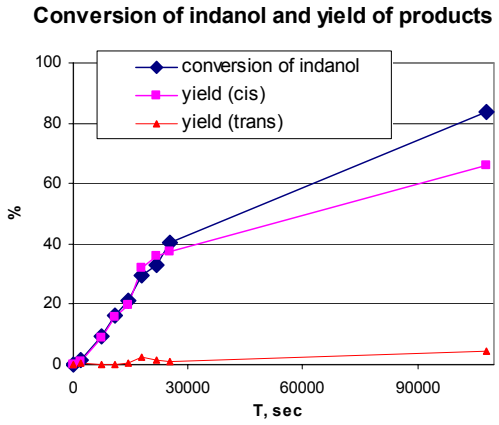
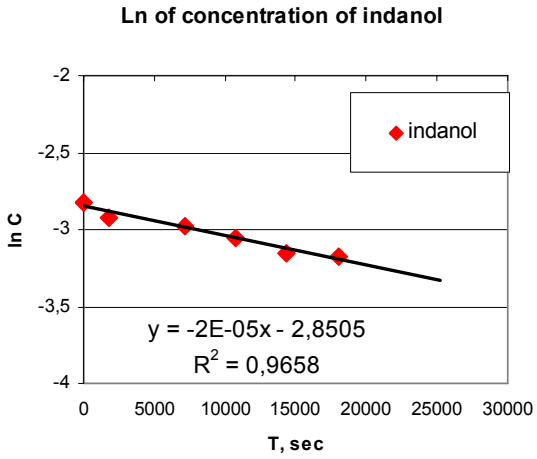
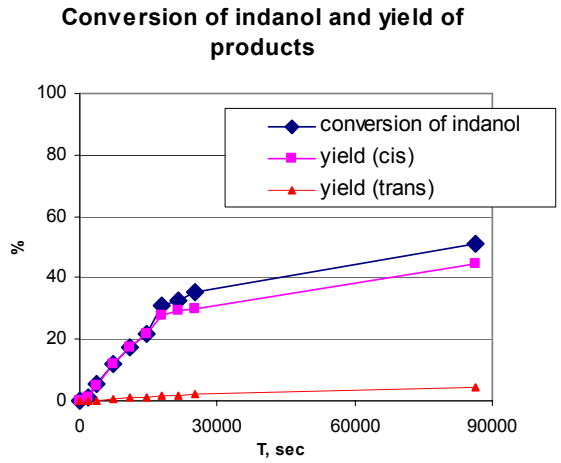
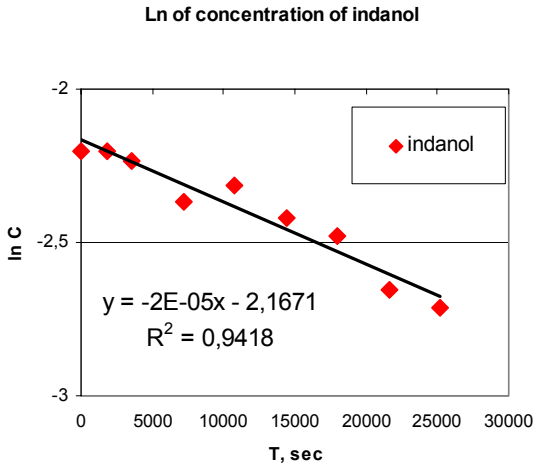




Graphics for experiment 5.





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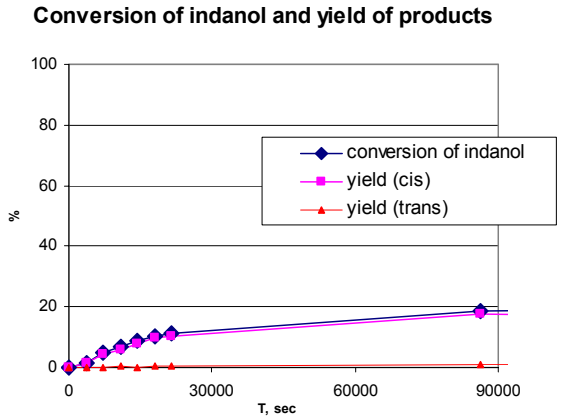
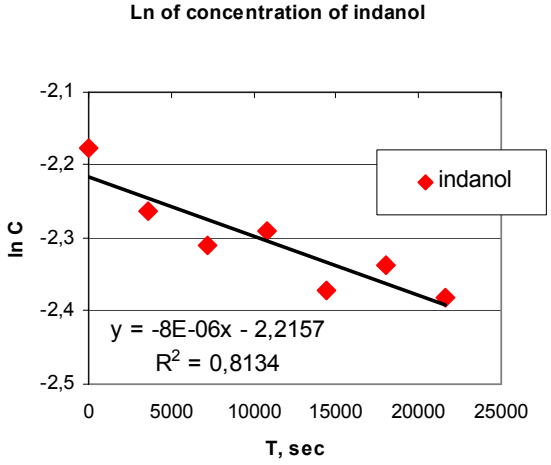
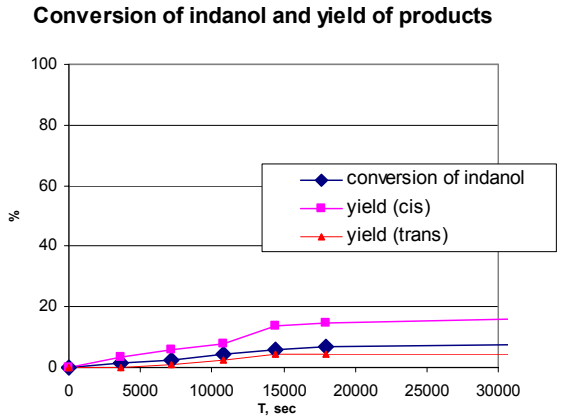
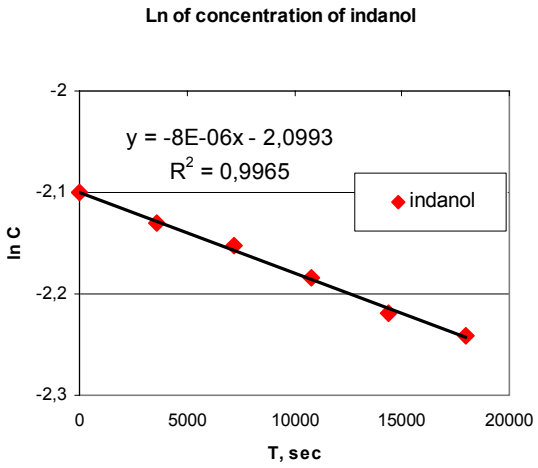




Graphics for experiment 7.





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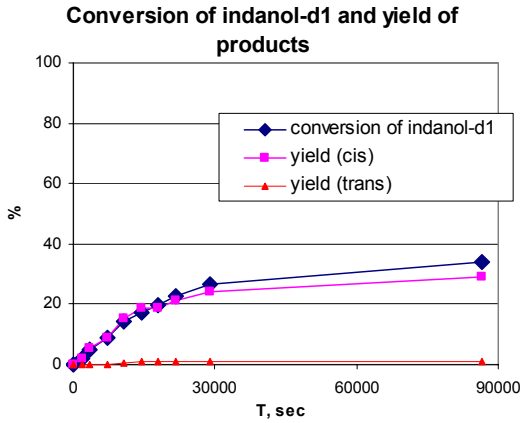
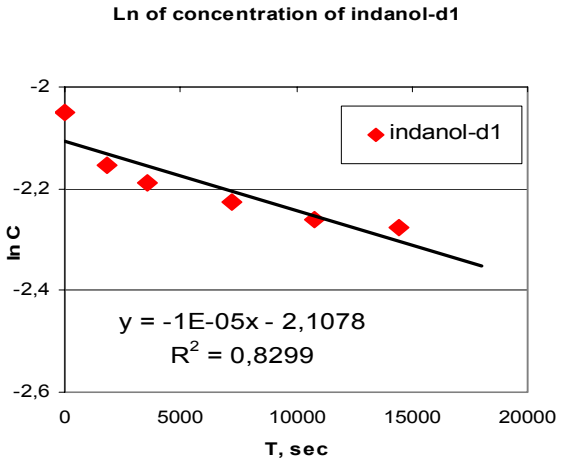
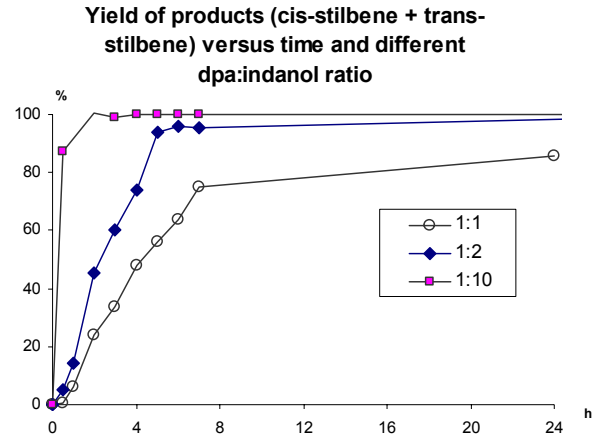
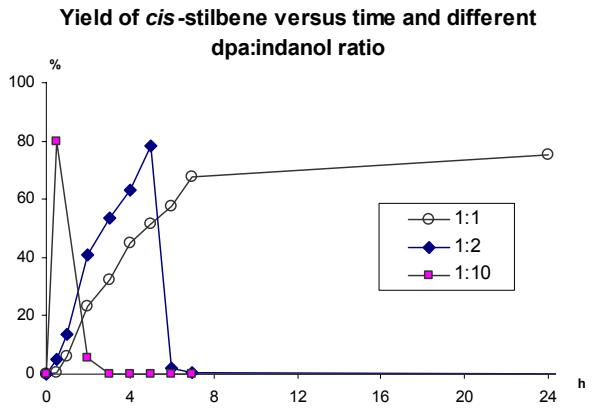
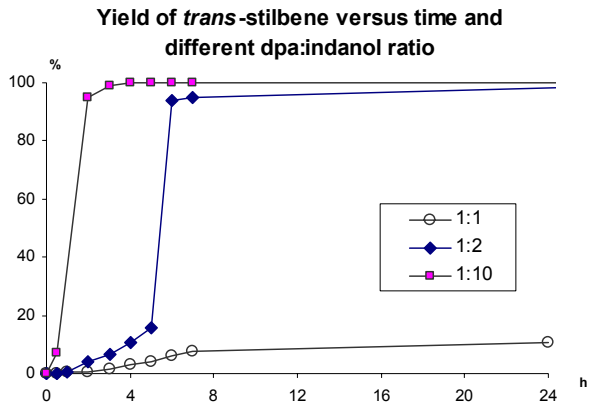


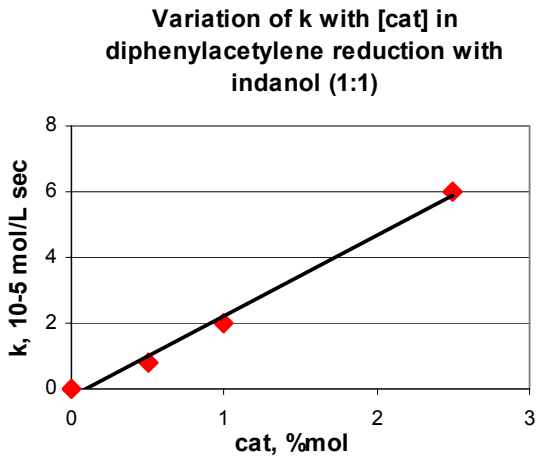


Summary graphs for kinetic study.



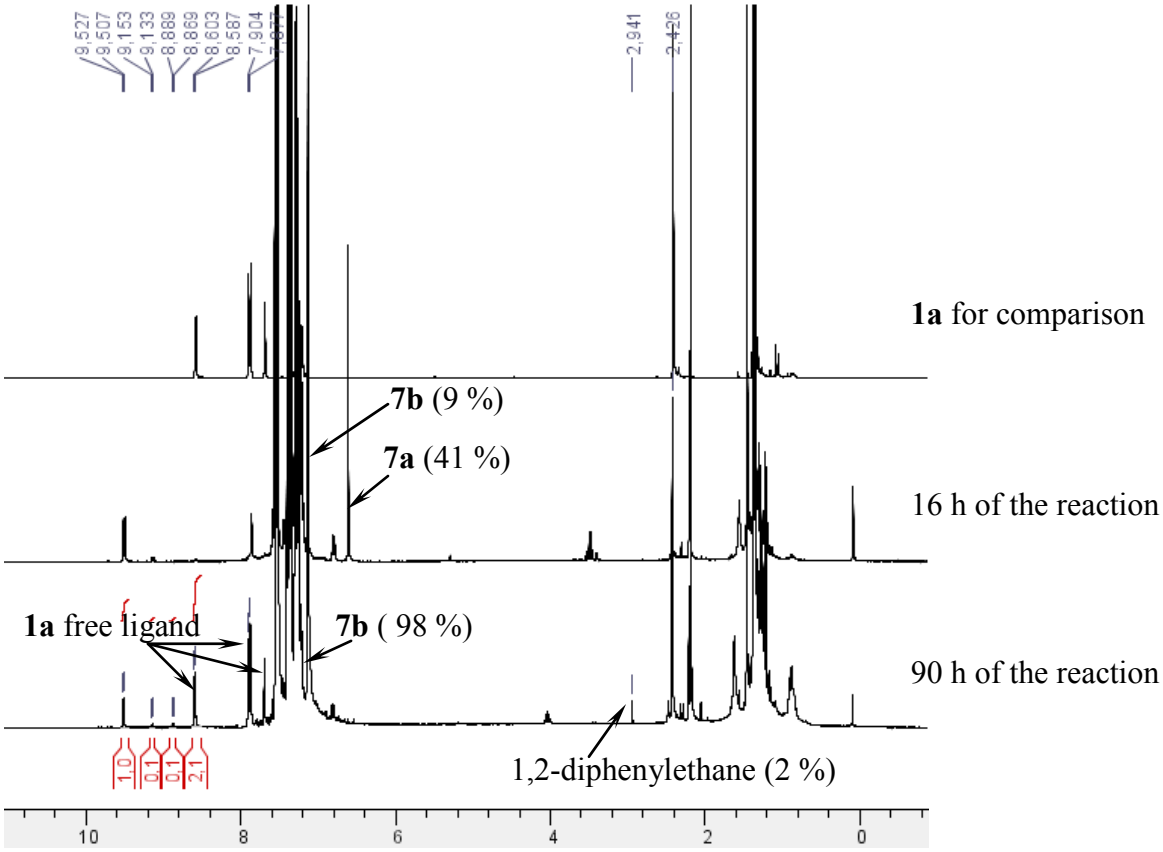



Yield of *trans*-stilbene versus time and different dpa:indanol ratio
%
100
80
60
40
20
0
0
4
8
12
16
20
24
h
1:1
1:2
1:10


Variation of k with [cat] in diphenylacetylene reduction with indanol (1:1)
k, 10-5 mol/L sec
8
6
4
2
0
0
1
2
3
cat, %mol

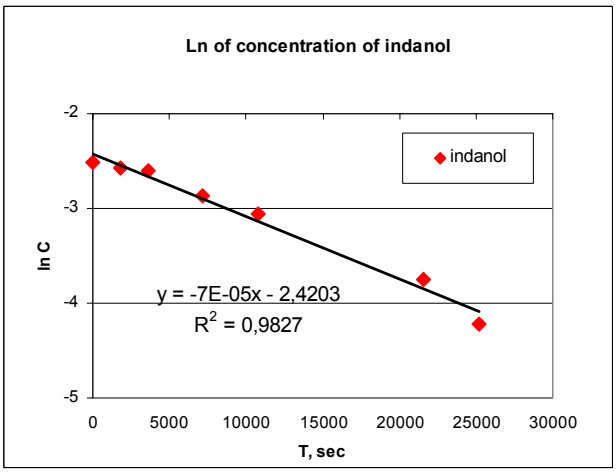
15. Hydrogenation of 7 in the presence of 10 %mol of 2a

2a (42 mg, 10 %mol, 0.05 mmol), diphenylacetylene **7** (89 mg, 0.5 mmol, 0.1 M), 1,3,5-tri-*tert*-butylbenzene (25 mg, 0.1 mmol), Na_2CO_3 (60 mg, 0.57 mmol), distilled water (0.25 mL) and *i*-PrOH (5 mL) were mixed in a 100 mL Schlenk tube. The mixture was brought to reflux using a silicone oil bath (~90 °C). 1 mL samples were withdrawn after 16 and 90 h of the reaction.



B. Evaluation of catalysis inhibition by the products

a) Hydrogenation of diphenylacetylene with 1-indanol (1:1)

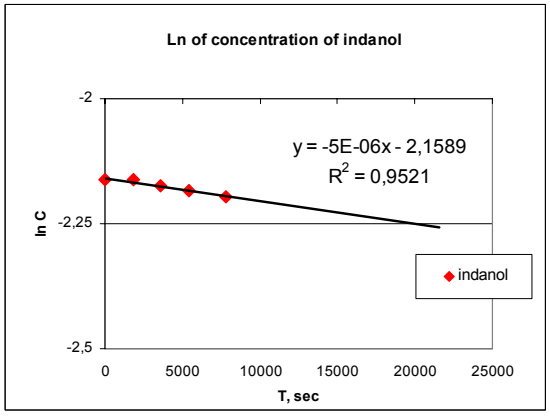


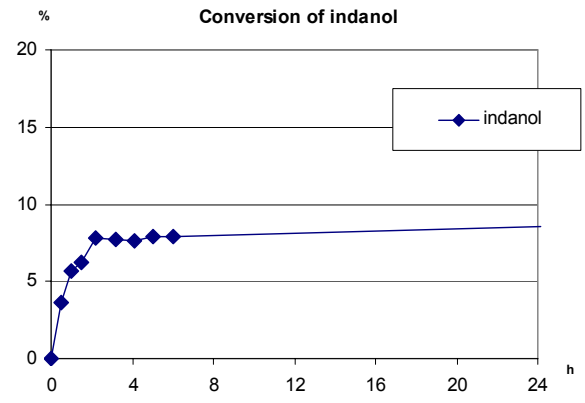
$k = 7 * 10^{-5}\ s^{-1}$

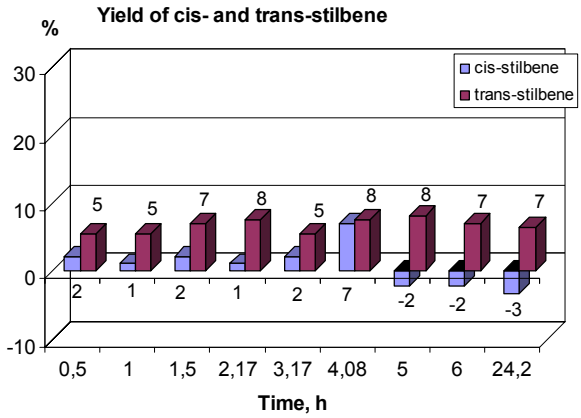
Hydrogenation of diphenylacetylene with 1-indanol in the presence of products:

b) Addition of 1 equivalent of cis-stilbene

$k = 5 * 10^{-6}\ s^{-1}$ at 1:1 ratio with added 1 eq of *cis*-stilbene



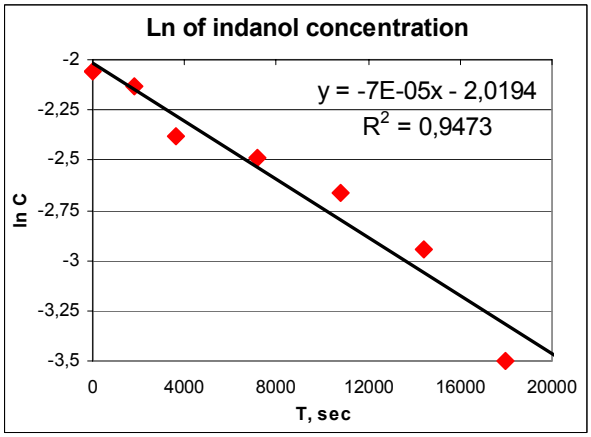


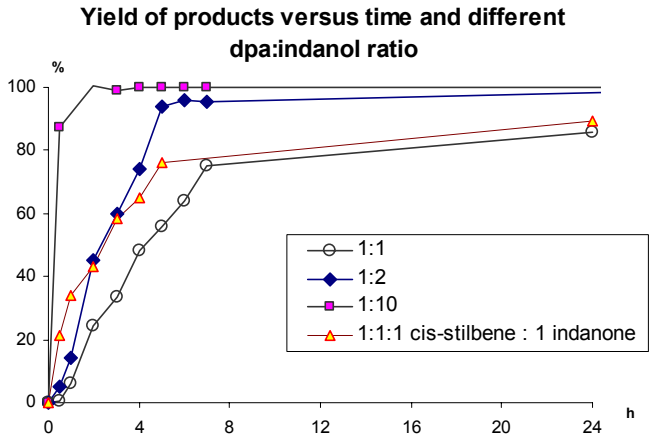


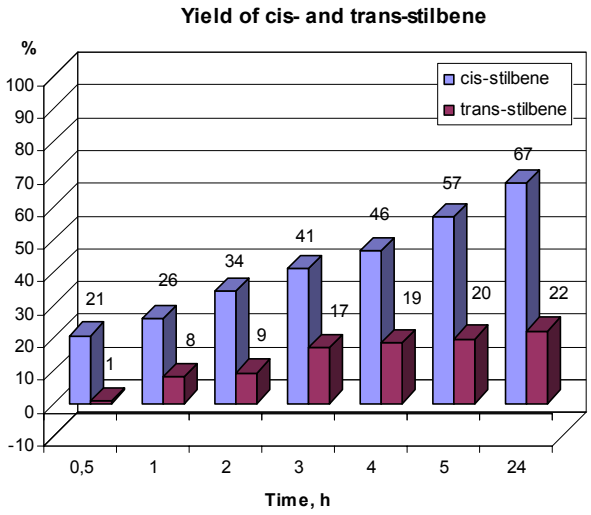
The rate of 1-indanol consumption in this case is 10 times slower in several few hours and this conversion does not exceed 10 %. This converted 10 % of alcohol serve to reduce diphenylacetylene to cis-stilbene (Δ of cis-stilbene concentration is about 2-7 %) and isomerise the latter into trans-stilbene starting from the beginning of the reaction (not consecutively as it is the case in 1:1 reaction).

c) Addition of 1 equivalent of cis-stilbene and 1 equivalent of 1-indanone

$k = 7 * 10^{-5}\ s^{-1}$ at 1:1 ratio with added 1 eq of cis-stilbene and 1 eq of 1-indanone



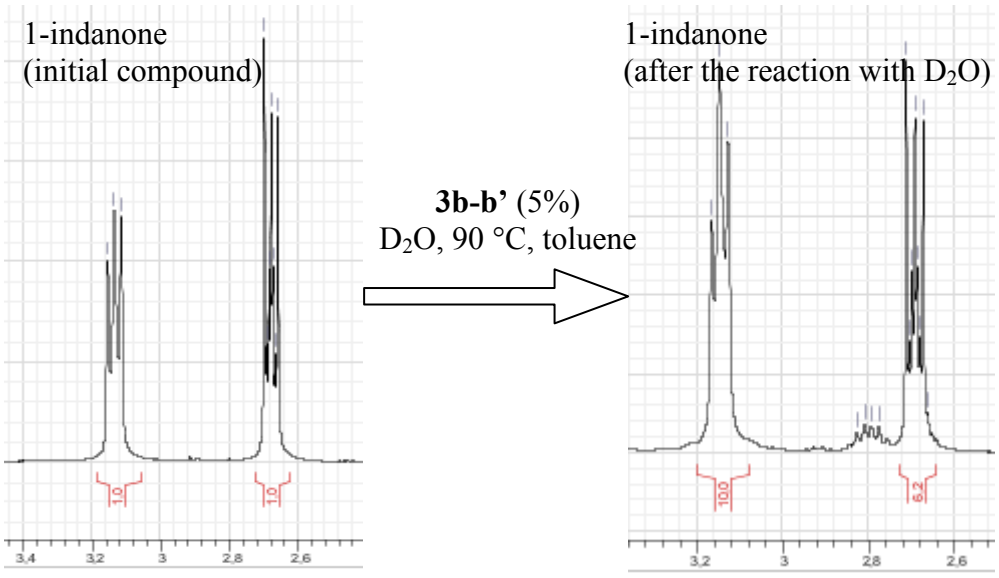




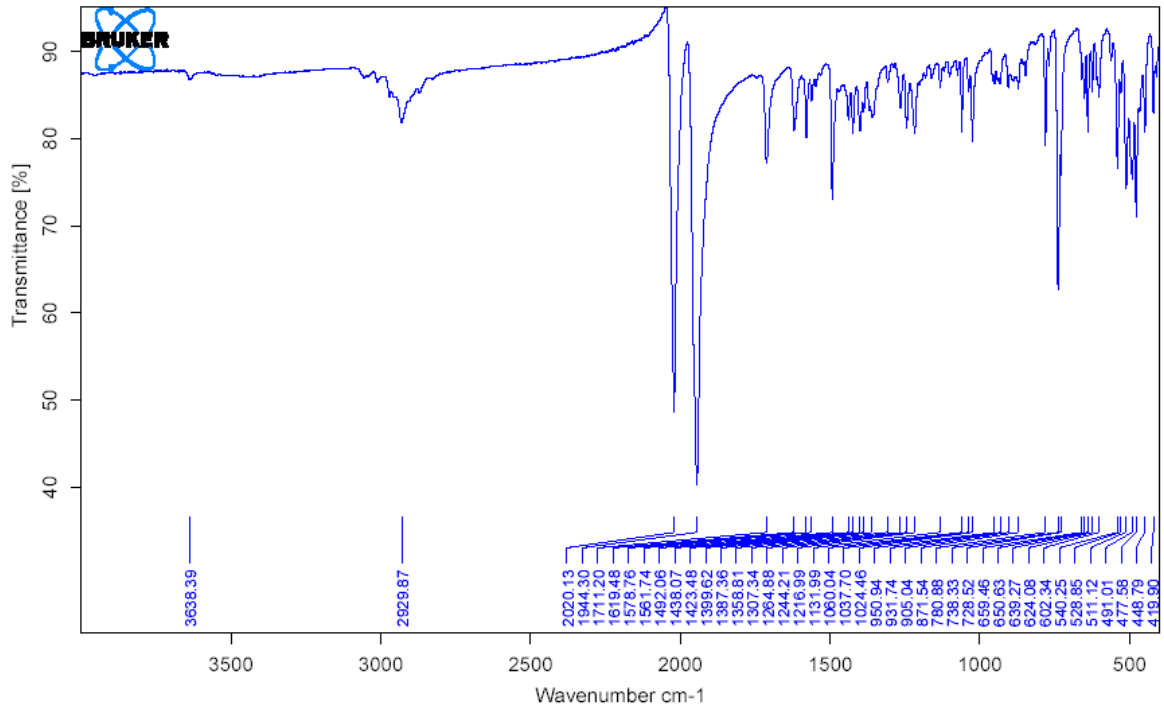
The rate of 1-indanol consumption in this case is the same as in the reaction '1:1' and the conversion after 24 h is 92 %. Summary yield of products complies with the conversion of alcohol (89 %). Here the intermediate moment of the reaction was demonstrated, which lead to the same quantitative results except selectivity. Trans-stilbene was forming as well as cis-stilbene from the beginning of the reaction while in the reaction of 1:1 (without products'addition) cis-stilbene is the major product after 24 h.

Catalytic reduction of diphenylacetylene with 1-indanol in the presence of products. Reactions were carried out using 2.5 molar % versus substrate of the catalyst **3b-b'** in a 100 mL Schlenk tube. Flush the Schlenk with argon, load calculated amount of the catalyst (24.2 mg), diphenylacetylene (200 mg, 1.122 mmol), 1-indanol (150.5 mg, 1.122 mmol), 1,3,5-tri-*tert*-butylbenzene as internal standard (30.7 mg, 0.125 mmol), **7a** (202 mg, 1.122 mmol) sole or together with 1-indanone (150 mg, 1.122 mmol), add 10 mL of toluene under argon atmosphere and bring the solution slowly to 90°C. Withdraw 1 mL aliquots in another Schlenk tube before heating and at 1, 2, 3, 4, 5, 6, 7, 24 h, evaporate the solvent and add deuterated chloroform for NMR analysis.

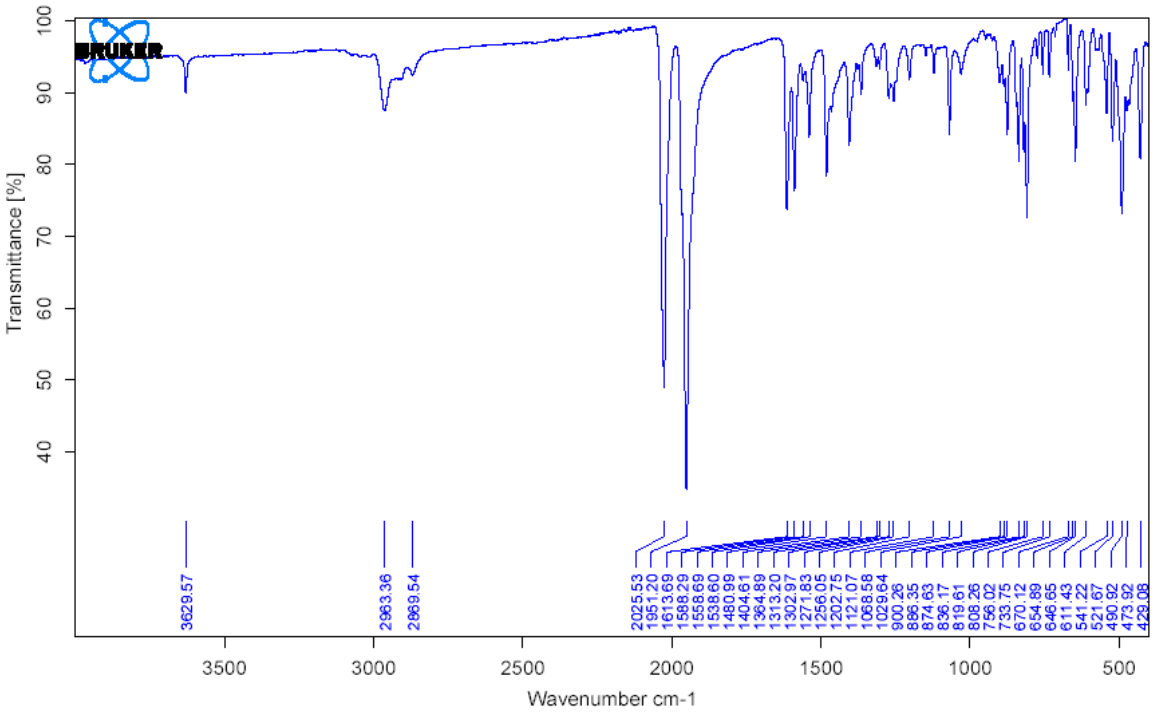
Reaction of 3b-b' with 1-indanone in the presence of D_2O in toluene. Reaction was carried out in a 100 mL Schlenk tube, which was filled with the catalyst **3b-b'** (5 molar %, 5 mg) and 1-indanone (15 mg, 0.11 mmol). Toluene (1.5 mL) and D_2O (0.2 mL) were added and the solution was warmed slowly to 90°C with vigorous stirring. After 4 h the suspension was cooled to the room temperature and organic layer was removed in another Schlenk tube after filtering over $MgSO_4$. D_2O was washed with 1 mL of toluene, which passed through the filter and was added to the organic phase in the Schlenk. Then toluene was evaporated under reduced pressure and the residue was was analysed by NMR using $CDCl_3$ as a solvent.



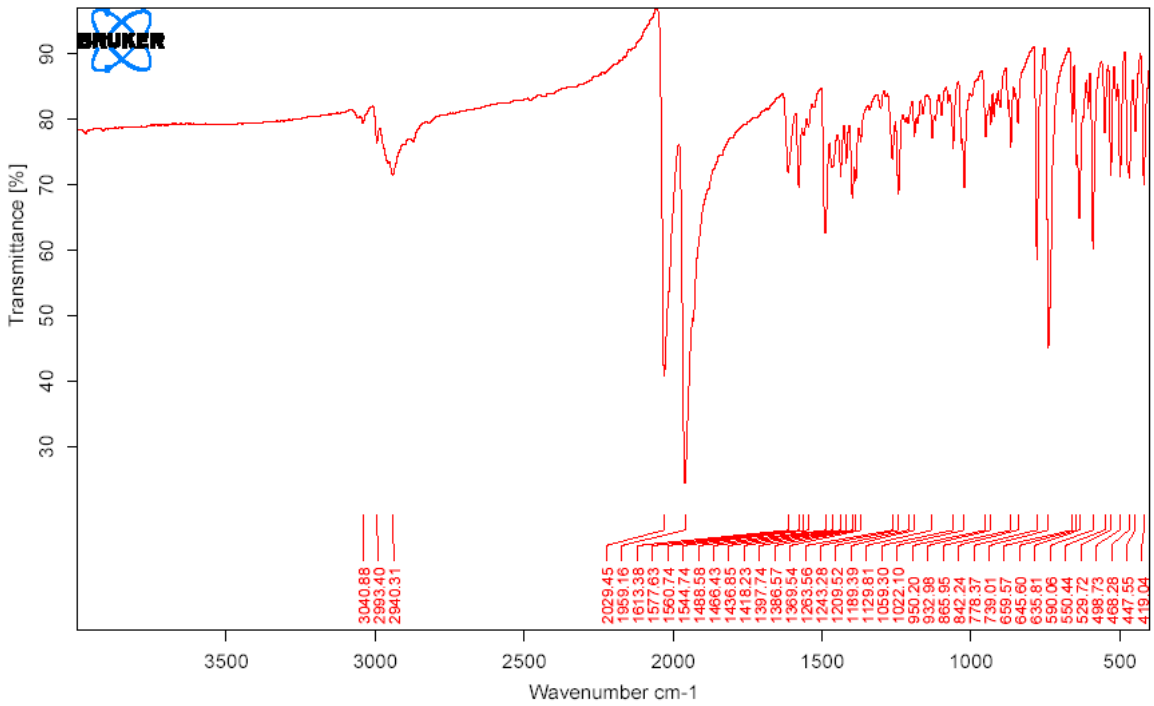
C. Infrared spectra (ATR)



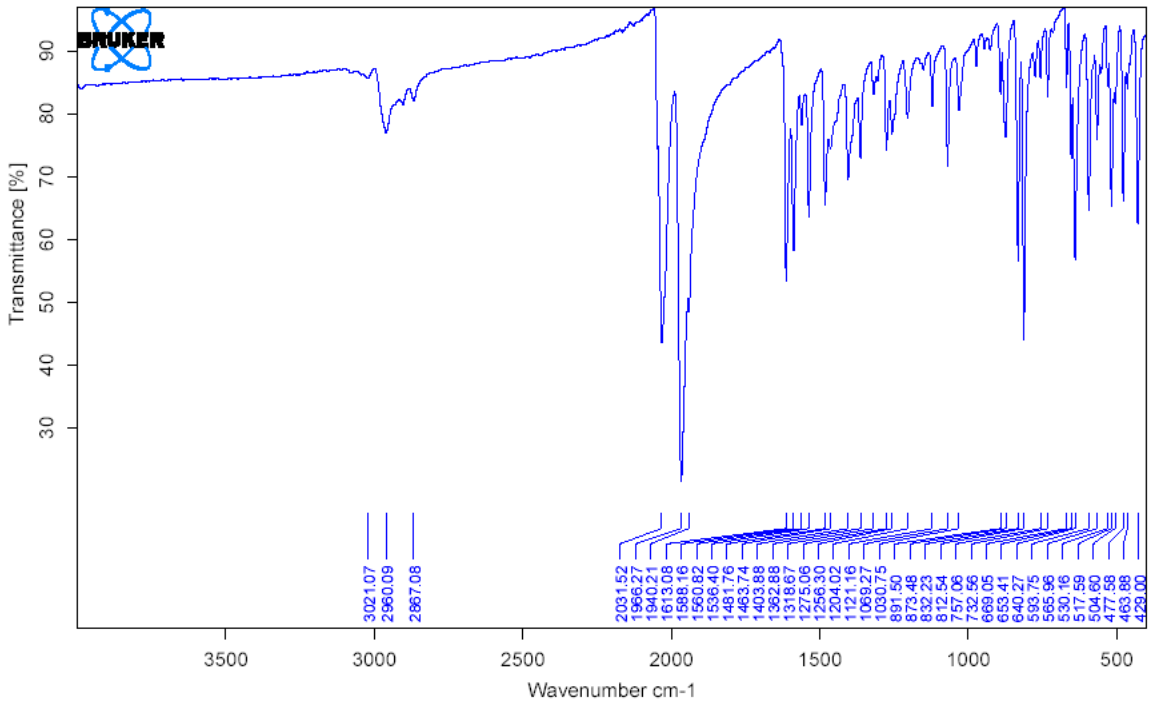
IR-spectrum of **3b-b'**



IR-spectrum of **3a**

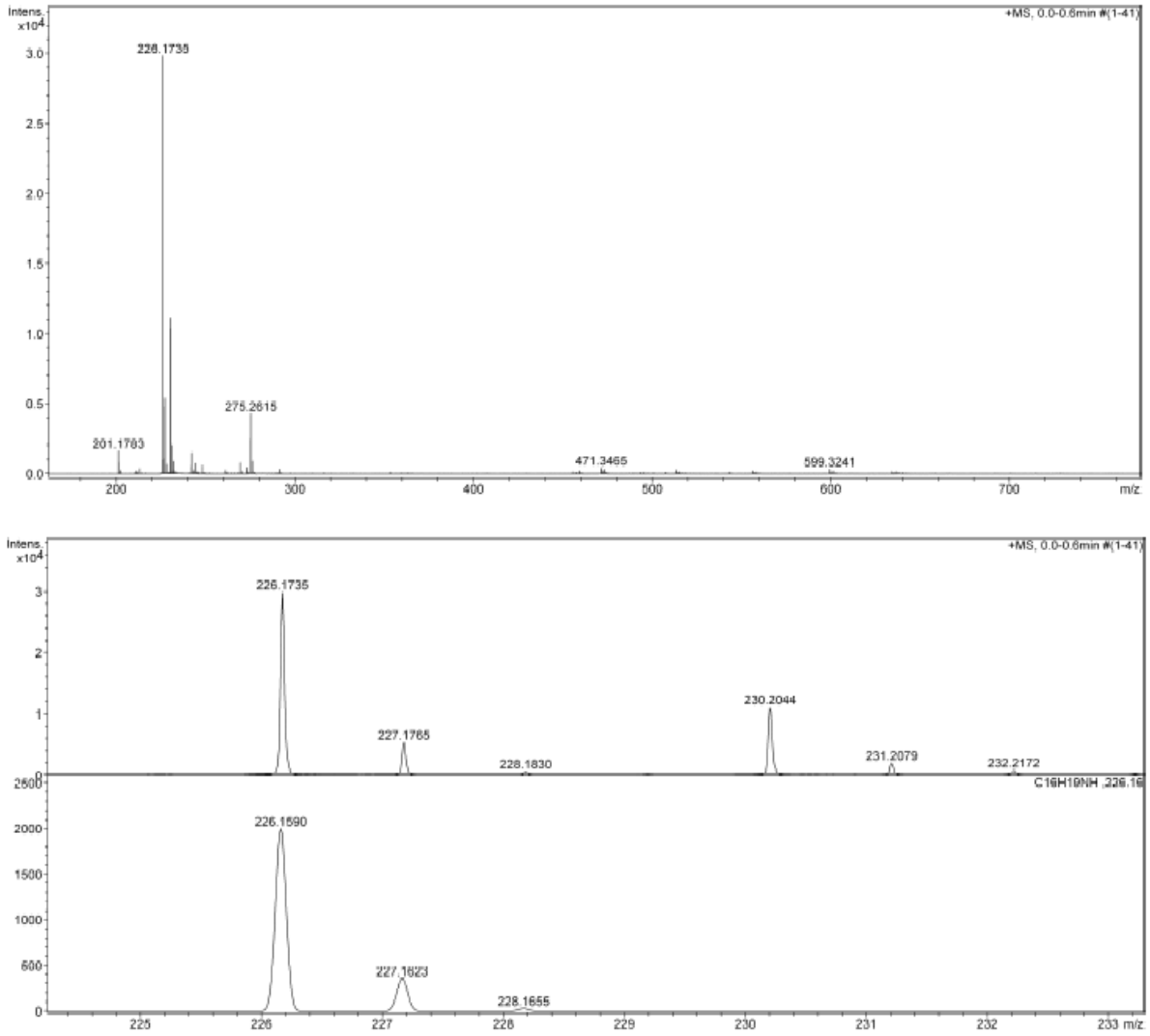


IR-spectrum of **2b**

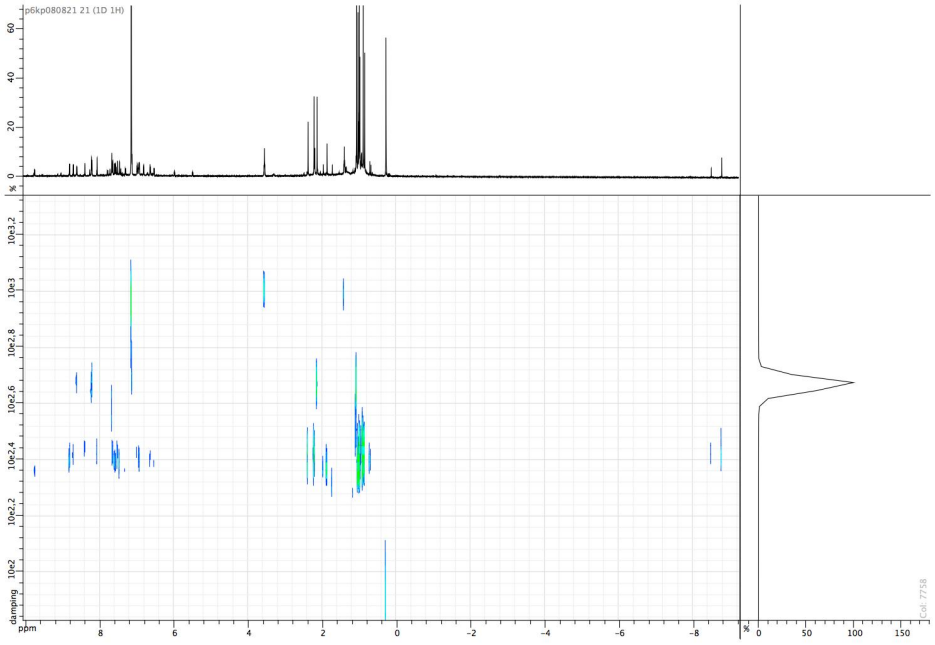


IR-spectrum of **2a**

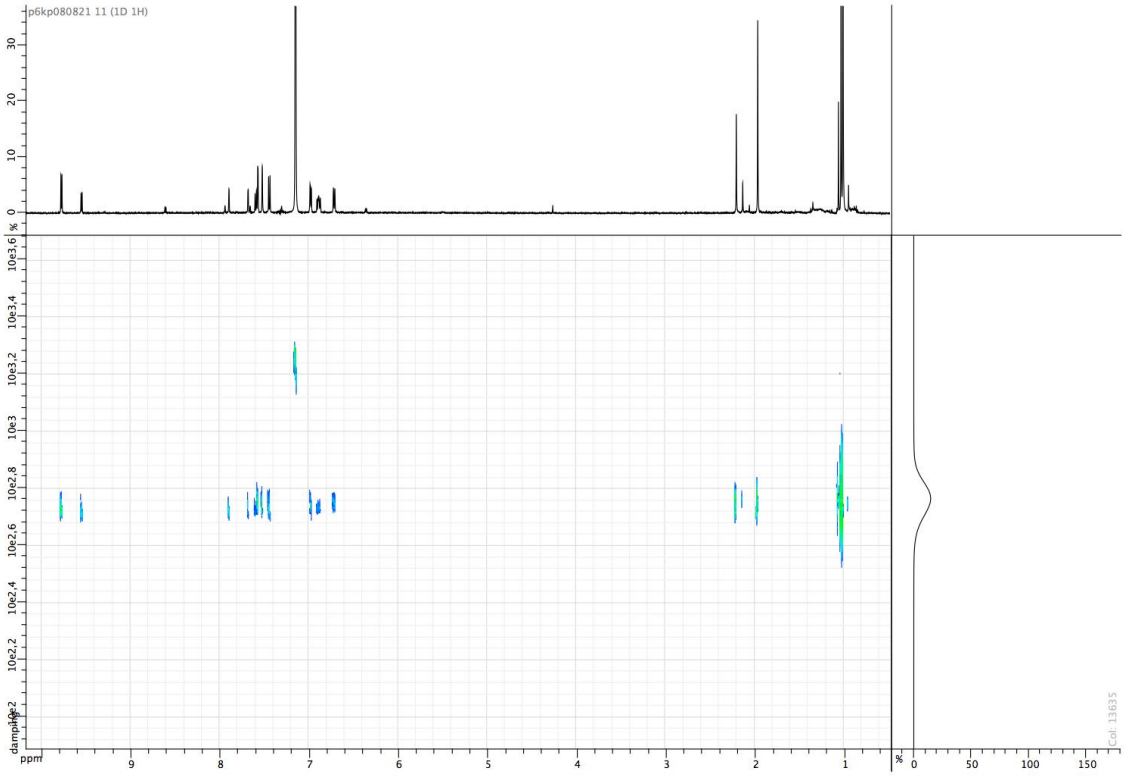
D. High Resolution MS (ESI+) of 1a



E. ^{1}H NMR diffusion ordered spectroscopy of 6a and 2a (reference).

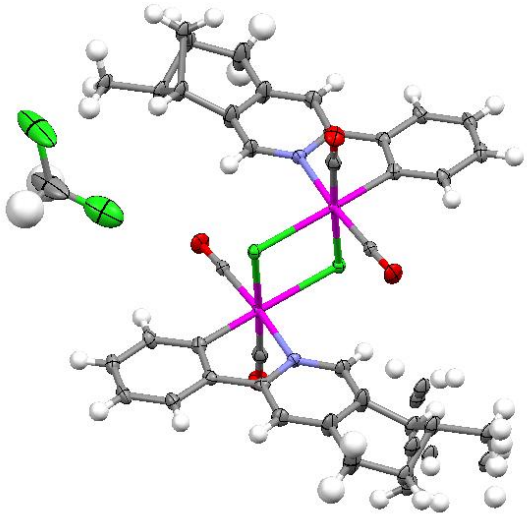


^{1}H NMR DOSY map for **6a** in C_6D_6.



^{1}H NMR DOSY map for **2a** in C_6D_6.

F. CIF of the aborted structure of 2b showing the parallel relationship between chelating ligands.



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C7 C 0.8495(5) -0.2759(9) 0.0601(4) 0.0364(19) Uani 1 1 d . . .
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C8 C 0.8329(4) -0.1384(8) 0.0657(4) 0.0305(17) Uani 1 1 d . . .
C9 C 0.7821(4) -0.0985(8) 0.0905(4) 0.0278(16) Uani 1 1 d . . .
C10 C 0.7464(5) -0.1926(9) 0.1133(5) 0.038(2) Uani 1 1 d . . .
H10 H 0.7516 -0.2894 0.1093 0.046 Uiso 1 1 calc R . .
C11 C 0.7043(6) -0.1450(10) 0.1412(6) 0.054(3) Uani 1 1 d . B .
C12 C 0.6989(7) -0.0003(10) 0.1486(6) 0.059(3) Uani 1 1 d . . .
C13 C 0.7338(5) 0.0861(9) 0.1249(5) 0.039(2) Uani 1 1 d . . .
H13 H 0.7297 0.1832 0.1291 0.046 Uiso 1 1 calc R . .
C14 C 0.6647(8) -0.2416(12) 0.1676(8) 0.080(5) Uani 1 1 d . . .
H14A H 0.6925 -0.3225 0.1891 0.097 Uiso 1 1 calc R A 1
H14B H 0.6242 -0.2756 0.1315 0.097 Uiso 1 1 calc R A 1
C15 C 0.6440(10) -0.159(2) 0.2181(10) 0.0428(15) Uani 0.50 1 d P B 1
H15 H 0.6210 -0.2159 0.2407 0.051 Uiso 0.50 1 calc PR B 1
C16 C 0.7040(10) -0.0585(19) 0.2670(10) 0.0428(15) Uani 0.50 1 d P B 1
H16A H 0.6972 -0.0242 0.3059 0.051 Uiso 0.50 1 calc PR B 1
H16B H 0.7502 -0.0921 0.2775 0.051 Uiso 0.50 1 calc PR B 1
C17 C 0.6733(11) 0.039(2) 0.2027(10) 0.0428(15) Uani 0.50 1 d P B 1
H17 H 0.6722 0.1404 0.2113 0.051 Uiso 0.50 1 calc PR B 1
C18 C 0.6024(10) -0.039(2) 0.1788(10) 0.0428(15) Uani 0.50 1 d P B 1
C19 C 0.5581(10) 0.024(2) 0.2113(10) 0.0428(15) Uani 0.50 1 d P B 1
H19A H 0.5776 0.0047 0.2581 0.064 Uiso 0.50 1 calc PR B 1
H19B H 0.5131 -0.0160 0.1922 0.064 Uiso 0.50 1 calc PR B 1
H19C H 0.5552 0.1247 0.2045 0.064 Uiso 0.50 1 calc PR B 1
C15B C 0.6038(11) -0.146(2) 0.1774(10) 0.0428(15) Uani 0.50 1 d P B 2
H15B H 0.5726 -0.1996 0.1920 0.051 Uiso 0.50 1 calc PR B 2
C16B C 0.5671(10) -0.0452(19) 0.1161(10) 0.0428(15) Uani 0.50 1 d P B 2
H16C H 0.5235 -0.0067 0.1129 0.051 Uiso 0.50 1 calc PR B 2
H16D H 0.5662 -0.0786 0.0738 0.051 Uiso 0.50 1 calc PR B 2
C17B C 0.6369(11) 0.050(2) 0.1624(11) 0.0428(15) Uani 0.50 1 d P B 2
H17B H 0.6308 0.1522 0.1643 0.051 Uiso 0.50 1 calc PR B 2
C18B C 0.6454(11) -0.036(2) 0.2260(10) 0.0428(15) Uani 0.50 1 d P B 2
C19B C 0.6016(10) 0.033(2) 0.2597(10) 0.0428(15) Uani 0.50 1 d P B 2
H19D H 0.6160 0.1291 0.2708 0.064 Uiso 0.50 1 calc PR B 2
H19E H 0.6071 -0.0180 0.2995 0.064 Uiso 0.50 1 calc PR B 2
H19F H 0.5544 0.0312 0.2300 0.064 Uiso 0.50 1 calc PR B 2
N1 N 0.7741(3) 0.0396(7) 0.0956(3) 0.0286(14) Uani 1 1 d . . .
O1 O 0.9126(3) 0.3117(7) -0.0066(4) 0.0497(17) Uani 1 1 d . . .
O2 O 0.9430(4) 0.2085(8) 0.1807(4) 0.0546(19) Uani 1 1 d . . .
Cl1 Cl 0.73861(10) 0.12022(19) -0.05282(9) 0.0282(4) Uani 1 1 d . . .
Ru1 Ru 0.82900(3) 0.16353(6) 0.05446(3) 0.0255(2) Uani 1 1 d . . .
Cl2 Cl 0.9022(3) 0.0840(5) -0.1308(3) 0.135(2) Uani 1 1 d . . .
Cl3 Cl 0.9040(4) 0.0932(7) -0.2618(3) 0.218(5) Uani 1 1 d . . .
C20 C 0.9440(14) 0.0683(19) -0.1779(8) 0.161(12) Uani 1 1 d . . .
H20A H 0.9635 -0.0258 -0.1711 0.193 Uiso 1 1 calc R . .
H20B H 0.9819 0.1342 -0.1619 0.193 Uiso 1 1 calc R . .

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C1 0.028(4) 0.032(4) 0.033(4) 0.003(3) 0.013(3) 0.006(3)
C2 0.047(6) 0.028(5) 0.053(6) 0.003(4) 0.028(5) 0.005(4)
C3 0.028(4) 0.026(4) 0.034(4) -0.005(3) 0.012(3) -0.005(3)
C4 0.024(4) 0.040(5) 0.054(6) 0.002(4) 0.018(4) 0.003(4)
C5 0.033(5) 0.044(5) 0.046(5) -0.011(4) 0.017(4) 0.004(4)
C6 0.038(5) 0.036(5) 0.050(5) -0.004(4) 0.013(4) 0.013(4)
C7 0.034(5) 0.029(4) 0.046(5) 0.000(4) 0.015(4) 0.005(4)
C8 0.032(4) 0.028(4) 0.028(4) 0.000(3) 0.007(3) 0.002(3)
C9 0.029(4) 0.027(4) 0.024(4) 0.000(3) 0.007(3) -0.003(3)

C10 0.047(5) 0.023(4) 0.050(5) -0.002(4) 0.024(4) -0.007(4)
C11 0.073(7) 0.032(5) 0.084(8) -0.001(5) 0.060(7) -0.007(5)
C12 0.082(8) 0.034(5) 0.093(9) 0.002(5) 0.070(7) -0.001(5)
C13 0.044(5) 0.028(4) 0.057(6) 0.005(4) 0.034(5) -0.002(4)
C14 0.111(11) 0.044(7) 0.137(13) 0.000(7) 0.103(11) -0.009(7)
C15 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
C16 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
C17 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
C18 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
C19 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
C15B 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
C16B 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
C17B 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
C18B 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
C19B 0.049(4) 0.040(3) 0.057(4) 0.000(3) 0.040(3) -0.010(3)
N1 0.027(3) 0.026(3) 0.036(4) 0.004(3) 0.016(3) -0.002(3)
O1 0.043(4) 0.049(4) 0.071(5) 0.010(3) 0.038(4) -0.008(3)
O2 0.037(4) 0.070(5) 0.046(4) -0.005(4) 0.005(3) 0.000(4)
Cl1 0.0289(9) 0.0256(9) 0.0317(10) -0.0023(7) 0.0134(8) -0.0004(7)
Ru1 0.0233(3) 0.0263(3) 0.0298(3) 0.0013(3) 0.0136(2) 0.0002(3)
Cl2 0.121(4) 0.079(3) 0.145(5) -0.006(3) -0.015(4) -0.019(3)
Cl3 0.252(8) 0.184(6) 0.086(3) -0.077(4) -0.082(4) 0.137(6)
C20 0.23(3) 0.099(13) 0.058(9) -0.038(9) -0.049(13) 0.077(15)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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C1 Ru1 1.868(8) . ?
C2 O2 1.115(12) . ?
C2 Ru1 1.858(11) . ?
C3 C4 1.386(12) . ?
C3 C8 1.426(11) . ?
C3 Ru1 2.048(8) . ?
C4 C5 1.405(13) . ?
C4 H4 0.9500 . ?
C5 C6 1.375(14) . ?
C5 H5 0.9500 . ?
C6 C7 1.397(13) . ?
C6 H6 0.9500 . ?
C7 C8 1.394(11) . ?
C7 H7 0.9500 . ?
C8 C9 1.458(12) . ?
C9 N1 1.356(10) . ?
C9 C10 1.411(11) . ?
C10 C11 1.365(13) . ?
C10 H10 0.9500 . ?
C11 C12 1.418(14) . ?
C11 C14 1.528(14) . ?
C12 C13 1.363(13) . ?
C12 C17 1.55(2) . ?
C12 C17B 1.56(2) . ?
C13 N1 1.351(11) . ?
C13 H13 0.9500 . ?

C14 C15 1.58(2) . ?
C14 C15B 1.69(2) . ?
C14 H14A 0.9900 . ?
C14 H14B 0.9900 . ?
C15 C18 1.52(3) . ?
C15 C16 1.65(3) . ?
C15 H15 1.0000 . ?
C16 C17 1.63(3) . ?
C16 H16A 0.9900 . ?
C16 H16B 0.9900 . ?
C17 C18 1.61(3) . ?
C17 H17 1.0000 . ?
C18 C19 1.53(2) . ?
C19 H19A 0.9800 . ?
C19 H19B 0.9800 . ?
C19 H19C 0.9800 . ?
C15B C18B 1.53(3) . ?
C15B C16B 1.61(3) . ?
C15B H15B 1.0000 . ?
C16B C17B 1.73(3) . ?
C16B H16C 0.9900 . ?
C16B H16D 0.9900 . ?
C17B C18B 1.59(3) . ?
C17B H17B 1.0000 . ?
C18B C19B 1.57(3) . ?
C19B H19D 0.9800 . ?
C19B H19E 0.9800 . ?
C19B H19F 0.9800 . ?
N1 Ru1 2.127(6) . ?
Cl1 Ru1 2.472(2) . ?
Cl1 Ru1 2.543(2) 7_655 ?
Ru1 Cl1 2.543(2) 7_655 ?
Cl2 C20 1.63(3) . ?
Cl3 C20 1.747(16) . ?
C20 H20A 0.9900 . ?
C20 H20B 0.9900 . ?

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O1 C1 Ru1 178.0(8) . . ?
O2 C2 Ru1 176.9(9) . . ?
C4 C3 C8 117.7(8) . . ?
C4 C3 Ru1 128.6(6) . . ?
C8 C3 Ru1 113.6(6) . . ?
C3 C4 C5 121.7(8) . . ?
C3 C4 H4 119.2 . . ?
C5 C4 H4 119.2 . . ?
C6 C5 C4 119.6(8) . . ?
C6 C5 H5 120.2 . . ?
C4 C5 H5 120.2 . . ?
C5 C6 C7 120.7(8) . . ?
C5 C6 H6 119.6 . . ?
C7 C6 H6 119.6 . . ?
C8 C7 C6 119.5(9) . . ?
C8 C7 H7 120.2 . . ?
C6 C7 H7 120.2 . . ?
C7 C8 C3 120.7(8) . . ?
C7 C8 C9 123.0(8) . . ?
C3 C8 C9 116.3(7) . . ?
N1 C9 C10 119.9(8) . . ?
N1 C9 C8 115.6(7) . . ?

C10 C9 C8 124.3(7) . . ?
C11 C10 C9 120.2(8) . . ?
C11 C10 H10 119.9 . . ?
C9 C10 H10 119.9 . . ?
C10 C11 C12 118.9(9) . . ?
C10 C11 C14 122.7(9) . . ?
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C11 C12 C17 113.6(11) . . ?
C13 C12 C17B 122.2(11) . . ?
C11 C12 C17B 116.3(11) . . ?
N1 C13 C12 122.8(8) . . ?
N1 C13 H13 118.6 . . ?
C12 C13 H13 118.6 . . ?
C11 C14 C15 108.6(11) . . ?
C11 C14 C15B 107.2(10) . . ?
C11 C14 H14A 110.0 . . ?
C15 C14 H14A 110.0 . . ?
C15B C14 H14A 136.7 . . ?
C11 C14 H14B 110.0 . . ?
C15 C14 H14B 110.0 . . ?
C15B C14 H14B 78.2 . . ?
H14A C14 H14B 108.4 . . ?
C18 C15 C14 104.1(15) . . ?
C18 C15 C16 94.3(15) . . ?
C14 C15 C16 113.7(14) . . ?
C18 C15 H15 114.2 . . ?
C14 C15 H15 114.2 . . ?
C16 C15 H15 114.2 . . ?
C17 C16 C15 78.9(14) . . ?
C17 C16 H16A 115.4 . . ?
C15 C16 H16A 115.4 . . ?
C17 C16 H16B 115.4 . . ?
C15 C16 H16B 115.4 . . ?
H16A C16 H16B 112.4 . . ?
C12 C17 C18 102.1(15) . . ?
C12 C17 C16 113.3(15) . . ?
C18 C17 C16 92.0(14) . . ?
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C18 C17 H17 115.5 . . ?
C16 C17 H17 115.5 . . ?
C15 C18 C19 111.7(16) . . ?
C15 C18 C17 83.5(15) . . ?
C19 C18 C17 110.4(16) . . ?
C18B C15B C16B 98.4(15) . . ?
C18B C15B C14 101.2(15) . . ?
C16B C15B C14 111.9(13) . . ?
C18B C15B H15B 114.5 . . ?
C16B C15B H15B 114.5 . . ?
C14 C15B H15B 114.5 . . ?
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C15B C16B H16C 115.6 . . ?
C17B C16B H16C 115.6 . . ?
C15B C16B H16D 115.6 . . ?
C17B C16B H16D 115.6 . . ?
H16C C16B H16D 112.6 . . ?
C12 C17B C18B 101.5(15) . . ?
C12 C17B C16B 109.7(14) . . ?
C18B C17B C16B 91.5(13) . . ?
C12 C17B H17B 116.8 . . ?
C18B C17B H17B 116.8 . . ?
C16B C17B H17B 116.8 . . ?
C15B C18B C19B 109.6(16) . . ?
C15B C18B C17B 84.1(15) . . ?
C19B C18B C17B 108.6(16) . . ?
C18B C19B H19D 109.5 . . ?

C18B C19B H19E 109.5 . . ?
H19D C19B H19E 109.5 . . ?
C18B C19B H19F 109.5 . . ?
H19D C19B H19F 109.5 . . ?
H19E C19B H19F 109.5 . . ?
C13 N1 C9 119.7(7) . . ?
C13 N1 Ru1 126.3(5) . . ?
C9 N1 Ru1 114.0(5) . . ?
Ru1 Cl1 Ru1 96.39(7) . 7_655 ?
C2 Ru1 C1 88.0(4) . . ?
C2 Ru1 C3 89.3(3) . . ?
C1 Ru1 C3 94.7(3) . . ?
C2 Ru1 N1 93.1(3) . . ?
C1 Ru1 N1 174.2(3) . . ?
C3 Ru1 N1 79.7(3) . . ?
C2 Ru1 Cl1 177.6(3) . . ?
C1 Ru1 Cl1 91.2(3) . . ?
C3 Ru1 Cl1 88.6(2) . . ?
N1 Ru1 Cl1 87.46(19) . . ?
C2 Ru1 Cl1 98.7(3) . 7_655 ?
C1 Ru1 Cl1 92.3(3) . 7_655 ?
C3 Ru1 Cl1 169.6(2) . 7_655 ?
N1 Ru1 Cl1 93.12(19) . 7_655 ?
Cl1 Ru1 Cl1 83.61(7) . 7_655 ?
Cl2 C20 Cl3 120.4(15) . . ?
Cl2 C20 H20A 107.2 . . ?
Cl3 C20 H20A 107.2 . . ?
Cl2 C20 H20B 107.2 . . ?
Cl3 C20 H20B 107.2 . . ?
H20A C20 H20B 106.9 . . ?

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Ru1 C3 C4 C5 -176.2(7) . . . . ?
C3 C4 C5 C6 1.7(14) . . . . ?
C4 C5 C6 C7 -0.9(14) . . . . ?
C5 C6 C7 C8 -0.4(14) . . . . ?
C6 C7 C8 C3 1.1(13) . . . . ?
C6 C7 C8 C9 -177.1(8) . . . . ?
C4 C3 C8 C7 -0.3(12) . . . . ?
Ru1 C3 C8 C7 175.5(6) . . . . ?
C4 C3 C8 C9 177.9(8) . . . . ?
Ru1 C3 C8 C9 -6.2(9) . . . . ?
C7 C8 C9 N1 177.2(8) . . . . ?
C3 C8 C9 N1 -1.0(10) . . . . ?
C7 C8 C9 C10 2.4(13) . . . . ?
C3 C8 C9 C10 -175.8(8) . . . . ?
N1 C9 C10 C11 -0.7(14) . . . . ?
C8 C9 C10 C11 173.9(9) . . . . ?
C9 C10 C11 C12 -2.0(18) . . . . ?
C9 C10 C11 C14 -179.4(12) . . . . ?
C10 C11 C12 C13 3(2) . . . . ?
C14 C11 C12 C13 -179.6(13) . . . . ?
C10 C11 C12 C17 -157.5(13) . . . . ?
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C11 C12 C13 N1 -1.1(19) . . . . ?
C17 C12 C13 N1 157.0(14) . . . . ?
C17B C12 C13 N1 -160.5(13) . . . . ?
C10 C11 C14 C15 159.0(14) . . . . ?
C12 C11 C14 C15 -18(2) . . . . ?
C10 C11 C14 C15B -164.1(13) . . . . ?
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C11 C14 C15 C18 59.4(18) . . . . ?
C15B C14 C15 C18 -34.3(15) . . . . ?
C11 C14 C15 C16 -42(2) . . . . ?
C15B C14 C15 C16 -135(2) . . . . ?
C18 C15 C16 C17 -25.4(13) . . . . ?
C14 C15 C16 C17 82.0(16) . . . . ?
C13 C12 C17 C18 142.9(15) . . . . ?
C11 C12 C17 C18 -58.1(18) . . . . ?
C17B C12 C17 C18 44.6(17) . . . . ?
C13 C12 C17 C16 -119.6(16) . . . . ?
C11 C12 C17 C16 39(2) . . . . ?
C17B C12 C17 C16 142(3) . . . . ?
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C15 C16 C17 C18 23.9(13) . . . . ?
C14 C15 C18 C19 160.3(15) . . . . ?
C16 C15 C18 C19 -84.0(17) . . . . ?
C14 C15 C18 C17 -90.2(14) . . . . ?
C16 C15 C18 C17 25.5(13) . . . . ?
C12 C17 C18 C15 88.6(15) . . . . ?
C16 C17 C18 C15 -25.8(13) . . . . ?
C12 C17 C18 C19 -160.7(15) . . . . ?
C16 C17 C18 C19 85.0(18) . . . . ?
C11 C14 C15B C18B -59.9(17) . . . . ?
C15 C14 C15B C18B 38.2(15) . . . . ?
C11 C14 C15B C16B 44.0(18) . . . . ?
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C18B C15B C16B C17B 21.8(13) . . . . ?
C14 C15B C16B C17B -83.9(14) . . . . ?
C13 C12 C17B C18B -143.9(14) . . . . ?
C11 C12 C17B C18B 56.3(18) . . . . ?
C17 C12 C17B C18B -38.0(16) . . . . ?
C13 C12 C17B C16B 120.3(15) . . . . ?
C11 C12 C17B C16B -39.5(19) . . . . ?
C17 C12 C17B C16B -134(2) . . . . ?
C15B C16B C17B C12 82.0(15) . . . . ?
C15B C16B C17B C18B -20.7(13) . . . . ?
C16B C15B C18B C19B 84.3(17) . . . . ?
C14 C15B C18B C19B -161.2(14) . . . . ?
C16B C15B C18B C17B -23.3(14) . . . . ?
C14 C15B C18B C17B 91.1(14) . . . . ?
C12 C17B C18B C15B -89.0(14) . . . . ?
C16B C17B C18B C15B 21.5(14) . . . . ?
C12 C17B C18B C19B 162.3(15) . . . . ?
C16B C17B C18B C19B -87.2(16) . . . . ?
C12 C13 N1 C9 -1.7(15) . . . . ?
C12 C13 N1 Ru1 178.3(9) . . . . ?
C10 C9 N1 C13 2.6(12) . . . . ?
C8 C9 N1 C13 -172.5(8) . . . . ?
C10 C9 N1 Ru1 -177.4(6) . . . . ?
C8 C9 N1 Ru1 7.5(9) . . . . ?
C4 C3 Ru1 C2 -83.7(8) . . . . ?
C8 C3 Ru1 C2 101.0(6) . . . . ?
C4 C3 Ru1 C1 4.3(8) . . . . ?
C8 C3 Ru1 C1 -171.1(6) . . . . ?
C4 C3 Ru1 N1 -177.0(8) . . . . ?
C8 C3 Ru1 N1 7.7(6) . . . . ?
C4 C3 Ru1 Cl1 95.3(8) . . . . ?
C8 C3 Ru1 Cl1 -80.0(6) . . . . ?
C4 C3 Ru1 Cl1 136.2(11) . . . 7_655 ?
C8 C3 Ru1 Cl1 -39.1(17) . . . 7_655 ?

```
C13 N1 Ru1 C2 82.8(8) . . . . ?
C9 N1 Ru1 C2 -97.1(6) . . . . ?
C13 N1 Ru1 C3 171.5(8) . . . . ?
C9 N1 Ru1 C3 -8.5(6) . . . . ?
C13 N1 Ru1 Cl1 -99.5(7) . . . . ?
C9 N1 Ru1 Cl1 80.5(6) . . . . ?
C13 N1 Ru1 Cl1 -16.0(7) . . . 7_655 ?
C9 N1 Ru1 Cl1 164.0(5) . . . 7_655 ?
Ru1 Cl1 Ru1 C1 -92.2(3) 7_655 . . . ?
Ru1 Cl1 Ru1 C3 173.2(2) 7_655 . . . ?
Ru1 Cl1 Ru1 N1 93.43(19) 7_655 . . . ?
Ru1 Cl1 Ru1 Cl1 0.0 7_655 . . 7_655 ?

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_diffrn_reflns_theta_full              27.47
_diffrn_measured_fraction_theta_full   0.999
_refine_diff_density_max    1.803
_refine_diff_density_min   -1.238
_refine_diff_density_rms    0.174
```

G. Crystallographic data for 1b, 2a, 2b and 3b

1. 1b

Crystal data

$C_{18}H_{19}N$	D_x = 1.176 Mg m^{-3}
M_r = 249.34	Melting point: ? K
Monoclinic, *C*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C 2Y	Cell parameters from 3291 reflections
a = 17.9479 (6) Å	θ = 1.0–30.0°
b = 6.2856 (4) Å	μ = 0.07 mm^{-1}
c = 12.5093 (7) Å	*T* = 173 (2) K
β = 93.780 (3)°	Cell measurement pressure: ? kPa
V = 1408.15 (13) Å^3	Block, colorless
Z = 4	0.50 × 0.50 × 0.50 mm
F_{000} = 536	

Data collection

KappaCCD diffractometer	2229 independent reflections
Radiation source: fine-focus sealed tube	1969 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.061
Detector resolution: ? pixels mm^{-1}	θ_{max} = 30.1°
T = 173(2) K	θ_{min} = 1.6°
P = ? kPa	*h* = −25→25
phi and ω scans	*k* = −8→8
Absorption correction: none	*l* = −12→17
5637 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.043	$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 0.1745P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.121	$(\Delta/\sigma)_{max} < 0.001$
S = 1.06	$\Delta\rho_{max}$ = 0.27 e Å^{-3}

2229 reflections

175 parameters

1 restraint

? constraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.030 (4)

Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881

Flack parameter: −10 (10)

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.18173 (12)	0.2801 (4)	0.82649 (14)	0.0476 (5)
H1	0.1998	0.1418	0.8116	0.057*
C2	0.18096 (15)	0.3488 (5)	0.93206 (16)	0.0633 (8)
H2	0.1993	0.2580	0.9885	0.076*
C3	0.15389 (12)	0.5466 (5)	0.95555 (15)	0.0529 (6)
H3	0.1519	0.5907	1.0279	0.064*
C4	0.12964 (11)	0.6803 (4)	0.87331 (15)	0.0504 (6)
H4	0.1118	0.8185	0.8888	0.060*
C5	0.13126 (10)	0.6133 (4)	0.76733 (14)	0.0436 (5)
H5	0.1149	0.7071	0.7110	0.052*
C6	0.15644 (8)	0.4112 (3)	0.74291 (12)	0.0285 (4)
C7	0.15592 (7)	0.3318 (3)	0.63058 (11)	0.0259 (3)
C8	0.12292 (8)	0.4454 (3)	0.54375 (12)	0.0270 (3)
H8	0.1011	0.5807	0.5548	0.032*
C9	0.12203 (8)	0.3602 (3)	0.44159 (12)	0.0258 (3)
C10	0.15498 (7)	0.1612 (3)	0.42772 (11)	0.0245 (3)
C11	0.18635 (8)	0.0596 (3)	0.51823 (11)	0.0279 (3)

H11	0.2087	−0.0756	0.5093	0.034*
C12	0.08613 (10)	0.4693 (3)	0.34285 (13)	0.0348 (4)
H12A	0.1087	0.6118	0.3352	0.042*
H12B	0.0321	0.4885	0.3514	0.042*
C13	0.09690 (10)	0.3387 (3)	0.24271 (13)	0.0364 (4)
H13	0.0770	0.4048	0.1739	0.044*
C14	0.17983 (10)	0.2651 (4)	0.24498 (12)	0.0389 (4)
H14A	0.1966	0.2218	0.1744	0.047*
H14B	0.2156	0.3648	0.2820	0.047*
C15	0.15569 (7)	0.0771 (3)	0.31581 (11)	0.0284 (3)
H15	0.1817	−0.0618	0.3067	0.034*
C16	0.07543 (8)	0.1002 (3)	0.25801 (12)	0.0316 (4)
C17	0.00784 (8)	0.0487 (4)	0.32158 (15)	0.0384 (4)
H17A	−0.0380	0.0878	0.2793	0.058*
H17B	0.0111	0.1292	0.3888	0.058*
H17C	0.0071	−0.1040	0.3374	0.058*
C18	0.06849 (10)	−0.0203 (4)	0.15160 (14)	0.0438 (5)
H18A	0.0619	−0.1724	0.1654	0.066*
H18B	0.1139	0.0011	0.1134	0.066*
H18C	0.0252	0.0331	0.1078	0.066*
N1	0.18711 (7)	0.1404 (3)	0.61778 (10)	0.0290 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0734 (13)	0.0403 (12)	0.0301 (8)	0.0134 (11)	0.0097 (8)	0.0049 (9)
C2	0.1010 (19)	0.0605 (18)	0.0289 (9)	0.0207 (16)	0.0093 (10)	0.0073 (11)
C3	0.0633 (11)	0.0639 (16)	0.0326 (8)	0.0048 (13)	0.0105 (8)	−0.0082 (11)
C4	0.0548	0.0526	0.0435	0.0116 (11)	0.0009 (8)	−0.0161

	(11)	(15)	(10)			(10)
C5	0.0467 (9)	0.0455 (13)	0.0376 (9)	0.0128 (9)	−0.0048 (7)	−0.0071 (9)
C6	0.0235 (6)	0.0339 (9)	0.0284 (7)	−0.0010 (6)	0.0029 (5)	0.0005 (7)
C7	0.0217 (6)	0.0282 (8)	0.0280 (6)	−0.0011 (6)	0.0032 (5)	0.0019 (7)
C8	0.0270 (6)	0.0219 (8)	0.0322 (7)	0.0021 (6)	0.0024 (5)	0.0015 (7)
C9	0.0254 (6)	0.0238 (8)	0.0279 (7)	−0.0026 (6)	−0.0004 (5)	0.0031 (6)
C10	0.0214 (5)	0.0245 (8)	0.0278 (6)	−0.0004 (6)	0.0023 (5)	0.0006 (6)
C11	0.0251 (6)	0.0267 (8)	0.0320 (7)	0.0037 (6)	0.0022 (5)	0.0015 (7)
C12	0.0458 (8)	0.0247 (8)	0.0330 (8)	0.0029 (7)	−0.0045 (6)	0.0033 (7)
C13	0.0494 (9)	0.0296 (10)	0.0292 (7)	−0.0009 (8)	−0.0048 (6)	0.0045 (7)
C14	0.0438 (9)	0.0442 (12)	0.0289 (7)	−0.0108 (8)	0.0045 (6)	0.0011 (8)
C15	0.0257 (6)	0.0301 (8)	0.0296 (7)	−0.0004 (6)	0.0025 (5)	−0.0010 (7)
C16	0.0314 (7)	0.0292 (9)	0.0333 (7)	−0.0005 (6)	−0.0039 (5)	−0.0016 (7)
C17	0.0262 (7)	0.0324 (9)	0.0561 (10)	0.0007 (7)	−0.0014 (6)	−0.0048 (9)
C18	0.0499 (10)	0.0410 (11)	0.0388 (9)	−0.0002 (9)	−0.0089 (7)	−0.0079 (9)
N1	0.0282 (5)	0.0304 (8)	0.0284 (6)	0.0040 (6)	0.0017 (4)	0.0024 (6)

Table 1
Geometric parameters (Å, °)

C1—C6	1.384 (3)	C11—H11	0.9500
C1—C2	1.390 (3)	C12—C13	1.521 (2)
C1—H1	0.9500	C12—H12A	0.9900
C2—C3	1.374 (4)	C12—H12B	0.9900

C2—H2	0.9500	C13—C14	1.557 (3)
C3—C4	1.377 (3)	C13—C16	1.563 (3)
C3—H3	0.9500	C13—H13	1.0000
C4—C5	1.393 (2)	C14—C15	1.556 (3)
C4—H4	0.9500	C14—H14A	0.9900
C5—C6	1.389 (3)	C14—H14B	0.9900
C5—H5	0.9500	C15—C16	1.575 (2)
C6—C7	1.491 (2)	C15—H15	1.0000
C7—N1	1.341 (2)	C16—C17	1.528 (2)
C7—C8	1.398 (2)	C16—C18	1.529 (2)
C8—C9	1.385 (2)	C17—H17A	0.9800
C8—H8	0.9500	C17—H17B	0.9800
C9—C10	1.399 (2)	C17—H17C	0.9800
C9—C12	1.519 (2)	C18—H18A	0.9800
C10—C11	1.387 (2)	C18—H18B	0.9800
C10—C15	1.4974 (19)	C18—H18C	0.9800
C11—N1	1.3440 (19)		

C6—C1—C2	120.6 (2)	H12A—C12—H12B	108.1
C6—C1—H1	119.7	C12—C13—C14	108.58 (14)
C2—C1—H1	119.7	C12—C13—C16	111.80 (14)
C3—C2—C1	120.7 (2)	C14—C13—C16	87.48 (14)
C3—C2—H2	119.7	C12—C13—H13	115.3
C1—C2—H2	119.7	C14—C13—H13	115.3
C2—C3—C4	119.45 (19)	C16—C13—H13	115.3
C2—C3—H3	120.3	C15—C14—C13	86.24 (12)
C4—C3—H3	120.3	C15—C14—H14A	114.3
C3—C4—C5	120.1 (2)	C13—C14—H14A	114.3
C3—C4—H4	120.0	C15—C14—H14B	114.3
C5—C4—H4	120.0	C13—C14—H14B	114.3
C6—C5—C4	120.9 (2)	H14A—C14—H14B	111.4

C6—C5—H5	119.6	C10—C15—C14	106.49 (14)
C4—C5—H5	119.6	C10—C15—C16	109.43 (11)
C1—C6—C5	118.28 (16)	C14—C15—C16	87.08 (12)
C1—C6—C7	119.59 (16)	C10—C15—H15	116.6
C5—C6—C7	122.12 (16)	C14—C15—H15	116.6
N1—C7—C8	121.60 (14)	C16—C15—H15	116.6
N1—C7—C6	115.87 (14)	C17—C16—C18	109.03 (14)
C8—C7—C6	122.49 (15)	C17—C16—C13	118.52 (15)
C9—C8—C7	119.86 (15)	C18—C16—C13	112.03 (15)
C9—C8—H8	120.1	C17—C16—C15	118.35 (13)
C7—C8—H8	120.1	C18—C16—C15	111.92 (13)
C8—C9—C10	118.75 (13)	C13—C16—C15	85.37 (13)
C8—C9—C12	123.66 (15)	C16—C17—H17A	109.5
C10—C9—C12	117.59 (14)	C16—C17—H17B	109.5
C11—C10—C9	117.56 (14)	H17A—C17—H17B	109.5
C11—C10—C15	124.93 (15)	C16—C17—H17C	109.5
C9—C10—C15	117.48 (13)	H17A—C17—H17C	109.5
N1—C11—C10	124.16 (16)	H17B—C17—H17C	109.5
N1—C11—H11	117.9	C16—C18—H18A	109.5
C10—C11—H11	117.9	C16—C18—H18B	109.5
C9—C12—C13	110.84 (15)	H18A—C18—H18B	109.5
C9—C12—H12A	109.5	C16—C18—H18C	109.5
C13—C12—H12A	109.5	H18A—C18—H18C	109.5
C9—C12—H12B	109.5	H18B—C18—H18C	109.5
C13—C12—H12B	109.5	C7—N1—C11	118.07 (13)

C6—C1—C2—C3	1.1 (4)	C9—C12—C13—C16	48.91 (19)
C1—C2—C3—C4	−2.2 (4)	C12—C13—C14—C15	84.34 (15)
C2—C3—C4—C5	1.3 (4)	C16—C13—C14—C15	−27.82 (12)
C3—C4—C5—C6	0.7 (3)	C11—C10—C15—C14	−133.29 (16)
C2—C1—C6—C5	0.8 (3)	C9—C10—C15—C14	44.79 (16)

C2—C1—C6—C7	−178.37 (19)	C11—C10—C15—C16	133.96 (16)
C4—C5—C6—C1	−1.7 (3)	C9—C10—C15—C16	−47.97 (18)
C4—C5—C6—C7	177.45 (16)	C13—C14—C15—C10	−81.81 (13)
C1—C6—C7—N1	−5.9 (2)	C13—C14—C15—C16	27.59 (12)
C5—C6—C7—N1	175.01 (15)	C12—C13—C16—C17	38.3 (2)
C1—C6—C7—C8	172.07 (16)	C14—C13—C16—C17	147.36 (14)
C5—C6—C7—C8	−7.0 (2)	C12—C13—C16—C18	166.68 (14)
N1—C7—C8—C9	0.0 (2)	C14—C13—C16—C18	−84.31 (14)
C6—C7—C8—C9	−177.87 (13)	C12—C13—C16—C15	−81.53 (14)
C7—C8—C9—C10	−0.4 (2)	C14—C13—C16—C15	27.48 (11)
C7—C8—C9—C12	178.68 (14)	C10—C15—C16—C17	−41.1 (2)
C8—C9—C10—C11	0.5 (2)	C14—C15—C16—C17	−147.55 (16)
C12—C9—C10—C11	−178.67 (14)	C10—C15—C16—C18	−169.15 (15)
C8—C9—C10—C15	−177.74 (13)	C14—C15—C16—C18	84.39 (17)
C12—C9—C10—C15	3.11 (19)	C10—C15—C16—C13	78.95 (14)
C9—C10—C11—N1	−0.1 (2)	C14—C15—C16—C13	−27.51 (12)
C15—C10—C11—N1	177.98 (13)	C8—C7—N1—C11	0.4 (2)
C8—C9—C12—C13	178.09 (14)	C6—C7—N1—C11	178.40 (13)
C10—C9—C12—C13	−2.8 (2)	C10—C11—N1—C7	−0.4 (2)
C9—C12—C13—C14	−45.9 (2)		

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

2. 2a

Crystal data

$C_{36}H_{36}Cl_2N_2O_4Ru_2$
M_r = 833.71
Monoclinic, $P2_1/c$

D_x = 1.572 Mg m^{-3}
Melting point: ? K
Mo $K\alpha$ radiation
λ = 0.71073 Å

Hall symbol: -P 2ybc	Cell parameters from 12571 reflections
a = 10.5024 (4) Å	θ = 1.0–27.5°
b = 17.3861 (6) Å	μ = 1.05 mm^{-1}
c = 19.4045 (6) Å	T = 173 (2) K
β = 96.247 (2)°	Cell measurement pressure: ? kPa
V = 3522.1 (2) $Å^3$	Prism, colorless
Z = 4	0.20 × 0.15 × 0.10 mm
F_{000} = 1680	

Data collection

KappaCCD diffractometer	8042 independent reflections
Radiation source: fine-focus sealed tube	5452 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.081
Detector resolution: ? pixels mm^{-1}	θ_{max} = 27.5°
T = 173(2) K	θ_{min} = 1.6°
P = ? kPa	h = −13→11
phi and ω scans	k = −20→22
Absorption correction: none	l = −24→25
22098 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H-atom parameters constrained
$wR(F^2)$ = 0.144	$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
8042 reflections	$\Delta\rho_{max}$ = 1.24 e $Å^{-3}$
423 parameters	$\Delta\rho_{min}$ = −1.62 e $Å^{-3}$
? constraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.1393 (5)	0.1506 (3)	0.1372 (3)	0.0328 (12)	
C2	0.3701 (5)	0.1539 (3)	0.1084 (3)	0.0341 (12)	
C3	0.3049 (4)	0.0177 (3)	0.1599 (2)	0.0255 (10)	
C4	0.2172 (5)	−0.0217 (3)	0.1138 (2)	0.0288 (11)	
H4	0.1448	0.0049	0.0920	0.035*	
C5	0.2331 (5)	−0.0992 (3)	0.0990 (2)	0.0316 (12)	
C6	0.3400 (5)	−0.1378 (3)	0.1296 (3)	0.0329 (12)	
H6	0.3518	−0.1906	0.1193	0.039*	
C7	0.4298 (5)	−0.1001 (3)	0.1750 (2)	0.0296 (11)	
H7	0.5033	−0.1270	0.1952	0.036*	
C8	0.4128 (5)	−0.0225 (3)	0.1913 (2)	0.0246 (10)	
C9	0.1338 (5)	−0.1400 (3)	0.0492 (3)	0.0447 (15)	
H9A	0.0492	−0.1347	0.0656	0.067*	
H9B	0.1558	−0.1947	0.0469	0.067*	
H9C	0.1324	−0.1171	0.0030	0.067*	
C10	0.5027 (4)	0.0201 (3)	0.2410 (2)	0.0250 (10)	
C11	0.6043 (5)	−0.0120 (3)	0.2835 (2)	0.0275 (11)	
H11	0.6230	−0.0652	0.2794	0.033*	
C12	0.6784 (4)	0.0322 (3)	0.3317 (2)	0.0275 (11)	
C13	0.6512 (5)	0.1106 (3)	0.3322 (3)	0.0336 (12)	
H13	0.7021	0.1439	0.3627	0.040*	
C14	0.5506 (5)	0.1398 (3)	0.2887 (3)	0.0312 (12)	
H14	0.5343	0.1935	0.2897	0.037*	
C15	0.7817 (5)	−0.0025 (3)	0.3845 (3)	0.0345 (12)	
C16	0.7997 (17)	−0.0924 (10)	0.3725 (10)	0.0595 (18)	0.50
H16A	0.8073	−0.1020	0.3233	0.089*	0.50
H16B	0.7255	−0.1202	0.3863	0.089*	0.50
H16C	0.8775	−0.1101	0.4004	0.089*	0.50

C17	0.9129 (14)	0.0347 (8)	0.3757 (7)	0.0595 (18)	0.50
H17A	0.9772	0.0161	0.4122	0.089*	0.50
H17B	0.9057	0.0908	0.3790	0.089*	0.50
H17C	0.9387	0.0209	0.3303	0.089*	0.50
C18	0.7451 (14)	0.0118 (8)	0.4560 (7)	0.0595 (18)	0.50
H18A	0.6584	−0.0077	0.4591	0.089*	0.50
H18B	0.7474	0.0672	0.4655	0.089*	0.50
H18C	0.8055	−0.0147	0.4900	0.089*	0.50
C16B	0.8358 (16)	−0.0721 (10)	0.3631 (10)	0.0595 (18)	0.50
H16D	0.8855	−0.0965	0.4030	0.089*	0.50
H16E	0.8922	−0.0612	0.3273	0.089*	0.50
H16F	0.7672	−0.1069	0.3443	0.089*	0.50
C17B	0.8840 (14)	0.0535 (8)	0.4108 (7)	0.0595 (18)	0.50
H17D	0.9401	0.0298	0.4486	0.089*	0.50
H17E	0.8444	0.0997	0.4280	0.089*	0.50
H17F	0.9345	0.0675	0.3731	0.089*	0.50
C18B	0.7088 (14)	−0.0234 (8)	0.4495 (7)	0.0595 (18)	0.50
H18D	0.6774	−0.0765	0.4451	0.089*	0.50
H18E	0.6363	0.0116	0.4515	0.089*	0.50
H18F	0.7677	−0.0184	0.4920	0.089*	0.50
C19	0.3519 (5)	0.2211 (3)	0.3990 (3)	0.0338 (12)	
C20	0.1151 (5)	0.2138 (3)	0.4243 (3)	0.0359 (12)	
C21	0.1845 (4)	0.3504 (3)	0.3596 (2)	0.0243 (10)	
C22	0.2708 (5)	0.3978 (3)	0.3985 (2)	0.0294 (11)	
H22	0.3397	0.3749	0.4271	0.035*	
C23	0.2605 (5)	0.4777 (3)	0.3973 (2)	0.0296 (11)	
C24	0.1572 (5)	0.5102 (3)	0.3569 (2)	0.0326 (12)	
H24	0.1471	0.5645	0.3566	0.039*	
C25	0.0690 (5)	0.4657 (3)	0.3172 (2)	0.0291 (11)	
H25	−0.0004	0.4894	0.2897	0.035*	

C26	0.0813 (4)	0.3856 (3)	0.3172 (2)	0.0240 (10)
C27	0.3594 (5)	0.5273 (3)	0.4385 (3)	0.0399 (13)
H27A	0.3397	0.5816	0.4292	0.060*
H27B	0.4445	0.5154	0.4250	0.060*
H27C	0.3581	0.5169	0.4881	0.060*
C28	−0.0075 (4)	0.3350 (3)	0.2751 (2)	0.0237 (10)
C29	−0.1098 (5)	0.3601 (3)	0.2281 (2)	0.0265 (11)
H29	−0.1252	0.4136	0.2219	0.032*
C30	−0.1886 (4)	0.3078 (3)	0.1905 (2)	0.0241 (10)
C31	−0.1654 (5)	0.2297 (3)	0.2056 (3)	0.0303 (11)
H31	−0.2213	0.1916	0.1841	0.036*
C32	−0.0633 (5)	0.2083 (3)	0.2509 (3)	0.0309 (11)
H32	−0.0493	0.1550	0.2595	0.037*
C33	−0.2933 (5)	0.3311 (3)	0.1342 (2)	0.0287 (11)
C34	−0.3037 (5)	0.4184 (3)	0.1256 (3)	0.0386 (13)
H34A	−0.3253	0.4415	0.1688	0.058*
H34B	−0.3707	0.4306	0.0880	0.058*
H34C	−0.2216	0.4390	0.1143	0.058*
C35	−0.4221 (5)	0.3005 (3)	0.1518 (3)	0.0417 (13)
H35A	−0.4176	0.2445	0.1566	0.063*
H35B	−0.4890	0.3142	0.1146	0.063*
H35C	−0.4423	0.3234	0.1955	0.063*
C36	−0.2629 (6)	0.2955 (3)	0.0655 (3)	0.0455 (14)
H36A	−0.1779	0.3124	0.0554	0.068*
H36B	−0.3273	0.3121	0.0281	0.068*
H36C	−0.2641	0.2393	0.0692	0.068*
N1	0.4747 (4)	0.0959 (2)	0.24505 (19)	0.0242 (8)
N2	0.0186 (4)	0.2589 (2)	0.28385 (19)	0.0249 (9)
O1	0.0445 (4)	0.1631 (2)	0.10452 (19)	0.0463 (10)
O2	0.4103 (4)	0.1660 (2)	0.05680 (18)	0.0468 (10)

O3	0.4470 (4)	0.2147 (2)	0.4338 (2)	0.0516 (11)
O4	0.0704 (4)	0.2038 (2)	0.4737 (2)	0.0518 (11)
Cl1	0.19787 (11)	0.09761 (7)	0.29483 (6)	0.0287 (3)
Cl2	0.30459 (11)	0.26371 (6)	0.24227 (6)	0.0279 (3)
Ru1	0.29805 (4)	0.13088 (2)	0.188289 (19)	0.02429 (12)
Ru2	0.19494 (4)	0.23358 (2)	0.344812 (19)	0.02500 (13)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.036 (3)	0.033 (3)	0.029 (3)	−0.003 (2)	0.005 (2)	−0.001 (2)
C2	0.037 (3)	0.031 (3)	0.033 (3)	−0.003 (2)	0.000 (2)	−0.006 (2)
C3	0.027 (3)	0.024 (3)	0.026 (2)	−0.005 (2)	0.005 (2)	−0.002 (2)
C4	0.027 (3)	0.030 (3)	0.029 (2)	−0.004 (2)	0.003 (2)	−0.007 (2)
C5	0.033 (3)	0.034 (3)	0.028 (3)	−0.010 (2)	0.007 (2)	−0.008 (2)
C6	0.041 (3)	0.022 (3)	0.037 (3)	−0.004 (2)	0.010 (2)	−0.008 (2)
C7	0.034 (3)	0.024 (3)	0.030 (3)	0.003 (2)	0.000 (2)	0.000 (2)
C8	0.031 (3)	0.020 (2)	0.023 (2)	−0.001 (2)	0.005 (2)	−0.0005 (19)
C9	0.039 (3)	0.052 (4)	0.043 (3)	−0.011 (3)	0.000 (3)	−0.017 (3)
C10	0.026 (3)	0.025 (3)	0.025 (2)	0.001 (2)	0.005 (2)	0.001 (2)
C11	0.031 (3)	0.026 (3)	0.026 (2)	0.005 (2)	0.004 (2)	0.000 (2)
C12	0.026 (3)	0.030 (3)	0.026 (2)	0.000 (2)	0.003 (2)	0.000 (2)
C13	0.030 (3)	0.032 (3)	0.037 (3)	−0.001 (2)	−0.002 (2)	−0.011 (2)
C14	0.034 (3)	0.024 (3)	0.035 (3)	0.000 (2)	0.001 (2)	−0.004 (2)
C15	0.037 (3)	0.034 (3)	0.031 (3)	0.000 (2)	−0.006 (2)	−0.001 (2)
C16	0.057 (5)	0.060 (5)	0.056 (3)	0.003 (3)	−0.018 (3)	0.004 (4)
C17	0.057 (5)	0.060 (5)	0.056 (3)	0.003 (3)	−0.018 (3)	0.004 (4)
C18	0.057 (5)	0.060 (5)	0.056 (3)	0.003 (3)	−0.018 (3)	0.004 (4)
C16B	0.057 (5)	0.060 (5)	0.056 (3)	0.003 (3)	−0.018 (3)	0.004 (4)
C17B	0.057 (5)	0.060 (5)	0.056 (3)	0.003 (3)	−0.018 (3)	0.004 (4)
C18B	0.057 (5)	0.060 (5)	0.056 (3)	0.003 (3)	−0.018 (3)	0.004 (4)

C19	0.043 (3)	0.031 (3)	0.027 (3)	0.008 (2)	0.004 (2)	−0.002 (2)
C20	0.041 (3)	0.032 (3)	0.036 (3)	0.009 (2)	0.007 (3)	0.007 (2)
C21	0.031 (3)	0.021 (2)	0.022 (2)	0.004 (2)	0.006 (2)	0.000 (2)
C22	0.030 (3)	0.031 (3)	0.027 (2)	0.006 (2)	0.000 (2)	−0.001 (2)
C23	0.031 (3)	0.029 (3)	0.029 (3)	0.001 (2)	0.003 (2)	−0.006 (2)
C24	0.039 (3)	0.025 (3)	0.033 (3)	−0.002 (2)	0.000 (2)	−0.004 (2)
C25	0.033 (3)	0.025 (3)	0.029 (3)	0.005 (2)	−0.001 (2)	0.003 (2)
C26	0.027 (3)	0.024 (3)	0.020 (2)	0.002 (2)	0.002 (2)	0.003 (2)
C27	0.033 (3)	0.045 (3)	0.039 (3)	0.001 (2)	−0.006 (2)	−0.010 (3)
C28	0.026 (3)	0.023 (2)	0.023 (2)	−0.001 (2)	0.0060 (19)	−0.001 (2)
C29	0.030 (3)	0.022 (2)	0.027 (2)	0.001 (2)	0.003 (2)	0.004 (2)
C30	0.026 (3)	0.022 (2)	0.025 (2)	0.003 (2)	0.005 (2)	−0.001 (2)
C31	0.028 (3)	0.023 (3)	0.038 (3)	−0.002 (2)	0.000 (2)	−0.003 (2)
C32	0.030 (3)	0.020 (2)	0.042 (3)	0.001 (2)	−0.001 (2)	0.004 (2)
C33	0.031 (3)	0.029 (3)	0.024 (2)	0.002 (2)	−0.001 (2)	−0.003 (2)
C34	0.040 (3)	0.030 (3)	0.042 (3)	0.003 (2)	−0.010 (3)	0.003 (2)
C35	0.027 (3)	0.047 (3)	0.051 (3)	−0.003 (2)	0.000 (3)	−0.001 (3)
C36	0.056 (4)	0.047 (3)	0.032 (3)	0.006 (3)	0.001 (3)	−0.010 (3)
N1	0.022 (2)	0.026 (2)	0.0247 (19)	0.0006 (17)	0.0009 (17)	−0.0030 (18)
N2	0.026 (2)	0.021 (2)	0.027 (2)	0.0008 (17)	0.0005 (18)	0.0007 (17)
O1	0.035 (2)	0.058 (3)	0.043 (2)	0.0029 (19)	−0.0105 (19)	0.003 (2)
O2	0.060 (3)	0.053 (2)	0.029 (2)	−0.009 (2)	0.0092 (19)	−0.0002 (19)
O3	0.044 (3)	0.065 (3)	0.042 (2)	0.019 (2)	−0.013 (2)	−0.007 (2)
O4	0.061 (3)	0.054 (2)	0.045 (2)	0.009 (2)	0.022 (2)	0.012 (2)
Cl1	0.0318 (7)	0.0208 (6)	0.0338 (6)	0.0021 (5)	0.0046 (5)	0.0039 (5)
Cl2	0.0316 (7)	0.0219 (6)	0.0304 (6)	−0.0011 (5)	0.0050 (5)	−0.0002 (5)
Ru1	0.0253 (2)	0.0222 (2)	0.0247 (2)	−0.00032 (16)	−0.00027 (16)	−0.00046 (16)
Ru2	0.0269	0.0232	0.0243 (2)	0.00409 (16)	0.00031 (16)	0.00252 (16)

(2) (2)

Table 2
Geometric parameters (Å, °)

C1—O1	1.142 (6)	C18B—H18D	0.9800
C1—Ru1	1.876 (5)	C18B—H18E	0.9800
C2—O2	1.149 (6)	C18B—H18F	0.9800
C2—Ru1	1.841 (6)	C19—O3	1.148 (6)
C3—C4	1.392 (6)	C19—Ru2	1.869 (6)
C3—C8	1.412 (6)	C20—O4	1.126 (6)
C3—Ru1	2.046 (5)	C20—Ru2	1.866 (6)
C4—C5	1.391 (7)	C21—C22	1.386 (6)
C4—H4	0.9500	C21—C26	1.425 (6)
C5—C6	1.385 (7)	C21—Ru2	2.056 (4)
C5—C9	1.519 (6)	C22—C23	1.393 (6)
C6—C7	1.383 (6)	C22—H22	0.9500
C6—H6	0.9500	C23—C24	1.387 (6)
C7—C8	1.402 (6)	C23—C27	1.510 (6)
C7—H7	0.9500	C24—C25	1.377 (6)
C8—C10	1.473 (6)	C24—H24	0.9500
C9—H9A	0.9800	C25—C26	1.397 (6)
C9—H9B	0.9800	C25—H25	0.9500
C9—H9C	0.9800	C26—C28	1.466 (6)
C10—N1	1.354 (6)	C27—H27A	0.9800
C10—C11	1.393 (6)	C27—H27B	0.9800
C11—C12	1.383 (6)	C27—H27C	0.9800
C11—H11	0.9500	C28—N2	1.357 (6)
C12—C13	1.392 (7)	C28—C29	1.402 (6)
C12—C15	1.533 (6)	C29—C30	1.382 (6)
C13—C14	1.376 (7)	C29—H29	0.9500

C13—H13	0.9500	C30—C31	1.404 (6)
C14—N1	1.337 (6)	C30—C33	1.518 (6)
C14—H14	0.9500	C31—C32	1.363 (7)
C15—C16B	1.42 (2)	C31—H31	0.9500
C15—C17B	1.498 (15)	C32—N2	1.343 (6)
C15—C18	1.500 (15)	C32—H32	0.9500
C15—C17	1.548 (16)	C33—C35	1.526 (7)
C15—C18B	1.588 (17)	C33—C34	1.530 (7)
C15—C16	1.593 (19)	C33—C36	1.534 (7)
C16—H16A	0.9800	C34—H34A	0.9800
C16—H16B	0.9800	C34—H34B	0.9800
C16—H16C	0.9800	C34—H34C	0.9800
C17—H17A	0.9800	C35—H35A	0.9800
C17—H17B	0.9800	C35—H35B	0.9800
C17—H17C	0.9800	C35—H35C	0.9800
C18—H18A	0.9800	C36—H36A	0.9800
C18—H18B	0.9800	C36—H36B	0.9800
C18—H18C	0.9800	C36—H36C	0.9800
C16B—H16D	0.9800	N1—Ru1	2.141 (4)
C16B—H16E	0.9800	N2—Ru2	2.132 (4)
C16B—H16F	0.9800	Cl1—Ru1	2.4878 (12)
C17B—H17D	0.9800	Cl1—Ru2	2.5565 (12)
C17B—H17E	0.9800	Cl2—Ru2	2.4614 (12)
C17B—H17F	0.9800	Cl2—Ru1	2.5338 (12)

O1—C1—Ru1	178.0 (5)	C24—C23—C27	121.1 (4)
O2—C2—Ru1	176.6 (5)	C22—C23—C27	120.8 (4)
C4—C3—C8	118.4 (4)	C25—C24—C23	121.6 (5)
C4—C3—Ru1	127.3 (4)	C25—C24—H24	119.2
C8—C3—Ru1	114.2 (3)	C23—C24—H24	119.2
C5—C4—C3	121.6 (5)	C24—C25—C26	120.2 (4)

C5—C4—H4	119.2	C24—C25—H25	119.9
C3—C4—H4	119.2	C26—C25—H25	119.9
C6—C5—C4	119.4 (4)	C25—C26—C21	119.5 (4)
C6—C5—C9	121.0 (5)	C25—C26—C28	123.0 (4)
C4—C5—C9	119.7 (5)	C21—C26—C28	117.5 (4)
C7—C6—C5	120.6 (4)	C23—C27—H27A	109.5
C7—C6—H6	119.7	C23—C27—H27B	109.5
C5—C6—H6	119.7	H27A—C27—H27B	109.5
C6—C7—C8	120.3 (5)	C23—C27—H27C	109.5
C6—C7—H7	119.8	H27A—C27—H27C	109.5
C8—C7—H7	119.8	H27B—C27—H27C	109.5
C7—C8—C3	119.7 (4)	N2—C28—C29	121.0 (4)
C7—C8—C10	122.9 (4)	N2—C28—C26	114.0 (4)
C3—C8—C10	117.4 (4)	C29—C28—C26	124.9 (4)
C5—C9—H9A	109.5	C30—C29—C28	120.7 (4)
C5—C9—H9B	109.5	C30—C29—H29	119.7
H9A—C9—H9B	109.5	C28—C29—H29	119.7
C5—C9—H9C	109.5	C29—C30—C31	116.5 (4)
H9A—C9—H9C	109.5	C29—C30—C33	123.3 (4)
H9B—C9—H9C	109.5	C31—C30—C33	120.2 (4)
N1—C10—C11	120.8 (4)	C32—C31—C30	120.3 (4)
N1—C10—C8	113.6 (4)	C32—C31—H31	119.8
C11—C10—C8	125.6 (4)	C30—C31—H31	119.8
C12—C11—C10	121.0 (4)	N2—C32—C31	123.1 (4)
C12—C11—H11	119.5	N2—C32—H32	118.4
C10—C11—H11	119.5	C31—C32—H32	118.4
C11—C12—C13	116.7 (4)	C30—C33—C35	109.6 (4)
C11—C12—C15	122.5 (4)	C30—C33—C34	112.4 (4)
C13—C12—C15	120.8 (4)	C35—C33—C34	108.4 (4)
C14—C13—C12	120.0 (4)	C30—C33—C36	108.3 (4)

C14—C13—H13	120.0	C35—C33—C36	109.1 (4)
C12—C13—H13	120.0	C34—C33—C36	108.9 (4)
N1—C14—C13	122.9 (4)	C33—C34—H34A	109.5
N1—C14—H14	118.6	C33—C34—H34B	109.5
C13—C14—H14	118.6	H34A—C34—H34B	109.5
C16B—C15—C17B	111.0 (9)	C33—C34—H34C	109.5
C16B—C15—C18	124.3 (10)	H34A—C34—H34C	109.5
C17B—C15—C18	79.8 (8)	H34B—C34—H34C	109.5
C16B—C15—C12	114.7 (8)	C33—C35—H35A	109.5
C17B—C15—C12	113.7 (6)	C33—C35—H35B	109.5
C18—C15—C12	108.5 (7)	H35A—C35—H35B	109.5
C16B—C15—C17	86.3 (9)	C33—C35—H35C	109.5
C18—C15—C17	110.7 (8)	H35A—C35—H35C	109.5
C12—C15—C17	109.6 (6)	H35B—C35—H35C	109.5
C16B—C15—C18B	106.2 (9)	C33—C36—H36A	109.5
C17B—C15—C18B	105.5 (8)	C33—C36—H36B	109.5
C12—C15—C18B	104.7 (6)	H36A—C36—H36B	109.5
C17—C15—C18B	134.0 (8)	C33—C36—H36C	109.5
C17B—C15—C16	126.5 (9)	H36A—C36—H36C	109.5
C18—C15—C16	110.1 (9)	H36B—C36—H36C	109.5
C12—C15—C16	112.0 (7)	C14—N1—C10	118.4 (4)
C17—C15—C16	105.8 (9)	C14—N1—Ru1	125.9 (3)
C18B—C15—C16	88.1 (9)	C10—N1—Ru1	115.3 (3)
C15—C16—H16A	109.5	C32—N2—C28	117.9 (4)
C15—C16—H16B	109.5	C32—N2—Ru2	127.0 (3)
C15—C16—H16C	109.5	C28—N2—Ru2	115.0 (3)
C15—C17—H17A	109.5	Ru1—Cl1—Ru2	97.12 (4)
C15—C17—H17B	109.5	Ru2—Cl2—Ru1	98.40 (4)
C15—C17—H17C	109.5	C2—Ru1—C1	86.5 (2)
C15—C18—H18A	109.5	C2—Ru1—C3	87.3 (2)

C15—C18—H18B	109.5	C1—Ru1—C3	95.1 (2)
C15—C18—H18C	109.5	C2—Ru1—N1	94.71 (19)
C15—C16B—H16D	109.5	C1—Ru1—N1	174.04 (18)
C15—C16B—H16E	109.5	C3—Ru1—N1	79.12 (16)
H16D—C16B—H16E	109.5	C2—Ru1—Cl1	178.77 (16)
C15—C16B—H16F	109.5	C1—Ru1—Cl1	92.84 (16)
H16D—C16B—H16F	109.5	C3—Ru1—Cl1	91.76 (13)
H16E—C16B—H16F	109.5	N1—Ru1—Cl1	85.85 (11)
C15—C17B—H17D	109.5	C2—Ru1—Cl2	98.91 (16)
C15—C17B—H17E	109.5	C1—Ru1—Cl2	91.94 (16)
H17D—C17B—H17E	109.5	C3—Ru1—Cl2	170.89 (13)
C15—C17B—H17F	109.5	N1—Ru1—Cl2	93.64 (10)
H17D—C17B—H17F	109.5	Cl1—Ru1—Cl2	82.14 (4)
H17E—C17B—H17F	109.5	C20—Ru2—C19	87.8 (2)
C15—C18B—H18D	109.5	C20—Ru2—C21	91.8 (2)
C15—C18B—H18E	109.5	C19—Ru2—C21	95.3 (2)
H18D—C18B—H18E	109.5	C20—Ru2—N2	93.16 (19)
C15—C18B—H18F	109.5	C19—Ru2—N2	174.72 (18)
H18D—C18B—H18F	109.5	C21—Ru2—N2	79.44 (16)
H18E—C18B—H18F	109.5	C20—Ru2—Cl2	177.83 (17)
O3—C19—Ru2	178.0 (5)	C19—Ru2—Cl2	91.03 (16)
O4—C20—Ru2	177.2 (5)	C21—Ru2—Cl2	86.51 (13)
C22—C21—C26	118.0 (4)	N2—Ru2—Cl2	87.83 (11)
C22—C21—Ru2	128.4 (3)	C20—Ru2—Cl1	99.71 (16)
C26—C21—Ru2	113.1 (3)	C19—Ru2—Cl1	93.45 (15)
C21—C22—C23	122.5 (4)	C21—Ru2—Cl1	165.79 (13)
C21—C22—H22	118.7	N2—Ru2—Cl1	91.50 (10)
C23—C22—H22	118.7	Cl2—Ru2—Cl1	82.19 (4)
C24—C23—C22	118.0 (4)		
C8—C3—C4—C5	0.7 (7)	C31—C30—C33—C36	−59.6 (6)

Ru1—C3—C4—C5	−179.9 (4)	C13—C14—N1—C10	−3.7 (7)
C3—C4—C5—C6	−1.4 (7)	C13—C14—N1—Ru1	168.7 (4)
C3—C4—C5—C9	179.1 (4)	C11—C10—N1—C14	3.0 (7)
C4—C5—C6—C7	0.6 (8)	C8—C10—N1—C14	−180.0 (4)
C9—C5—C6—C7	−179.9 (4)	C11—C10—N1—Ru1	−170.2 (3)
C5—C6—C7—C8	0.8 (8)	C8—C10—N1—Ru1	6.8 (5)
C6—C7—C8—C3	−1.4 (7)	C31—C32—N2—C28	4.8 (7)
C6—C7—C8—C10	177.9 (4)	C31—C32—N2—Ru2	−171.1 (4)
C4—C3—C8—C7	0.7 (7)	C29—C28—N2—C32	−5.9 (7)
Ru1—C3—C8—C7	−178.8 (4)	C26—C28—N2—C32	175.5 (4)
C4—C3—C8—C10	−178.7 (4)	C29—C28—N2—Ru2	170.4 (3)
Ru1—C3—C8—C10	1.9 (5)	C26—C28—N2—Ru2	−8.2 (5)
C7—C8—C10—N1	174.9 (4)	C4—C3—Ru1—C2	−82.7 (4)
C3—C8—C10—N1	−5.8 (6)	C8—C3—Ru1—C2	96.7 (4)
C7—C8—C10—C11	−8.3 (7)	C4—C3—Ru1—C1	3.5 (4)
C3—C8—C10—C11	171.1 (4)	C8—C3—Ru1—C1	−177.1 (4)
N1—C10—C11—C12	0.8 (7)	C4—C3—Ru1—N1	−178.1 (4)
C8—C10—C11—C12	−175.8 (4)	C8—C3—Ru1—N1	1.3 (3)
C10—C11—C12—C13	−3.8 (7)	C4—C3—Ru1—Cl1	96.5 (4)
C10—C11—C12—C15	173.5 (4)	C8—C3—Ru1—Cl1	−84.1 (3)
C11—C12—C13—C14	3.2 (7)	C14—N1—Ru1—C2	96.4 (4)
C15—C12—C13—C14	−174.2 (5)	C10—N1—Ru1—C2	−91.0 (3)
C12—C13—C14—N1	0.6 (8)	C14—N1—Ru1—C3	−177.3 (4)
C11—C12—C15—C16B	26.8 (10)	C10—N1—Ru1—C3	−4.7 (3)
C13—C12—C15—C16B	−155.9 (8)	C14—N1—Ru1—Cl1	−84.7 (4)
C11—C12—C15—C17B	156.1 (8)	C10—N1—Ru1—Cl1	87.9 (3)
C13—C12—C15—C17B	−26.6 (9)	C14—N1—Ru1—Cl2	−2.9 (4)
C11—C12—C15—C18	−117.1 (7)	C10—N1—Ru1—Cl2	169.8 (3)

C13—C12—C15—C18	60.1 (8)	Ru2—Cl1—Ru1—C1	−88.73 (16)
C11—C12—C15—C17	121.9 (7)	Ru2—Cl1—Ru1—C3	176.05 (13)
C13—C12—C15—C17	−60.9 (8)	Ru2—Cl1—Ru1—N1	97.10 (11)
C11—C12—C15—C18B	−89.2 (7)	Ru2—Cl1—Ru1—Cl2	2.84 (4)
C13—C12—C15—C18B	88.0 (7)	Ru2—Cl2—Ru1—C2	176.39 (16)
C11—C12—C15—C16	4.7 (9)	Ru2—Cl2—Ru1—C1	89.65 (16)
C13—C12—C15—C16	−178.0 (8)	Ru2—Cl2—Ru1—N1	−88.25 (11)
C26—C21—C22—C23	−0.3 (7)	Ru2—Cl2—Ru1—Cl1	−2.96 (4)
Ru2—C21—C22—C23	171.7 (4)	C22—C21—Ru2—C20	87.5 (5)
C21—C22—C23—C24	1.9 (8)	C26—C21—Ru2—C20	−100.1 (4)
C21—C22—C23—C27	−177.8 (5)	C22—C21—Ru2—C19	−0.4 (5)
C22—C23—C24—C25	−2.1 (8)	C26—C21—Ru2—C19	171.9 (4)
C27—C23—C24—C25	177.7 (5)	C22—C21—Ru2—N2	−179.6 (5)
C23—C24—C25—C26	0.6 (8)	C26—C21—Ru2—N2	−7.2 (3)
C24—C25—C26—C21	1.1 (7)	C22—C21—Ru2—Cl2	−91.1 (4)
C24—C25—C26—C28	−178.7 (4)	C26—C21—Ru2—Cl2	81.2 (3)
C22—C21—C26—C25	−1.2 (7)	C22—C21—Ru2—Cl1	−128.5 (5)
Ru2—C21—C26—C25	−174.4 (4)	C26—C21—Ru2—Cl1	43.9 (8)
C22—C21—C26—C28	178.6 (4)	C32—N2—Ru2—C20	−84.1 (4)
Ru2—C21—C26—C28	5.4 (5)	C28—N2—Ru2—C20	99.9 (3)
C25—C26—C28—N2	−178.2 (4)	C32—N2—Ru2—C21	−175.3 (4)
C21—C26—C28—N2	2.0 (6)	C28—N2—Ru2—C21	8.7 (3)
C25—C26—C28—C29	3.2 (7)	C32—N2—Ru2—Cl2	97.8 (4)
C21—C26—C28—C29	−176.5 (4)	C28—N2—Ru2—Cl2	−78.1 (3)
N2—C28—C29—C30	1.5 (7)	C32—N2—Ru2—Cl1	15.7 (4)
C26—C28—C29—C30	179.9 (4)	C28—N2—Ru2—Cl1	−160.2 (3)
C28—C29—C30—C31	4.1 (7)	Ru1—Cl2—Ru2—C19	96.22 (15)
C28—C29—C30—C33	−174.3 (4)	Ru1—Cl2—Ru2—C21	−168.49 (13)
C29—C30—C31—C32	−5.3 (7)	Ru1—Cl2—Ru2—N2	−88.94 (10)

C33—C30—C31—C32	173.2 (5)	Ru1—Cl2—Ru2—Cl1	2.88 (4)
C30—C31—C32—N2	0.9 (8)	Ru1—Cl1—Ru2—C20	178.14 (17)
C29—C30—C33—C35	−122.3 (5)	Ru1—Cl1—Ru2—C19	−93.49 (16)
C31—C30—C33—C35	59.4 (6)	Ru1—Cl1—Ru2—C21	34.7 (6)
C29—C30—C33—C34	−1.6 (6)	Ru1—Cl1—Ru2—N2	84.68 (11)
C31—C30—C33—C34	−180.0 (4)	Ru1—Cl1—Ru2—Cl2	−2.92 (4)
C29—C30—C33—C36	118.7 (5)		

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

3. 2b

Crystal data

C40H36Cl2N2O4Ru2?	D_x = 1.365 Mg m^{-3}
M_r = 966.67	Melting point: ? K
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: ?	Cell parameters from 9172 reflections
a = 10.845 (1) Å	θ = 1.0–30.0°
b = 15.601 (1) Å	μ = 0.91 mm^{-1}
c = 27.808 (1) Å	T = 150.0 (1) K
V = 4704.9 (6) Å^3	Cell measurement pressure: ? kPa
Z = 4	Needle, colorless
F_{000} = 1944	0.40 × 0.10 × 0.10 mm

Data collection

KappaCCD diffractometer	40814 measured reflections
Radiation source: fine-focus sealed tube	13705 independent reflections
Monochromator: graphite	11962 reflections with $I > 2\sigma(I)$
Detector resolution: ? pixels mm^{-1}	R_{int} = 0.037
T = 150.0(1) K	θ_{max} = 30.0°
P = ? kPa	θ_{min} = 2.7°
phi and ω scans	h = −15→14

Absorption correction: multi-scan
?

T_{min} = 0.713, T_{max} = 0.915

k = −21→17

l = −38→38

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.034

$wR(F^2)$ = 0.093

S = 1.02

13705 reflections

455 parameters

? constraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.002

$\Delta\rho_{max}$ = 0.44 e Å^{-3}

$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Extinction correction: none

Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881

Flack parameter: −0.02 (2)

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

One highly disordered CH2Cl2 molecule was accounted for using the Platon SQUEEZE function.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.27323 (2)	1.024432 (14)	0.234902 (7)	0.02440 (5)
Ru2	0.09936 (2)	0.936973 (15)	0.130672 (8)	0.02801 (6)
Cl2	0.17994 (7)	0.88221 (4)	0.21066 (2)	0.02872 (14)
Cl1	0.18744 (7)	1.07401 (5)	0.15800 (2)	0.03358 (15)
O1	−0.1483 (2)	0.99042 (17)	0.17069 (9)	0.0477 (6)
O2	0.0003 (2)	0.77386 (16)	0.08983 (8)	0.0433 (6)
O3	0.5161 (2)	0.99773 (17)	0.18407 (8)	0.0413 (6)

O4	0.3692 (2)	0.96862 (19)	0.33088 (8)	0.0495 (6)
N1	0.2705 (2)	0.90979 (16)	0.09660 (7)	0.0282 (5)
N2	0.1048 (2)	1.06248 (15)	0.26755 (8)	0.0268 (4)
C1	0.0722 (3)	0.9942 (2)	0.06525 (11)	0.0373 (7)
C2	−0.0329 (4)	1.0370 (3)	0.04886 (13)	0.0491 (9)
H2	−0.1058	1.0356	0.0678	0.059*
C3	−0.0336 (4)	1.0814 (3)	0.00595 (14)	0.0570 (11)
H3	−0.1060	1.1102	−0.0044	0.068*
C4	0.0732 (5)	1.0836 (3)	−0.02213 (14)	0.0601 (12)
H4	0.0734	1.1146	−0.0516	0.072*
C5	0.1778 (4)	1.0415 (3)	−0.00752 (12)	0.0489 (9)
H5	0.2501	1.0429	−0.0268	0.059*
C6	0.1773 (3)	0.9963 (2)	0.03604 (10)	0.0368 (7)
C7	0.2849 (3)	0.9456 (2)	0.05246 (10)	0.0324 (6)
C8	0.3923 (3)	0.9323 (2)	0.02656 (10)	0.0387 (7)
H8	0.4028	0.9588	−0.0039	0.046*
C9	0.4842 (3)	0.8804 (2)	0.04499 (10)	0.0357 (7)
C10	0.4683 (3)	0.8435 (2)	0.09047 (10)	0.0288 (6)
C11	0.3614 (3)	0.85953 (19)	0.11429 (9)	0.0268 (6)
H11	0.3499	0.8341	0.1450	0.032*
C12	0.6044 (4)	0.8590 (3)	0.01890 (11)	0.0471 (9)
H12A	0.5852	0.8302	−0.0119	0.057*
H12B	0.6492	0.9127	0.0116	0.057*
C13	0.6845 (3)	0.8020 (3)	0.04866 (11)	0.0478 (9)
H13	0.7662	0.7881	0.0339	0.057*
C14	0.6138 (3)	0.7235 (2)	0.06930 (11)	0.0396 (7)
C15	0.5698 (3)	0.7889 (2)	0.10970 (10)	0.0342 (7)
H15	0.5578	0.7648	0.1427	0.041*
C16	0.6912 (3)	0.8380 (3)	0.10073 (11)	0.0416 (8)
H16A	0.7622	0.8169	0.1197	0.050*

H16B	0.6834	0.9011	0.1029	0.050*
C17	0.5173 (4)	0.6817 (3)	0.03830 (13)	0.0517 (10)
H17A	0.5573	0.6432	0.0152	0.078*
H17B	0.4711	0.7258	0.0209	0.078*
H17C	0.4607	0.6487	0.0586	0.078*
C18	0.7006 (4)	0.6557 (3)	0.09043 (14)	0.0544 (10)
H18A	0.6539	0.6174	0.1116	0.082*
H18B	0.7658	0.6841	0.1090	0.082*
H18C	0.7377	0.6224	0.0643	0.082*
C19	0.3120 (3)	1.14973 (19)	0.25080 (9)	0.0287 (6)
C20	0.4232 (3)	1.1938 (2)	0.24517 (10)	0.0354 (7)
H20	0.4944	1.1632	0.2351	0.043*
C21	0.4322 (3)	1.2816 (2)	0.25402 (11)	0.0377 (7)
H21	0.5086	1.3103	0.2498	0.045*
C22	0.3287 (3)	1.3267 (2)	0.26899 (11)	0.0367 (7)
H22	0.3341	1.3865	0.2750	0.044*
C23	0.2193 (3)	1.28502 (19)	0.27511 (10)	0.0334 (6)
H23	0.1487	1.3164	0.2851	0.040*
C24	0.2093 (3)	1.19622 (18)	0.26686 (10)	0.0291 (6)
C25	0.0958 (3)	1.14828 (18)	0.27579 (9)	0.0285 (6)
C26	−0.0139 (3)	1.1829 (2)	0.29340 (11)	0.0361 (7)
H26	−0.0209	1.2430	0.2982	0.043*
C27	−0.1130 (3)	1.1295 (2)	0.30402 (10)	0.0332 (6)
C28	−0.1001 (3)	1.04116 (18)	0.29788 (9)	0.0285 (6)
C29	0.0100 (3)	1.01079 (19)	0.27839 (9)	0.0276 (6)
H29	0.0182	0.9511	0.2725	0.033*
C30	−0.2339 (3)	1.1610 (2)	0.32411 (13)	0.0437 (8)
H30A	−0.2722	1.2014	0.3010	0.052*
H30B	−0.2187	1.1923	0.3545	0.052*
C31	−0.3221 (3)	1.0867 (2)	0.33358 (11)	0.0395 (7)

H31	−0.4054	1.1033	0.3459	0.047*
C32	−0.2580 (3)	1.0127 (2)	0.36114 (10)	0.0379 (7)
C33	−0.2058 (3)	0.9856 (2)	0.31082 (10)	0.0311 (6)
H33	−0.1952	0.9227	0.3051	0.037*
C34	−0.3226 (3)	1.0276 (2)	0.28915 (10)	0.0350 (6)
H34A	−0.3083	1.0577	0.2583	0.042*
H34B	−0.3948	0.9889	0.2872	0.042*
C35	−0.3495 (4)	0.9485 (3)	0.38074 (12)	0.0496 (9)
H35A	−0.3050	0.9012	0.3962	0.074*
H35B	−0.3998	0.9259	0.3543	0.074*
H35C	−0.4029	0.9766	0.4044	0.074*
C36	−0.1695 (4)	1.0349 (3)	0.40155 (12)	0.0568 (11)
H36A	−0.2161	1.0573	0.4290	0.085*
H36B	−0.1109	1.0783	0.3904	0.085*
H36C	−0.1245	0.9833	0.4113	0.085*
C37	0.0355 (3)	0.8359 (2)	0.10625 (11)	0.0328 (6)
C38	−0.0552 (3)	0.9693 (2)	0.15618 (11)	0.0359 (7)
C39	0.4252 (3)	1.00509 (19)	0.20386 (10)	0.0290 (6)
C40	0.3345 (3)	0.9890 (2)	0.29425 (11)	0.0324 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.02102 (9)	0.02548 (10)	0.02671 (10)	0.00067 (9)	−0.00038 (8)	−0.00106 (8)
Ru2	0.02474 (10)	0.02848 (11)	0.03080 (11)	−0.00145 (9)	−0.00249 (9)	−0.00398 (9)
Cl2	0.0291 (3)	0.0261 (3)	0.0310 (3)	−0.0002 (3)	0.0039 (3)	−0.0020 (3)
Cl1	0.0381 (4)	0.0301 (4)	0.0325 (3)	−0.0018 (3)	−0.0059 (3)	−0.0006 (3)
O1	0.0299 (12)	0.0525 (16)	0.0609 (14)	0.0054 (11)	0.0039 (11)	−0.0117 (12)
O2	0.0395 (13)	0.0406 (14)	0.0497 (13)	−0.0051	0.0020 (11)	−0.0114

				(11)		(11)
O3	0.0263 (11)	0.0551 (15)	0.0426 (12)	0.0016 (10)	0.0023 (9)	−0.0054 (10)
O4	0.0432 (14)	0.0694 (17)	0.0359 (11)	0.0082 (13)	−0.0053 (10)	0.0114 (11)
N1	0.0289 (11)	0.0316 (12)	0.0241 (10)	−0.0016 (11)	−0.0007 (9)	−0.0018 (9)
N2	0.0247 (10)	0.0269 (11)	0.0287 (10)	0.0008 (10)	−0.0005 (9)	−0.0022 (10)
C1	0.0428 (18)	0.0350 (17)	0.0340 (14)	−0.0012 (14)	−0.0131 (13)	−0.0041 (12)
C2	0.0421 (19)	0.058 (2)	0.0469 (19)	0.0028 (18)	−0.0184 (15)	−0.0004 (17)
C3	0.060 (3)	0.058 (3)	0.054 (2)	0.010 (2)	−0.0267 (19)	0.0013 (18)
C4	0.077 (3)	0.060 (3)	0.0437 (19)	−0.003 (2)	−0.026 (2)	0.0127 (18)
C5	0.056 (2)	0.055 (2)	0.0356 (16)	−0.0081 (18)	−0.0087 (15)	0.0036 (14)
C6	0.0438 (17)	0.0350 (17)	0.0315 (14)	−0.0064 (14)	−0.0104 (13)	−0.0005 (12)
C7	0.0341 (15)	0.0357 (16)	0.0273 (12)	−0.0084 (13)	−0.0034 (11)	−0.0024 (11)
C8	0.0425 (17)	0.0468 (19)	0.0269 (13)	−0.0096 (17)	0.0024 (12)	0.0038 (13)
C9	0.0325 (16)	0.0447 (18)	0.0298 (14)	−0.0090 (14)	0.0008 (12)	−0.0039 (13)
C10	0.0285 (14)	0.0320 (15)	0.0258 (13)	−0.0072 (12)	0.0024 (10)	−0.0063 (11)
C11	0.0283 (13)	0.0296 (14)	0.0226 (12)	−0.0036 (11)	−0.0012 (10)	−0.0019 (10)
C12	0.046 (2)	0.064 (2)	0.0319 (15)	−0.0060 (19)	0.0152 (15)	0.0004 (15)
C13	0.0285 (15)	0.080 (3)	0.0348 (16)	−0.0049 (18)	0.0073 (13)	−0.0021 (17)
C14	0.0332 (16)	0.051 (2)	0.0344 (15)	0.0061 (15)	0.0023 (13)	−0.0040 (14)
C15	0.0279 (14)	0.0482 (19)	0.0266 (13)	−0.0042	0.0040 (11)	0.0001 (12)

				(13)		
C16	0.0263 (15)	0.059 (2)	0.0393 (16)	−0.0031 (15)	0.0036 (12)	−0.0052 (15)
C17	0.066 (3)	0.047 (2)	0.0414 (18)	0.005 (2)	−0.0011 (17)	−0.0136 (16)
C18	0.047 (2)	0.066 (3)	0.0502 (19)	0.020 (2)	0.0057 (16)	−0.0110 (18)
C19	0.0303 (14)	0.0291 (14)	0.0267 (12)	−0.0018 (12)	−0.0025 (10)	−0.0019 (11)
C20	0.0309 (16)	0.0375 (16)	0.0379 (15)	−0.0041 (13)	0.0007 (12)	−0.0034 (13)
C21	0.0369 (17)	0.0376 (17)	0.0387 (16)	−0.0111 (14)	−0.0042 (12)	0.0024 (13)
C22	0.0465 (18)	0.0266 (15)	0.0370 (15)	−0.0101 (13)	−0.0085 (14)	0.0039 (12)
C23	0.0365 (15)	0.0272 (14)	0.0366 (15)	0.0032 (13)	−0.0063 (13)	0.0014 (11)
C24	0.0326 (15)	0.0269 (13)	0.0279 (12)	0.0007 (11)	−0.0011 (12)	0.0042 (11)
C25	0.0287 (13)	0.0248 (13)	0.0321 (13)	0.0033 (12)	0.0007 (11)	−0.0023 (10)
C26	0.0345 (16)	0.0256 (15)	0.0481 (17)	0.0052 (13)	0.0006 (13)	−0.0049 (13)
C27	0.0245 (14)	0.0367 (16)	0.0383 (15)	0.0031 (12)	0.0005 (12)	−0.0074 (12)
C28	0.0241 (12)	0.0335 (16)	0.0278 (12)	0.0029 (12)	−0.0014 (11)	−0.0057 (10)
C29	0.0256 (13)	0.0253 (14)	0.0317 (13)	0.0039 (11)	−0.0007 (10)	−0.0058 (11)
C30	0.0327 (16)	0.0417 (19)	0.0567 (19)	0.0046 (15)	0.0059 (15)	−0.0109 (15)
C31	0.0299 (15)	0.0465 (19)	0.0421 (17)	0.0051 (14)	0.0116 (13)	−0.0072 (14)
C32	0.0316 (15)	0.0509 (19)	0.0312 (14)	−0.0005 (14)	0.0027 (11)	−0.0023 (13)
C33	0.0288 (15)	0.0327 (15)	0.0316 (13)	0.0016 (13)	0.0013 (11)	−0.0064 (12)

C34	0.0282 (14)	0.0440 (17)	0.0328 (14)	0.0002 (14)	−0.0013 (11)	−0.0047 (14)
C35	0.0422 (19)	0.063 (3)	0.0440 (17)	−0.0023 (18)	0.0104 (15)	0.0074 (16)
C36	0.060 (2)	0.078 (3)	0.0331 (16)	−0.009 (2)	−0.0032 (15)	−0.0077 (17)
C37	0.0250 (14)	0.0379 (17)	0.0354 (15)	−0.0029 (13)	0.0017 (12)	−0.0038 (13)
C38	0.0313 (15)	0.0353 (16)	0.0412 (15)	−0.0038 (14)	−0.0048 (12)	−0.0057 (14)
C39	0.0247 (14)	0.0330 (15)	0.0294 (13)	0.0003 (11)	−0.0021 (10)	−0.0021 (11)
C40	0.0243 (13)	0.0351 (16)	0.0377 (15)	0.0024 (12)	0.0022 (11)	0.0009 (13)

Table 3
Geometric parameters (Å, °)

Ru1—C40	1.863 (3)	C15—C16	1.543 (4)
Ru1—C39	1.885 (3)	C15—H15	1.0000
Ru1—C19	2.048 (3)	C16—H16A	0.9900
Ru1—N2	2.124 (2)	C16—H16B	0.9900
Ru1—Cl1	2.4570 (7)	C17—H17A	0.9800
Ru1—Cl2	2.5301 (7)	C17—H17B	0.9800
Ru2—C37	1.851 (3)	C17—H17C	0.9800
Ru2—C38	1.889 (3)	C18—H18A	0.9800
Ru2—C1	2.048 (3)	C18—H18B	0.9800
Ru2—N1	2.126 (3)	C18—H18C	0.9800
Ru2—Cl1	2.4618 (8)	C19—C20	1.397 (4)
Ru2—Cl2	2.5380 (7)	C19—C24	1.402 (4)
O1—C38	1.136 (4)	C20—C21	1.395 (5)
O2—C37	1.137 (4)	C20—H20	0.9500
O3—C39	1.135 (3)	C21—C22	1.388 (5)
O4—C40	1.132 (3)	C21—H21	0.9500

N1—C11	1.352 (4)	C22—C23	1.363 (5)
N1—C7	1.358 (4)	C22—H22	0.9500
N2—C29	1.341 (4)	C23—C24	1.408 (4)
N2—C25	1.362 (4)	C23—H23	0.9500
C1—C2	1.397 (5)	C24—C25	1.461 (4)
C1—C6	1.400 (5)	C25—C26	1.395 (4)
C2—C3	1.379 (5)	C26—C27	1.392 (4)
C2—H2	0.9500	C26—H26	0.9500
C3—C4	1.397 (7)	C27—C28	1.395 (4)
C3—H3	0.9500	C27—C30	1.508 (4)
C4—C5	1.373 (6)	C28—C29	1.395 (4)
C4—H4	0.9500	C28—C33	1.481 (4)
C5—C6	1.401 (5)	C29—H29	0.9500
C5—H5	0.9500	C30—C31	1.527 (5)
C6—C7	1.482 (5)	C30—H30A	0.9900
C7—C8	1.385 (4)	C30—H30B	0.9900
C8—C9	1.382 (5)	C31—C34	1.541 (4)
C8—H8	0.9500	C31—C32	1.550 (5)
C9—C10	1.400 (4)	C31—H31	1.0000
C9—C12	1.529 (5)	C32—C35	1.513 (5)
C10—C11	1.358 (4)	C32—C36	1.517 (5)
C10—C15	1.491 (4)	C32—C33	1.568 (4)
C11—H11	0.9500	C33—C34	1.548 (4)
C12—C13	1.493 (6)	C33—H33	1.0000
C12—H12A	0.9900	C34—H34A	0.9900
C12—H12B	0.9900	C34—H34B	0.9900
C13—C14	1.555 (5)	C35—H35A	0.9800
C13—C16	1.555 (5)	C35—H35B	0.9800
C13—H13	1.0000	C35—H35C	0.9800
C14—C17	1.505 (5)	C36—H36A	0.9800

C14—C18	1.533 (5)	C36—H36B	0.9800
C14—C15	1.591 (4)	C36—H36C	0.9800

C40—Ru1—C39	92.67 (12)	C15—C16—H16A	114.3
C40—Ru1—C19	91.08 (12)	C13—C16—H16A	114.3
C39—Ru1—C19	94.14 (12)	C15—C16—H16B	114.3
C40—Ru1—N2	90.62 (11)	C13—C16—H16B	114.3
C39—Ru1—N2	172.89 (11)	H16A—C16—H16B	111.4
C19—Ru1—N2	79.49 (11)	C14—C17—H17A	109.5
C40—Ru1—Cl1	178.13 (9)	C14—C17—H17B	109.5
C39—Ru1—Cl1	89.02 (8)	H17A—C17—H17B	109.5
C19—Ru1—Cl1	88.01 (8)	C14—C17—H17C	109.5
N2—Ru1—Cl1	87.61 (6)	H17A—C17—H17C	109.5
C40—Ru1—Cl2	96.80 (10)	H17B—C17—H17C	109.5
C39—Ru1—Cl2	95.01 (9)	C14—C18—H18A	109.5
C19—Ru1—Cl2	167.63 (9)	C14—C18—H18B	109.5
N2—Ru1—Cl2	90.86 (6)	H18A—C18—H18B	109.5
Cl1—Ru1—Cl2	83.84 (2)	C14—C18—H18C	109.5
C37—Ru2—C38	91.92 (13)	H18A—C18—H18C	109.5
C37—Ru2—C1	89.51 (13)	H18B—C18—H18C	109.5
C38—Ru2—C1	95.13 (14)	C20—C19—C24	117.9 (3)
C37—Ru2—N1	89.60 (11)	C20—C19—Ru1	128.5 (2)
C38—Ru2—N1	174.35 (12)	C24—C19—Ru1	113.5 (2)
C1—Ru2—N1	79.44 (11)	C21—C20—C19	121.6 (3)
C37—Ru2—Cl1	176.43 (10)	C21—C20—H20	119.2
C38—Ru2—Cl1	89.80 (10)	C19—C20—H20	119.2
C1—Ru2—Cl1	87.22 (9)	C22—C21—C20	119.6 (3)
N1—Ru2—Cl1	88.40 (7)	C22—C21—H21	120.2
C37—Ru2—Cl2	99.42 (10)	C20—C21—H21	120.2
C38—Ru2—Cl2	93.81 (10)	C23—C22—C21	120.0 (3)
C1—Ru2—Cl2	167.14 (10)	C23—C22—H22	120.0

N1—Ru2—Cl2	91.31 (6)	C21—C22—H22	120.0
Cl1—Ru2—Cl2	83.58 (2)	C22—C23—C24	121.0 (3)
Ru1—Cl2—Ru2	94.36 (2)	C22—C23—H23	119.5
Ru1—Cl1—Ru2	98.18 (3)	C24—C23—H23	119.5
C11—N1—C7	118.9 (3)	C19—C24—C23	119.9 (3)
C11—N1—Ru2	126.15 (18)	C19—C24—C25	117.3 (3)
C7—N1—Ru2	114.9 (2)	C23—C24—C25	122.7 (3)
C29—N2—C25	119.9 (2)	N2—C25—C26	120.1 (3)
C29—N2—Ru1	125.96 (18)	N2—C25—C24	114.5 (3)
C25—N2—Ru1	114.11 (19)	C26—C25—C24	125.4 (3)
C2—C1—C6	117.6 (3)	C27—C26—C25	120.1 (3)
C2—C1—Ru2	128.0 (3)	C27—C26—H26	120.0
C6—C1—Ru2	114.1 (2)	C25—C26—H26	120.0
C3—C2—C1	121.8 (4)	C26—C27—C28	119.2 (3)
C3—C2—H2	119.1	C26—C27—C30	123.7 (3)
C1—C2—H2	119.1	C28—C27—C30	117.1 (3)
C2—C3—C4	119.5 (4)	C29—C28—C27	117.9 (3)
C2—C3—H3	120.3	C29—C28—C33	123.9 (3)
C4—C3—H3	120.3	C27—C28—C33	118.1 (3)
C5—C4—C3	120.5 (3)	N2—C29—C28	122.7 (3)
C5—C4—H4	119.8	N2—C29—H29	118.7
C3—C4—H4	119.8	C28—C29—H29	118.7
C4—C5—C6	119.6 (4)	C27—C30—C31	111.1 (3)
C4—C5—H5	120.2	C27—C30—H30A	109.4
C6—C5—H5	120.2	C31—C30—H30A	109.4
C1—C6—C5	121.1 (3)	C27—C30—H30B	109.4
C1—C6—C7	116.7 (3)	C31—C30—H30B	109.4
C5—C6—C7	122.1 (3)	H30A—C30—H30B	108.0
N1—C7—C8	120.3 (3)	C30—C31—C34	108.5 (3)
N1—C7—C6	114.0 (3)	C30—C31—C32	111.7 (3)

C8—C7—C6	125.6 (3)	C34—C31—C32	87.3 (2)
C9—C8—C7	120.1 (3)	C30—C31—H31	115.3
C9—C8—H8	119.9	C34—C31—H31	115.3
C7—C8—H8	119.9	C32—C31—H31	115.3
C8—C9—C10	119.1 (3)	C35—C32—C36	107.4 (3)
C8—C9—C12	124.5 (3)	C35—C32—C31	112.1 (3)
C10—C9—C12	116.3 (3)	C36—C32—C31	118.7 (3)
C11—C10—C9	118.0 (3)	C35—C32—C33	112.3 (3)
C11—C10—C15	124.1 (3)	C36—C32—C33	119.6 (3)
C9—C10—C15	117.9 (3)	C31—C32—C33	85.5 (2)
N1—C11—C10	123.5 (3)	C28—C33—C34	106.9 (2)
N1—C11—H11	118.3	C28—C33—C32	109.8 (2)
C10—C11—H11	118.3	C34—C33—C32	86.4 (2)
C13—C12—C9	111.3 (3)	C28—C33—H33	116.6
C13—C12—H12A	109.4	C34—C33—H33	116.6
C9—C12—H12A	109.4	C32—C33—H33	116.6
C13—C12—H12B	109.4	C31—C34—C33	86.5 (2)
C9—C12—H12B	109.4	C31—C34—H34A	114.2
H12A—C12—H12B	108.0	C33—C34—H34A	114.2
C12—C13—C14	112.7 (3)	C31—C34—H34B	114.2
C12—C13—C16	109.2 (3)	C33—C34—H34B	114.2
C14—C13—C16	87.9 (2)	H34A—C34—H34B	111.4
C12—C13—H13	114.7	C32—C35—H35A	109.5
C14—C13—H13	114.7	C32—C35—H35B	109.5
C16—C13—H13	114.7	H35A—C35—H35B	109.5
C17—C14—C18	110.3 (3)	C32—C35—H35C	109.5
C17—C14—C13	118.2 (3)	H35A—C35—H35C	109.5
C18—C14—C13	112.4 (3)	H35B—C35—H35C	109.5
C17—C14—C15	118.3 (3)	C32—C36—H36A	109.5
C18—C14—C15	110.9 (3)	C32—C36—H36B	109.5

C13—C14—C15	84.5 (3)	H36A—C36—H36B	109.5
C10—C15—C16	106.8 (3)	C32—C36—H36C	109.5
C10—C15—C14	109.5 (2)	H36A—C36—H36C	109.5
C16—C15—C14	87.1 (2)	H36B—C36—H36C	109.5
C10—C15—H15	116.5	O2—C37—Ru2	177.1 (3)
C16—C15—H15	116.5	O1—C38—Ru2	178.3 (3)
C14—C15—H15	116.5	O3—C39—Ru1	176.3 (3)
C15—C16—C13	86.1 (2)	O4—C40—Ru1	178.2 (3)

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

4. 3b

Crystal data

$C_{40}H_{37}ClN_2O_5Ru_2$·	D_x = 1.368 Mg m^{-3}
M_r = 963.50	Melting point: ? K
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: ?	Cell parameters from 7309 reflections
a = 10.8220 (10) Å	θ = 1.0–30.0°
b = 15.8210 (10) Å	μ = 0.75 mm^{-1}
c = 27.3240 (10) Å	T = 150.0 (1) K
V = 4678.3 (6) Å^3	Cell measurement pressure: ? kPa
Z = 4	Block, colorless
F_{000} = 1976	0.20 × 0.20 × 0.20 mm

Data collection

KappaCCD diffractometer	39432 measured reflections
Radiation source: fine-focus sealed tube	13604 independent reflections

Monochromator: graphite	12769 reflections with $I > 2\sigma(I)$
Detector resolution: ? pixels mm^{-1}	R_{int} = 0.032
T = 150.0(1) K	θ_{max} = 30.1°
P = ? kPa	θ_{min} = 2.9°
phi and ω scans	h = −15→14
Absorption correction: multi-scan ?	k = −22→19
T_{min} = 0.865, T_{max} = 0.865	l = −38→35

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2 + 0.3756P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.098	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.79 e $Å^{-3}$
13604 reflections	$\Delta\rho_{min}$ = −1.65 e $Å^{-3}$
459 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
? constraints	Extinction coefficient: 0.0038 (4)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881
Secondary atom site location: difference Fourier map	Flack parameter: 0.03 (2)

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

A large cavity near -0.2 0.25 0.00 contains ill defined solvent that was interpreted as an heptane molecule and accounted for using the Platon SQUEEZE function.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}
Ru1	0.777573 (17)	−0.020897 (12)	0.244578 (7)	0.02623 (6)
Ru2	0.605947 (18)	−0.099907 (13)	0.146024 (8)	0.02918 (6)
Cl1	0.68716 (6)	−0.16531 (4)	0.22506 (2)	0.03057 (12)

O1	0.69235 (18)	0.00454 (12)	0.17772 (7)	0.0320 (4)
H1	0.642 (3)	0.037 (2)	0.1741 (14)	0.038*
O2	0.8801 (2)	−0.06163 (19)	0.34312 (8)	0.0532 (6)
O3	1.02243 (19)	−0.04608 (15)	0.19457 (9)	0.0414 (5)
O4	0.3574 (2)	−0.05187 (16)	0.18765 (10)	0.0473 (5)
O5	0.5038 (2)	−0.25127 (15)	0.09350 (9)	0.0439 (5)
N1	0.6097 (2)	0.01982 (14)	0.27683 (8)	0.0282 (4)
N2	0.7776 (2)	−0.11995 (13)	0.10998 (8)	0.0296 (4)
C1	0.8131 (2)	0.10489 (15)	0.25370 (10)	0.0290 (4)
C2	0.9229 (2)	0.14889 (18)	0.24456 (11)	0.0359 (5)
H2	0.9953	0.1183	0.2360	0.043*
C3	0.9278 (3)	0.23649 (18)	0.24778 (11)	0.0398 (6)
H3	1.0036	0.2652	0.2421	0.048*
C4	0.8215 (3)	0.28230 (18)	0.25934 (11)	0.0399 (6)
H4	0.8241	0.3423	0.2605	0.048*
C5	0.7135 (3)	0.24057 (17)	0.26903 (10)	0.0344 (5)
H5	0.6417	0.2719	0.2774	0.041*
C6	0.7076 (2)	0.15197 (16)	0.26673 (9)	0.0306 (5)
C7	0.5966 (2)	0.10419 (16)	0.27976 (10)	0.0306 (5)
C8	0.4846 (3)	0.13961 (18)	0.29584 (11)	0.0370 (6)
H8	0.4748	0.1993	0.2963	0.044*
C9	0.3897 (2)	0.08879 (17)	0.31081 (11)	0.0337 (5)
C10	0.4060 (2)	0.00112 (16)	0.30942 (10)	0.0300 (5)
C11	0.5166 (2)	−0.03098 (16)	0.29237 (9)	0.0281 (5)
H11	0.5278	−0.0905	0.2915	0.034*
C12	0.2676 (3)	0.1228 (2)	0.32877 (14)	0.0479 (8)
H12A	0.2288	0.1573	0.3027	0.057*
H12B	0.2815	0.1597	0.3575	0.057*
C13	0.1806 (3)	0.0501 (2)	0.34295 (12)	0.0415 (7)
H13	0.0968	0.0677	0.3545	0.050*

C14	0.1817 (2)	−0.0164 (2)	0.30186 (10)	0.0348 (5)
H14A	0.1948	0.0072	0.2687	0.042*
H14B	0.1104	−0.0557	0.3025	0.042*
C15	0.3015 (2)	−0.05231 (17)	0.32645 (10)	0.0317 (5)
H15	0.3136	−0.1149	0.3249	0.038*
C16	0.2485 (3)	−0.0153 (2)	0.37640 (10)	0.0414 (6)
C17	0.3353 (4)	0.0183 (4)	0.41527 (14)	0.0686 (12)
H17A	0.2871	0.0441	0.4417	0.103*
H17B	0.3901	0.0608	0.4008	0.103*
H17C	0.3848	−0.0283	0.4285	0.103*
C18	0.1587 (4)	−0.0780 (3)	0.40017 (14)	0.0561 (9)
H18A	0.2056	−0.1212	0.4179	0.084*
H18B	0.1086	−0.1051	0.3747	0.084*
H18C	0.1046	−0.0479	0.4230	0.084*
C19	0.5783 (3)	−0.03114 (17)	0.08419 (10)	0.0343 (5)
C20	0.4710 (3)	0.0118 (2)	0.06983 (13)	0.0484 (8)
H20	0.3977	0.0059	0.0886	0.058*
C21	0.4703 (4)	0.0631 (3)	0.02827 (14)	0.0576 (10)
H21	0.3965	0.0911	0.0187	0.069*
C22	0.5795 (4)	0.0735 (2)	0.00031 (14)	0.0553 (9)
H22	0.5801	0.1096	−0.0275	0.066*
C23	0.6836 (3)	0.0311 (2)	0.01370 (13)	0.0457 (7)
H23	0.7566	0.0379	−0.0052	0.055*
C24	0.6861 (3)	−0.02254 (18)	0.05480 (10)	0.0359 (5)
C25	0.7925 (3)	−0.07384 (16)	0.06855 (10)	0.0321 (5)
C26	0.9019 (3)	−0.08158 (19)	0.04152 (11)	0.0387 (6)
H26	0.9124	−0.0492	0.0125	0.046*
C27	0.9938 (3)	−0.13524 (19)	0.05635 (10)	0.0362 (6)
C28	0.9761 (2)	−0.18377 (17)	0.09938 (9)	0.0297 (5)
C29	0.8665 (2)	−0.17290 (17)	0.12447 (9)	0.0294 (5)

H29	0.8536	−0.2047	0.1535	0.035*
C30	1.1133 (3)	−0.1489 (2)	0.02807 (11)	0.0458 (7)
H30A	1.1583	−0.0947	0.0251	0.055*
H30B	1.0941	−0.1694	−0.0053	0.055*
C31	1.1946 (3)	−0.2135 (2)	0.05427 (11)	0.0456 (7)
H31	1.2767	−0.2239	0.0386	0.055*
C32	1.1999 (3)	−0.1907 (2)	0.10960 (11)	0.0429 (7)
H32A	1.2710	−0.2156	0.1273	0.051*
H32B	1.1915	−0.1296	0.1166	0.051*
C33	1.0780 (2)	−0.24159 (19)	0.11467 (10)	0.0335 (5)
H33	1.0658	−0.2728	0.1461	0.040*
C34	1.1216 (3)	−0.2956 (2)	0.06940 (11)	0.0408 (6)
C35	1.2080 (4)	−0.3654 (2)	0.08464 (13)	0.0537 (8)
H35A	1.1600	−0.4155	0.0937	0.081*
H35B	1.2572	−0.3468	0.1127	0.081*
H35C	1.2632	−0.3794	0.0574	0.081*
C36	1.0252 (3)	−0.3293 (2)	0.03455 (13)	0.0500 (8)
H36A	1.0661	−0.3562	0.0066	0.075*
H36B	0.9735	−0.2825	0.0229	0.075*
H36C	0.9735	−0.3708	0.0515	0.075*
C37	0.8430 (2)	−0.0465 (2)	0.30569 (11)	0.0368 (6)
C38	0.9306 (2)	−0.03991 (16)	0.21357 (10)	0.0304 (5)
C39	0.4516 (3)	−0.07123 (18)	0.17264 (11)	0.0352 (6)
C40	0.5405 (3)	−0.19406 (18)	0.11502 (11)	0.0349 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.02450 (9)	0.02500 (9)	0.02918 (10)	0.00062 (6)	0.00012 (7)	−0.00133 (7)
Ru2	0.02816 (9)	0.02711 (10)	0.03227 (10)	0.00002 (7)	−0.00206 (7)	−0.00519 (7)

Cl1	0.0326 (3)	0.0249 (3)	0.0342 (3)	0.0003 (2)	0.0045 (2)	−0.0011 (2)
O1	0.0373 (9)	0.0276 (9)	0.0312 (9)	0.0000 (7)	−0.0067 (7)	−0.0044 (7)
O2	0.0413 (12)	0.0825 (18)	0.0360 (12)	0.0070 (12)	−0.0055 (9)	0.0124 (11)
O3	0.0325 (10)	0.0446 (11)	0.0470 (12)	0.0021 (9)	0.0051 (9)	−0.0062 (9)
O4	0.0325 (10)	0.0537 (14)	0.0557 (14)	0.0036 (10)	0.0011 (10)	−0.0126 (11)
O5	0.0420 (11)	0.0384 (10)	0.0514 (13)	−0.0065 (9)	0.0004 (10)	−0.0142 (9)
N1	0.0259 (9)	0.0268 (9)	0.0320 (10)	0.0036 (9)	0.0004 (8)	−0.0042 (8)
N2	0.0337 (10)	0.0252 (9)	0.0300 (10)	−0.0044 (8)	−0.0010 (9)	−0.0037 (7)
C1	0.0317 (10)	0.0245 (10)	0.0309 (11)	−0.0055 (9)	−0.0042 (9)	0.0003 (9)
C2	0.0338 (12)	0.0364 (13)	0.0376 (14)	−0.0039 (10)	0.0004 (11)	−0.0016 (11)
C3	0.0412 (13)	0.0366 (13)	0.0417 (15)	−0.0114 (11)	−0.0014 (12)	−0.0024 (12)
C4	0.0523 (16)	0.0291 (12)	0.0382 (14)	−0.0069 (12)	−0.0037 (13)	0.0000 (11)
C5	0.0405 (13)	0.0272 (12)	0.0357 (13)	−0.0012 (10)	−0.0019 (11)	−0.0028 (9)
C6	0.0335 (12)	0.0282 (11)	0.0301 (12)	−0.0018 (9)	−0.0024 (9)	−0.0032 (9)
C7	0.0312 (11)	0.0265 (11)	0.0340 (12)	0.0008 (10)	−0.0028 (10)	0.0001 (9)
C8	0.0372 (13)	0.0269 (12)	0.0470 (16)	0.0046 (10)	0.0015 (12)	−0.0054 (11)
C9	0.0297 (11)	0.0316 (12)	0.0397 (14)	0.0034 (10)	0.0019 (10)	−0.0084 (10)
C10	0.0257 (11)	0.0336 (12)	0.0306 (12)	−0.0001 (9)	−0.0005 (9)	−0.0065 (9)
C11	0.0306 (11)	0.0243 (11)	0.0295 (11)	−0.0005 (9)	0.0014 (9)	−0.0009 (9)
C12	0.0412 (15)	0.0378 (15)	0.065 (2)	0.0054 (12)	0.0101 (15)	−0.0154 (14)

C13	0.0351 (13)	0.0438 (15)	0.0456 (17)	0.0048 (12)	0.0116 (12)	−0.0109 (12)
C14	0.0287 (11)	0.0427 (14)	0.0330 (13)	0.0007 (11)	0.0022 (9)	−0.0051 (11)
C15	0.0289 (12)	0.0331 (12)	0.0330 (13)	−0.0001 (10)	0.0005 (9)	−0.0031 (10)
C16	0.0392 (14)	0.0555 (17)	0.0296 (13)	−0.0022 (13)	0.0065 (10)	−0.0072 (12)
C17	0.061 (2)	0.106 (3)	0.0382 (18)	−0.016 (2)	−0.0051 (16)	−0.013 (2)
C18	0.0509 (19)	0.070 (2)	0.0478 (19)	−0.0048 (17)	0.0178 (16)	0.0041 (16)
C19	0.0404 (14)	0.0316 (12)	0.0309 (12)	0.0029 (11)	−0.0080 (10)	−0.0052 (10)
C20	0.0494 (17)	0.0510 (18)	0.0447 (16)	0.0126 (15)	−0.0152 (14)	−0.0103 (14)
C21	0.063 (2)	0.062 (2)	0.0478 (19)	0.0172 (19)	−0.0225 (17)	0.0000 (16)
C22	0.069 (2)	0.0509 (19)	0.0465 (19)	0.0049 (17)	−0.0223 (17)	0.0044 (14)
C23	0.0537 (17)	0.0400 (16)	0.0434 (16)	−0.0046 (14)	−0.0106 (14)	0.0067 (13)
C24	0.0423 (14)	0.0310 (12)	0.0345 (13)	−0.0024 (11)	−0.0110 (10)	−0.0026 (10)
C25	0.0365 (13)	0.0282 (11)	0.0317 (12)	−0.0060 (10)	−0.0040 (10)	−0.0012 (9)
C26	0.0434 (14)	0.0417 (14)	0.0310 (13)	−0.0101 (12)	0.0002 (11)	0.0065 (11)
C27	0.0366 (13)	0.0447 (15)	0.0272 (12)	−0.0064 (12)	0.0012 (10)	0.0013 (11)
C28	0.0296 (11)	0.0326 (12)	0.0269 (11)	−0.0049 (10)	−0.0002 (9)	−0.0009 (9)
C29	0.0303 (11)	0.0304 (12)	0.0276 (12)	−0.0043 (9)	0.0009 (9)	−0.0014 (9)
C30	0.0376 (14)	0.068 (2)	0.0320 (14)	−0.0056 (15)	0.0102 (12)	0.0084 (13)
C31	0.0366 (14)	0.068 (2)	0.0324 (14)	−0.0011 (14)	0.0085 (11)	−0.0001 (13)

C32	0.0335 (14)	0.0593 (19)	0.0358 (15)	−0.0054 (13)	0.0016 (11)	−0.0012 (13)
C33	0.0303 (12)	0.0433 (14)	0.0269 (12)	0.0007 (10)	0.0015 (9)	−0.0003 (10)
C34	0.0363 (14)	0.0524 (17)	0.0338 (14)	0.0075 (13)	0.0029 (11)	−0.0032 (12)
C35	0.058 (2)	0.061 (2)	0.0414 (17)	0.0165 (17)	0.0079 (15)	−0.0055 (15)
C36	0.0567 (19)	0.0538 (19)	0.0394 (16)	0.0042 (16)	−0.0052 (14)	−0.0142 (14)
C37	0.0286 (12)	0.0452 (15)	0.0367 (14)	0.0023 (11)	0.0015 (11)	0.0016 (11)
C38	0.0280 (11)	0.0292 (12)	0.0340 (13)	0.0024 (9)	−0.0025 (9)	−0.0030 (9)
C39	0.0338 (13)	0.0341 (13)	0.0376 (14)	−0.0021 (10)	−0.0043 (11)	−0.0073 (10)
C40	0.0319 (12)	0.0355 (13)	0.0375 (14)	0.0000 (11)	0.0021 (10)	−0.0033 (11)

Table 4
Geometric parameters (Å, °)

Ru1—C37	1.859 (3)	C15—C16	1.592 (4)
Ru1—C38	1.884 (3)	C15—H15	1.0000
Ru1—C1	2.042 (2)	C16—C17	1.514 (5)
Ru1—O1	2.0856 (19)	C16—C18	1.533 (5)
Ru1—N1	2.119 (2)	C17—H17A	0.9800
Ru1—Cl1	2.5420 (6)	C17—H17B	0.9800
Ru2—C40	1.854 (3)	C17—H17C	0.9800
Ru2—C39	1.878 (3)	C18—H18A	0.9800
Ru2—C19	2.032 (3)	C18—H18B	0.9800
Ru2—O1	2.0869 (18)	C18—H18C	0.9800
Ru2—N2	2.126 (2)	C19—C20	1.401 (4)
Ru2—Cl1	2.5508 (7)	C19—C24	1.423 (4)
O1—H1	0.76 (4)	C20—C21	1.396 (5)

O2—C37	1.124 (4)	C20—H20	0.9500
O3—C38	1.126 (3)	C21—C22	1.417 (6)
O4—C39	1.140 (4)	C21—H21	0.9500
O5—C40	1.150 (4)	C22—C23	1.361 (5)
N1—C7	1.345 (3)	C22—H22	0.9500
N1—C11	1.358 (3)	C23—C24	1.408 (4)
N2—C29	1.336 (3)	C23—H23	0.9500
N2—C25	1.356 (3)	C24—C25	1.458 (4)
C1—C2	1.399 (3)	C25—C26	1.400 (4)
C1—C6	1.409 (4)	C26—C27	1.369 (4)
C2—C3	1.390 (4)	C26—H26	0.9500
C2—H2	0.9500	C27—C28	1.417 (4)
C3—C4	1.396 (4)	C27—C30	1.522 (4)
C3—H3	0.9500	C28—C29	1.381 (4)
C4—C5	1.368 (4)	C28—C33	1.492 (4)
C4—H4	0.9500	C29—H29	0.9500
C5—C6	1.405 (4)	C30—C31	1.526 (5)
C5—H5	0.9500	C30—H30A	0.9900
C6—C7	1.463 (4)	C30—H30B	0.9900
C7—C8	1.406 (4)	C31—C32	1.555 (4)
C8—C9	1.367 (4)	C31—C34	1.577 (5)
C8—H8	0.9500	C31—H31	1.0000
C9—C10	1.399 (4)	C32—C33	1.552 (4)
C9—C12	1.509 (4)	C32—H32A	0.9900
C10—C11	1.381 (3)	C32—H32B	0.9900
C10—C15	1.487 (4)	C33—C34	1.576 (4)
C11—H11	0.9500	C33—H33	1.0000
C12—C13	1.536 (5)	C34—C35	1.506 (5)
C12—H12A	0.9900	C34—C36	1.509 (4)
C12—H12B	0.9900	C35—H35A	0.9800

C13—C14	1.539 (4)	C35—H35B	0.9800
C13—C16	1.564 (5)	C35—H35C	0.9800
C13—H13	1.0000	C36—H36A	0.9800
C14—C15	1.567 (4)	C36—H36B	0.9800
C14—H14A	0.9900	C36—H36C	0.9800
C14—H14B	0.9900		

C37—Ru1—C38	91.97 (12)	C17—C16—C18	108.8 (3)
C37—Ru1—C1	91.79 (12)	C17—C16—C13	118.0 (3)
C38—Ru1—C1	92.57 (11)	C18—C16—C13	112.2 (3)
C37—Ru1—O1	175.99 (10)	C17—C16—C15	120.5 (3)
C38—Ru1—O1	91.46 (10)	C18—C16—C15	110.7 (3)
C1—Ru1—O1	90.13 (9)	C13—C16—C15	84.9 (2)
C37—Ru1—N1	91.11 (10)	C16—C17—H17A	109.5
C38—Ru1—N1	171.41 (10)	C16—C17—H17B	109.5
C1—Ru1—N1	79.31 (9)	H17A—C17—H17B	109.5
O1—Ru1—N1	85.79 (8)	C16—C17—H17C	109.5
C37—Ru1—Cl1	97.98 (10)	H17A—C17—H17C	109.5
C38—Ru1—Cl1	95.76 (8)	H17B—C17—H17C	109.5
C1—Ru1—Cl1	166.90 (7)	C16—C18—H18A	109.5
O1—Ru1—Cl1	79.60 (5)	C16—C18—H18B	109.5
N1—Ru1—Cl1	91.75 (6)	H18A—C18—H18B	109.5
C40—Ru2—C39	91.78 (12)	C16—C18—H18C	109.5
C40—Ru2—C19	89.65 (12)	H18A—C18—H18C	109.5
C39—Ru2—C19	93.53 (12)	H18B—C18—H18C	109.5
C40—Ru2—O1	175.48 (11)	C20—C19—C24	118.4 (3)
C39—Ru2—O1	92.67 (10)	C20—C19—Ru2	127.9 (2)
C19—Ru2—O1	89.26 (9)	C24—C19—Ru2	113.55 (19)
C40—Ru2—N2	90.14 (10)	C21—C20—C19	120.9 (4)
C39—Ru2—N2	173.08 (11)	C21—C20—H20	119.5
C19—Ru2—N2	79.82 (10)	C19—C20—H20	119.5

O1—Ru2—N2	85.35 (8)	C20—C21—C22	120.1 (3)
C40—Ru2—Cl1	101.10 (9)	C20—C21—H21	120.0
C39—Ru2—Cl1	94.40 (9)	C22—C21—H21	120.0
C19—Ru2—Cl1	166.41 (8)	C23—C22—C21	119.3 (3)
O1—Ru2—Cl1	79.37 (6)	C23—C22—H22	120.4
N2—Ru2—Cl1	91.76 (6)	C21—C22—H22	120.4
Ru1—Cl1—Ru2	86.88 (2)	C22—C23—C24	121.8 (3)
Ru1—O1—Ru2	114.13 (9)	C22—C23—H23	119.1
Ru1—O1—H1	124 (3)	C24—C23—H23	119.1
Ru2—O1—H1	99 (3)	C23—C24—C19	119.5 (3)
C7—N1—C11	119.4 (2)	C23—C24—C25	123.8 (3)
C7—N1—Ru1	114.66 (18)	C19—C24—C25	116.7 (2)
C11—N1—Ru1	125.93 (16)	N2—C25—C26	119.6 (3)
C29—N2—C25	119.9 (2)	N2—C25—C24	114.8 (2)
C29—N2—Ru2	125.85 (17)	C26—C25—C24	125.5 (3)
C25—N2—Ru2	114.25 (18)	C27—C26—C25	120.8 (3)
C2—C1—C6	118.0 (2)	C27—C26—H26	119.6
C2—C1—Ru1	128.5 (2)	C25—C26—H26	119.6
C6—C1—Ru1	113.15 (17)	C26—C27—C28	118.9 (3)
C3—C2—C1	121.2 (3)	C26—C27—C30	123.8 (3)
C3—C2—H2	119.4	C28—C27—C30	117.3 (3)
C1—C2—H2	119.4	C29—C28—C27	117.4 (3)
C2—C3—C4	120.0 (3)	C29—C28—C33	124.9 (2)
C2—C3—H3	120.0	C27—C28—C33	117.7 (2)
C4—C3—H3	120.0	N2—C29—C28	123.4 (2)
C5—C4—C3	119.8 (3)	N2—C29—H29	118.3
C5—C4—H4	120.1	C28—C29—H29	118.3
C3—C4—H4	120.1	C27—C30—C31	110.3 (2)
C4—C5—C6	120.8 (3)	C27—C30—H30A	109.6
C4—C5—H5	119.6	C31—C30—H30A	109.6

C6—C5—H5	119.6	C27—C30—H30B	109.6
C5—C6—C1	120.1 (3)	C31—C30—H30B	109.6
C5—C6—C7	122.8 (3)	H30A—C30—H30B	108.1
C1—C6—C7	117.0 (2)	C30—C31—C32	108.8 (3)
N1—C7—C8	120.4 (2)	C30—C31—C34	112.7 (3)
N1—C7—C6	114.3 (2)	C32—C31—C34	87.4 (2)
C8—C7—C6	125.3 (2)	C30—C31—H31	114.9
C9—C8—C7	120.4 (2)	C32—C31—H31	114.9
C9—C8—H8	119.8	C34—C31—H31	114.9
C7—C8—H8	119.8	C33—C32—C31	86.3 (2)
C8—C9—C10	118.7 (2)	C33—C32—H32A	114.3
C8—C9—C12	123.0 (3)	C31—C32—H32A	114.3
C10—C9—C12	118.2 (3)	C33—C32—H32B	114.3
C11—C10—C9	118.9 (2)	C31—C32—H32B	114.3
C11—C10—C15	123.8 (2)	H32A—C32—H32B	111.4
C9—C10—C15	117.4 (2)	C28—C33—C32	106.6 (2)
N1—C11—C10	122.1 (2)	C28—C33—C34	109.5 (2)
N1—C11—H11	118.9	C32—C33—C34	87.5 (2)
C10—C11—H11	118.9	C28—C33—H33	116.5
C9—C12—C13	110.6 (2)	C32—C33—H33	116.5
C9—C12—H12A	109.5	C34—C33—H33	116.5
C13—C12—H12A	109.5	C35—C34—C36	110.2 (3)
C9—C12—H12B	109.5	C35—C34—C33	111.5 (3)
C13—C12—H12B	109.5	C36—C34—C33	118.7 (2)
H12A—C12—H12B	108.1	C35—C34—C31	111.5 (3)
C12—C13—C14	108.9 (2)	C36—C34—C31	118.1 (3)
C12—C13—C16	110.8 (3)	C33—C34—C31	84.7 (2)
C14—C13—C16	88.3 (2)	C34—C35—H35A	109.5
C12—C13—H13	115.3	C34—C35—H35B	109.5
C14—C13—H13	115.3	H35A—C35—H35B	109.5

C16—C13—H13	115.3	C34—C35—H35C	109.5
C13—C14—C15	86.6 (2)	H35A—C35—H35C	109.5
C13—C14—H14A	114.2	H35B—C35—H35C	109.5
C15—C14—H14A	114.2	C34—C36—H36A	109.5
C13—C14—H14B	114.2	C34—C36—H36B	109.5
C15—C14—H14B	114.2	H36A—C36—H36B	109.5
H14A—C14—H14B	111.4	C34—C36—H36C	109.5
C10—C15—C14	106.8 (2)	H36A—C36—H36C	109.5
C10—C15—C16	109.4 (2)	H36B—C36—H36C	109.5
C14—C15—C16	86.4 (2)	O2—C37—Ru1	178.4 (3)
C10—C15—H15	116.7	O3—C38—Ru1	175.8 (2)
C14—C15—H15	116.7	O4—C39—Ru2	177.8 (3)
C16—C15—H15	116.7	O5—C40—Ru2	176.1 (3)

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Data collection:

(akram4)	Collect (Nonius B.V., 1998)
(ksenia2)	Collect (Nonius B.V., 1998)
(ah621_cl)	?
(jpd-f1)	?

Cell refinement:

(akram4)	*DENZO* (Nonius B.V., 1998)
(ksenia2)	*DENZO* (Nonius B.V., 1998)
(ah621_cl)	?
(jpd-f1)	?

Data reduction:

(akram4) *DENZO* (Nonius B.V., 1998)

(ksenia2) *DENZO* (Nonius B.V., 1998)

(ah621_cl) ?

(jpd-f1) ?

Program(s) used to solve structure:

(akram4) *SHELXS97* (Sheldrick, 1997)

(ksenia2) *SHELXS97* (Sheldrick, 1997)

(ah621_cl) *SHELXS97* (Sheldrick, 1990)

(jpd-f1) *SHELXS97* (Sheldrick, 1990)

Program(s) used to refine structure:

(akram4) *SHELXL97* (Sheldrick, 1997)

(ksenia2) *SHELXL97* (Sheldrick, 1997)

(ah621_cl) *SHELXL97* (Sheldrick, 1997)

(jpd-f1) *SHELXL97* (Sheldrick, 1997)

H. Computational Supplementary Material

1. Geometry Optimizations with the BP/TZP method (all electrons on C, H, N, O; frozen core to 3d for Ru)

a) 3b

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                              Build 200711141748           *
*                                                                           *
*                                                                           *
*                               =================                           *
*                               |               |                           *
*                               |     A D F     |                           *
*                               |               |                           *
*                               =================                           *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  pentium64_linux  *****************************

ADF 2007.01  RunTime: Jul28-2008 16:12:30
terpRuOHax


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
----------------
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul28-2008 16:12:29
        title: Ruthenium (TZP, 3d frozen)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jul28-2008 16:12:28
        title: Chlorine (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul28-2008 16:12:28
        title: Oxygen (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul28-2008 16:12:27
        title: Hydrogen (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul28-2008 16:12:28
        title: Nitrogen (TZP)
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul28-2008 16:12:28
        title: Carbon (TZP)



                                  ******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ******************************************


==========================
Geometry Convergence Tests
==========================

Energy  old :        -20.46856965
        new :        -20.46855914

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-----------------------------------------------------------------------
change in energy       0.00001051     0.00100000    YES        0.08103025
gradient max           0.00090484     0.00100000    YES        0.82872419
gradient rms           0.00014690     0.00066667    YES        0.81498129
cart. step max         0.00165474     0.01000000    YES        0.30080149
cart. step rms         0.00042344     0.00666667    YES        0.29463002

prediction dE :       -0.00000495
```

```
*****************************************************************************************
                          Geometry CONVERGED
*****************************************************************************************


                                    ********************
                                    *  Final Geometry  *
                                    ********************


Coordinates (Cartesian)
=======================
```

Atom	bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1 Ru	15.918751	-0.618087	12.757357	8.423840	-0.327078	6.750903	1	2	3
2 Ru	12.387478	-3.057168	7.486613	6.555171	-1.617784	3.961745	4	5	6
3 Cl	14.096524	-5.066311	11.667301	7.459559	-2.680976	6.174070	7	8	9
4 O	14.433819	0.061705	9.046728	7.638048	0.032653	4.787322	10	11	12
5 H	13.515612	1.656206	8.969822	7.152154	0.876426	4.746625	13	14	15
6 O	17.971947	-1.665824	18.043485	9.510345	-0.881516	9.548201	16	17	18
7 O	21.243713	-1.614151	10.775307	11.241689	-0.854172	5.702047	19	20	21
8 O	7.174915	-1.663692	9.509082	3.796802	-0.880388	5.031990	22	23	24
9 O	9.874307	-7.677417	5.117926	5.225258	-4.062714	2.708290	25	26	27
10 N	12.353661	0.689833	14.337747	6.537276	0.365044	7.587209	28	29	30
11 N	15.907956	-3.745356	5.470945	8.418128	-1.981957	2.895100	31	32	33
12 C	16.586924	3.222528	13.105028	8.777422	1.705288	6.934882	34	35	36
13 C	18.815740	4.536422	12.523235	9.956861	2.400571	6.627011	37	38	39
14 H	20.506176	3.507585	11.951814	10.851401	1.856134	6.324627	40	41	42
15 C	18.930327	7.175199	12.648779	10.017497	3.796952	6.693446	43	44	45
16 H	20.691962	8.142196	12.181649	10.949715	4.308665	6.446251	46	47	48
17 C	16.802007	8.576082	13.363351	8.891239	4.538267	7.071581	49	50	51
18 H	16.885253	10.633356	13.451981	8.935291	5.626929	7.118482	52	53	54
19 C	14.573470	7.315731	13.967533	7.711948	3.871318	7.391300	55	56	57
20 H	12.921508	8.413439	14.528863	6.837768	4.452200	7.688343	58	59	60
21 C	14.446638	4.657010	13.862659	7.644832	2.464383	7.335803	61	62	63
22 C	12.171265	3.248313	14.576226	6.440756	1.718933	7.713407	64	65	66
23 C	9.932788	4.330198	15.504880	5.256205	2.291442	8.204829	67	68	69
24 H	9.786206	6.378602	15.656954	5.178637	3.375411	8.285303	70	71	72
25 C	7.923244	2.810627	16.251987	4.192800	1.487320	8.600181	73	74	75
26 C	8.187650	0.158968	16.074071	4.332718	0.084122	8.506032	76	77	78
27 C	10.428137	-0.801057	15.090575	5.518332	-0.423901	7.985589	79	80	81
28 H	10.726211	-2.825057	14.837428	5.676066	-1.494956	7.851629	82	83	84
29 C	5.448156	3.846597	17.277935	2.883040	2.035532	9.143090	85	86	87
30 H	4.605997	5.136250	15.874745	2.437389	2.717986	8.400554	88	89	90
31 H	5.820889	4.996683	18.973981	3.080282	2.644131	10.040598	91	92	93
32 C	3.591363	1.688664	17.871385	1.900467	0.893602	9.457129	94	95	96
33 H	1.771230	2.426928	18.550838	0.937295	1.284275	9.816681	97	98	99
34 C	3.577372	-0.201567	15.618629	1.893064	-0.106665	8.265023	100	101	102
35 H	3.836867	0.570186	13.710138	2.030383	0.301729	7.255093	103	104	105
36 H	1.934944	-1.460033	15.632325	1.023928	-0.772616	8.272270	106	107	108
37 C	5.960250	-1.421792	16.873660	3.154028	-0.752380	8.929156	109	110	111
38 H	6.295324	-3.456921	16.648680	3.331342	-1.829324	8.810102	112	113	114
39 C	4.889515	-0.442642	19.498686	2.587420	-0.234236	10.318260	115	116	117
40 C	6.731307	0.317719	21.591036	3.562054	0.168130	11.425484	118	119	120
41 H	5.704472	1.265743	23.135962	3.018677	0.669802	12.243024	121	122	123
42 H	8.238408	1.592190	20.947736	4.359578	0.842551	11.085065	124	125	126
43 H	7.645546	-1.367865	22.400858	4.045848	-0.723843	11.854024	127	128	129
44 C	2.946089	-2.291301	20.607614	1.559003	-1.212505	10.905080	130	131	132
45 H	3.906240	-3.969816	21.374720	2.067093	-2.100736	11.311015	133	134	135
46 H	1.545049	-2.942550	19.222913	0.817604	-1.557130	10.172327	136	137	138
47 H	1.914416	-1.389489	22.174065	1.013065	-0.735286	11.734010	139	140	141
48 C	11.836049	-0.935419	4.245515	6.263367	-0.495003	2.246630	142	143	144
49 C	9.687613	0.462653	3.569507	5.126464	0.244826	1.888902	145	146	147
50 H	7.977460	0.360339	4.714419	4.221490	0.190683	2.494763	148	149	150
51 C	9.678740	2.021883	1.430918	5.121769	1.069934	0.757209	151	152	153
52 H	7.981600	3.095624	0.957594	4.223681	1.638133	0.506737	154	155	156
53 C	11.833430	2.211370	-0.091385	6.261981	1.170206	-0.048359	157	158	159
54 H	11.839447	3.438892	-1.746899	6.265165	1.819783	-0.924419	160	161	162
55 C	13.975652	0.810404	0.523701	7.395596	0.428848	0.277130	163	164	165
56 H	15.647497	0.961797	-0.672677	8.280299	0.508961	-0.355965	166	167	168
57 C	13.995953	-0.775643	2.661126	7.406339	-0.410453	1.408207	169	170	171
58 C	16.177642	-2.345495	3.328846	8.560839	-1.241182	1.761549	172	173	174
59 C	18.413244	-2.525759	1.909667	9.743869	-1.336574	1.010552	175	176	177
60 H	18.622272	-1.394805	0.201355	9.854482	-0.738099	0.106552	178	179	180
61 C	20.345687	-4.141246	2.657621	10.766474	-2.191453	1.406352	181	182	183
62 C	20.013564	-5.595872	4.872316	10.590722	-2.961208	2.578319	184	185	186
63 C	17.765801	-5.323908	6.208212	9.401257	-2.817291	3.285244	187	188	189
64 H	17.409286	-6.356841	7.956254	9.212597	-3.363895	4.210268	190	191	192
65 C	22.806807	-4.447974	1.207772	12.068843	-2.353767	0.639125	193	194	195
66 H	23.729459	-2.590645	1.008166	12.557089	-1.370910	0.533499	196	197	198
67 H	22.399510	-5.105547	-0.726373	11.853310	-2.701739	-0.384380	199	200	201
68 C	24.589876	-6.292101	2.577815	13.012402	-3.329637	1.364121	202	203	204
69 H	26.405390	-6.465354	1.580871	13.973131	-3.421318	0.836561	205	206	207
70 C	24.627173	-5.623904	5.441742	13.032139	-2.976042	2.879646	208	209	210
71 H	26.238263	-6.450960	6.442723	13.884691	-3.413701	3.409342	211	212	213
72 H	24.444344	-3.624296	5.965408	12.935390	-1.917895	3.156758	214	215	216
73 C	22.178737	-7.266506	5.662575	11.736482	-3.845270	2.996505	217	218	219
74 H	21.802114	-8.292314	7.426508	11.537182	-4.388104	3.929939	220	221	222
75 C	23.192266	-8.820715	3.307933	12.272818	-4.667721	1.750483	223	224	225
76 C	25.058527	-10.888607	4.123591	13.260401	-5.762003	2.182111	226	227	228
77 H	24.040069	-12.462740	5.025096	12.721456	-6.594998	2.659166	229	230	231
78 H	26.496457	-10.218511	5.460692	14.021321	-5.407403	2.889674	232	233	234
79 H	26.049690	-11.653898	2.461233	13.784902	-6.166977	1.302428	235	236	237
80 C	21.300172	-9.969779	1.451551	11.271566	-5.275780	0.768127	238	239	240
81 H	22.294453	-10.692155	-0.230331	11.797716	-5.658045	-0.121886	241	242	243
82 H	19.848511	-8.630396	0.812772	10.503380	-4.567009	0.430100	244	245	246
83 H	20.316473	-11.582169	2.327017	10.751014	-6.129020	1.231404	247	248	249
84 C	17.181151	-1.276747	16.030476	9.091874	-0.675626	8.482963	250	251	252
85 C	19.176046	-1.293875	11.447789	10.147527	-0.684689	6.057909	253	254	255
86 C	9.207833	-2.179323	8.841469	4.872575	-1.153248	4.678704	256	257	258
87 C	10.862901	-5.932710	6.016054	5.748400	-3.139455	3.183559	259	260	261

```
Number of elements of the density matrix on this node (used, total):    206153    832695


=====================================================
Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
=====================================================
```

```
 General Accuracy Parameter :                          4.50

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
    Nr. of used Symmetry Operators                     1

    Points in the Atomic Spheres                   50260
    Points in the Atomic Polyhedra                521244
    Points in the Outer Region                     38933
    ------------------------------------------------------
    Total                                         610437

    Sum of Weights                                183595.259189

 Total nr. of points:     610437
 Nr. of blocks:             4770
 Block length:               128
 Nr. of dummy points:        123


 Test of Precision of the Numerical Integration Grid
 ===================================================

 Integral of the Total Core Density:                 55.99998076397415
 Relative Error:                                     -3.435E-07



 ============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

                                        hartree             eV         kcal/mol          kJ/mol
                                    --------------    ----------    ----------    ----------

Pauli Repulsion
  Kinetic (Delta T^0):             221.571342234667668    6029.2630     139038.13     581735.48
  Delta V^Pauli Coulomb:          -111.532789938814034   -3034.9616     -69987.89    -292829.30
  Delta V^Pauli LDA-XC:            -28.480996447973073    -775.0073     -17872.10     -74776.85
  Delta V^Pauli GGA-Exchange:        1.672183251095404      45.5024       1049.31       4390.32
  Delta V^Pauli GGA-Correlation:    -0.470468378497849     -12.8021       -295.22      -1235.21
                                    --------------    ----------    ----------    ----------
  Total Pauli Repulsion:           82.759270720478128    2251.9943      51932.23     217284.43
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  82.759270720478128    2251.9943      51932.23     217284.43
  Electrostatic Interaction:       -17.470990322308907    -475.4098     -10963.21     -45870.08
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                    --------------    ----------    ----------    ----------
  Total Steric Interaction:         65.288280398169221    1776.5845      40969.02     171414.36
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -85.742753210822642   -2333.1790     -53804.40    -225117.57
                                    --------------    ----------    ----------    ----------
  Total Orbital Interactions:      -85.756852781072681   -2333.5627     -53813.24    -225154.59

Alternative Decomposition Orb.Int.
  Kinetic:                        -202.361553266726247   -5506.5380    -126983.81    -531300.18
  Coulomb:                         107.681543735460380    2930.1639      67571.20     282717.85
  XC:                                8.923156750193328     242.8114       5599.37      23427.74
                                    --------------    ----------    ----------    ----------
  Total Orbital Interactions:      -85.756852781072539   -2333.5627     -53813.24    -225154.59

  Residu (E=Steric+OrbInt+Res):      0.000014331969659       0.0004          0.01          0.04

Total Bonding Energy:              -20.468558050933801    -556.9778     -12844.22     -53740.19


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
======================================================================================

  Electrostatic Energy:            -17.470990322308907    -475.4098     -10963.21     -45870.08
  Kinetic Energy:                   19.209788967941421     522.7250      12054.33      50435.29
  Coulomb (Steric+OrbInt) Energy:   -3.851231871383987    -104.7974      -2416.68     -10111.41
  XC Energy:                       -18.356124825182192    -499.4956     -11518.64     -48194.00
                                    --------------    ----------    ----------    ----------
  Total Bonding Energy:            -20.468558050933666    -556.9778     -12844.22     -53740.19


Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree):  -0.0061019483
2. Electrostatic (Fit correction):   0.0000000000
```

```
====================================
B O N D - O R D E R  A N A L Y S I S
====================================
```

			DIST. [A]	BOND-ORDERS (THRESHOLD = 0.050)				
				MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
Ru	1 - Cl	3	2.6083	0.4184	0.2577	0.3392	0.5799	0.3874
Ru	1 - O	4	2.1453	0.3359	0.3126	0.3980	0.7798	0.4394
Ru	1 - O	6	3.0517	0.2075	0.2496	0.2922	0.4166	0.2880
Ru	1 - O	7	3.0526	0.2151	0.2456	0.2875	0.4143	0.2836
Ru	1 - N	10	2.1766	0.2743	0.3258	0.3683	0.4917	0.3587
Ru	1 - C	12	2.0711	0.6292	0.7450	0.8177	0.8662	0.7827
Ru	1 - C	84	1.8889	1.1025	1.0860	1.1894	1.0303	1.0905
Ru	1 - C	85	1.8919	1.0471	1.0672	1.1699	1.0077	1.0715
Ru	2 - Cl	3	2.6159	0.4130	0.2532	0.3327	0.5743	0.3802
Ru	2 - O	4	2.1397	0.3552	0.3214	0.4085	0.7888	0.4511
Ru	2 - O	8	3.0492	0.2198	0.2535	0.2963	0.4263	0.2927
Ru	2 - O	9	3.0525	0.2062	0.2482	0.2901	0.4145	0.2859
Ru	2 - N	11	2.1774	0.2615	0.3224	0.3637	0.4825	0.3538
Ru	2 - C	48	2.0706	0.6390	0.7470	0.8181	0.8642	0.7827
Ru	2 - C	86	1.8870	1.0869	1.0846	1.1856	1.0350	1.0889
Ru	2 - C	87	1.8900	1.0949	1.0794	1.1801	1.0214	1.0820
Cl	3 - C	12	4.6427	0.0519	0.1043	0.1283	0.0492	0.1563
Cl	3 - C	48	4.6513	0.0516	0.1033	0.1270	0.0502	0.1546
O	4 - H	5	0.9745	1.1203	0.8506	1.0775	1.1654	1.0677
O	4 - C	84	4.0340	0.0556	0.1254	0.1484	0.2793	0.1697
O	4 - C	87	4.0256	0.0587	0.1279	0.1514	0.2818	0.1730
O	6 - C	84	1.1629	2.0422	2.1902	2.3687	2.3791	2.4126
O	7 - C	85	1.1630	2.0208	2.1882	2.3687	2.3797	2.4120
O	8 - C	86	1.1647	2.0086	2.1708	2.3487	2.3574	2.4007
O	9 - C	87	1.1627	2.0429	2.1909	2.3697	2.3801	2.4135
N	10 - C	22	1.3632	1.2762	1.3117	1.3794	1.3967	1.4035
N	10 - C	25	2.7897	0.0361	0.0896	0.0942	0.1042	0.0968
N	10 - C	27	1.3488	1.3551	1.3812	1.4596	1.4399	1.5131
N	10 - C	85	4.0589	0.0414	0.1144	0.1192	0.1663	0.1200
N	11 - C	58	1.3616	1.2802	1.3148	1.3820	1.4009	1.4029
N	11 - C	61	2.7884	0.0359	0.0907	0.0953	0.1048	0.0978
N	11 - C	63	1.3478	1.3575	1.3848	1.4628	1.4442	1.5147
N	11 - C	86	4.0545	0.0417	0.1142	0.1188	0.1598	0.1197
C	12 - C	13	1.4033	1.4118	1.4161	1.4516	1.4197	1.5064
C	12 - C	17	2.8386	0.0426	0.0995	0.1022	0.0767	0.1062
C	12 - C	21	1.4212	1.3473	1.3218	1.3515	1.3432	1.3801
C	13 - H	14	1.0900	1.0257	0.9217	0.9608	0.9732	0.9025
C	13 - C	15	1.3993	1.3953	1.4325	1.4883	1.4499	1.5486
C	13 - C	19	2.7905	0.0611	0.1094	0.1137	0.0837	0.1184
C	15 - H	16	1.0918	1.0311	0.9275	0.9692	0.9801	0.9074
C	15 - C	17	1.4004	1.3704	1.4075	1.4650	1.4244	1.5262
C	15 - C	21	2.7961	0.0534	0.0943	0.0977	0.0913	0.1000
C	17 - H	18	1.0906	1.0322	0.9288	0.9724	0.9860	0.9140
C	17 - C	19	1.3920	1.4125	1.4629	1.5231	1.4806	1.5878
C	19 - H	20	1.0908	1.0270	0.9268	0.9633	0.9749	0.9108
C	19 - C	21	1.4096	1.3405	1.3461	1.3954	1.3841	1.4301
C	21 - C	22	1.4656	1.1648	1.0937	1.1270	1.1294	1.1145
C	22 - C	23	1.4044	1.3598	1.3480	1.3947	1.4103	1.4053
C	22 - C	26	2.7829	0.0522	0.0844	0.0868	0.0873	0.0855
C	23 - H	24	1.0897	1.0136	0.9210	0.9605	0.9751	0.9056
C	23 - C	25	1.3906	1.4252	1.4419	1.4907	1.4923	1.5172
C	23 - C	27	2.7368	0.0563	0.0954	0.0992	0.0924	0.1019
C	25 - C	26	1.4133	1.3502	1.3093	1.3441	1.3440	1.3377
C	25 - C	29	1.5201	0.9402	1.0166	1.0521	1.0530	1.0877
C	26 - C	27	1.3909	1.4259	1.4082	1.4541	1.4537	1.4610
C	26 - C	37	1.5060	0.9721	1.0154	1.0432	1.0397	1.0624
C	27 - H	28	1.0909	1.0211	0.8994	0.9390	0.9294	0.8581
C	29 - H	30	1.1026	1.0135	0.9142	0.9566	0.9865	0.9126
C	29 - H	31	1.1022	1.0097	0.9148	0.9559	0.9851	0.9140
C	29 - C	32	1.5389	0.9551	1.0082	1.0429	0.9834	1.1011
C	32 - H	33	1.0998	1.0529	0.9246	0.9534	0.9612	0.9005
C	32 - C	34	1.5562	0.9377	0.9912	1.0220	0.9657	1.0775
C	32 - C	39	1.5765	0.9038	0.9453	0.9620	0.9676	0.9711
C	34 - H	35	1.0980	1.0207	0.9349	0.9724	0.9983	0.9328
C	34 - H	36	1.0950	1.0127	0.9327	0.9708	0.9970	0.9305
C	34 - C	37	1.5646	0.9268	0.9729	1.0045	0.9455	1.0601
C	37 - H	38	1.0979	1.0521	0.9226	0.9535	0.9623	0.8984
C	37 - C	39	1.5872	0.8957	0.9269	0.9446	0.9504	0.9545
C	39 - C	40	1.5290	0.9753	1.0172	1.0527	1.0501	1.1095
C	39 - C	44	1.5359	0.9969	1.0083	1.0427	1.0408	1.0982
C	40 - H	41	1.1024	0.9775	0.9440	0.9918	1.0295	0.9746
C	40 - H	42	1.0985	0.9576	0.9430	0.9899	1.0288	0.9710
C	40 - H	43	1.1015	0.9777	0.9425	0.9918	1.0318	0.9711
C	44 - H	45	1.1009	0.9784	0.9451	0.9931	1.0316	0.9733
C	44 - H	46	1.0979	0.9517	0.9477	0.9937	1.0297	0.9775
C	44 - H	47	1.1013	0.9765	0.9447	0.9923	1.0301	0.9735
C	48 - C	49	1.4028	1.4157	1.4222	1.4576	1.4251	1.5133
C	48 - C	53	2.8355	0.0429	0.1005	0.1032	0.0785	0.1071
C	48 - C	57	1.4200	1.3448	1.3202	1.3490	1.3428	1.3749
C	49 - H	50	1.0904	1.0254	0.9226	0.9613	0.9746	0.9052
C	49 - C	51	1.4006	1.3897	1.4265	1.4824	1.4416	1.5444
C	49 - C	55	2.7894	0.0601	0.1083	0.1125	0.0816	0.1173
C	51 - H	52	1.0919	1.0308	0.9279	0.9694	0.9807	0.9086
C	51 - C	53	1.3997	1.3772	1.4132	1.4709	1.4295	1.5329
C	51 - C	57	2.7990	0.0554	0.0961	0.0996	0.0950	0.1019
C	53 - H	54	1.0906	1.0320	0.9290	0.9725	0.9861	0.9144
C	53 - C	55	1.3931	1.4055	1.4573	1.5171	1.4753	1.5811
C	55 - H	56	1.0908	1.0272	0.9266	0.9632	0.9744	0.9102
C	55 - C	57	1.4085	1.3481	1.3521	1.4011	1.3921	1.4335
C	57 - C	58	1.4655	1.1578	1.0912	1.1242	1.1250	1.1087
C	58 - C	59	1.4045	1.3606	1.3478	1.3944	1.4113	1.4029
C	58 - C	62	2.7832	0.0538	0.0853	0.0876	0.0884	0.0862
C	59 - H	60	1.0898	1.0138	0.9212	0.9604	0.9747	0.9057
C	59 - C	61	1.3904	1.4247	1.4427	1.4914	1.4930	1.5175
C	59 - C	63	2.7357	0.0568	0.0964	0.1002	0.0934	0.1029
C	61 - C	62	1.4131	1.3518	1.3106	1.3456	1.3455	1.3394
C	61 - C	65	1.5202	0.9402	1.0164	1.0520	1.0527	1.0877
C	62 - C	63	1.3911	1.4256	1.4074	1.4534	1.4530	1.4606
C	62 - C	73	1.5064	0.9727	1.0151	1.0430	1.0393	1.0623
C	63 - H	64	1.0909	1.0210	0.9000	0.9396	0.9302	0.8592
C	65 - H	66	1.1025	1.0137	0.9147	0.9571	0.9868	0.9134
C	65 - H	67	1.1023	1.0099	0.9147	0.9557	0.9849	0.9140

C	65 - C	68	1.5389	0.9554	1.0083	1.0429	0.9834	1.1012
C	68 - H	69	1.0999	1.0529	0.9248	0.9534	0.9612	0.9007
C	68 - C	70	1.5564	0.9373	0.9912	1.0219	0.9655	1.0775
C	68 - C	75	1.5769	0.9039	0.9452	0.9618	0.9674	0.9709
C	70 - H	71	1.0950	1.0127	0.9330	0.9710	0.9971	0.9309
C	70 - H	72	1.0981	1.0208	0.9351	0.9728	0.9988	0.9332
C	70 - C	73	1.5646	0.9278	0.9735	1.0050	0.9461	1.0606
C	73 - H	74	1.0980	1.0520	0.9228	0.9535	0.9623	0.8987
C	73 - C	75	1.5864	0.8956	0.9270	0.9446	0.9505	0.9545
C	75 - C	76	1.5359	0.9964	1.0083	1.0426	1.0408	1.0981
C	75 - C	80	1.5288	0.9753	1.0171	1.0526	1.0500	1.1095
C	76 - H	77	1.1009	0.9785	0.9453	0.9931	1.0314	0.9735
C	76 - H	78	1.0979	0.9517	0.9477	0.9937	1.0296	0.9776
C	76 - H	79	1.1013	0.9765	0.9449	0.9923	1.0300	0.9737
C	80 - H	81	1.1023	0.9776	0.9442	0.9920	1.0295	0.9749
C	80 - H	82	1.0985	0.9580	0.9430	0.9900	1.0290	0.9709
C	80 - H	83	1.1016	0.9777	0.9426	0.9918	1.0316	0.9713
C	84 - C	85	2.6449	0.0714	0.0719	0.0724	0.0317	0.0684
C	86 - C	87	2.6358	0.0734	0.0747	0.0752	0.0384	0.0713
Sum :				110.7742	111.5212	117.3547	117.3547	117.3547
Atomic summation :								
Ru	1			4.3448	4.5009	5.0982	5.1620	4.9228
Ru	2			4.3910	4.5177	5.1069	5.1713	4.9346
Cl	3			1.0794	0.9743	1.2480	1.3450	1.4613
O	4			1.9806	1.9464	2.4374	2.6375	2.5999
H	5			1.1444	0.8821	1.1134	1.0524	1.0970
O	6			2.2865	2.5101	2.7420	2.7459	2.7894
O	7			2.2776	2.5074	2.7399	2.7449	2.7862
O	8			2.2737	2.5024	2.7339	2.7424	2.7892
O	9			2.2864	2.5102	2.7418	2.7456	2.7893
N	10			3.1856	3.4750	3.6899	3.6998	3.7723
N	11			3.1896	3.4798	3.6928	3.7001	3.7704
C	12			3.7506	3.9717	4.1473	4.1048	4.2342
C	13			4.0327	3.9877	4.1297	4.1210	4.1909
H	14			1.0693	0.9833	1.0258	1.0356	0.9624
C	15			3.9765	3.9856	4.1511	4.1372	4.2144
H	16			1.0397	0.9799	1.0240	1.0351	0.9579
C	17			3.9606	3.9857	4.1545	4.1465	4.2254
H	18			1.0426	0.9809	1.0270	1.0369	0.9641
C	19			3.9574	3.9926	4.1511	4.1455	4.2050
H	20			1.0357	0.9873	1.0263	1.0344	0.9691
C	21			4.0441	4.0191	4.1441	4.1318	4.1952
C	22			4.0872	4.0059	4.1636	4.1524	4.1810
C	23			3.9476	3.9888	4.1358	4.1367	4.1254
H	24			1.0489	0.9838	1.0262	1.0351	0.9660
C	25			3.8914	4.0116	4.1410	4.1196	4.1940
C	26			3.8965	4.0194	4.1388	4.1327	4.1545
C	27			4.0013	3.9637	4.1426	4.1120	4.1289
H	28			1.0783	0.9789	1.0262	1.0404	0.9421
C	29			3.9113	3.9609	4.1193	4.1399	4.1305
H	30			1.0858	0.9793	1.0244	1.0273	0.9743
H	31			1.0871	0.9809	1.0248	1.0267	0.9777
C	32			3.7968	3.9911	4.1060	4.0783	4.1731
H	33			1.0918	0.9877	1.0187	1.0268	0.9611
C	34			3.8642	3.9569	4.0998	4.1166	4.1341
H	35			1.0753	0.9837	1.0232	1.0244	0.9792
H	36			1.1049	0.9821	1.0222	1.0237	0.9778
C	37			3.7963	3.9899	4.1034	4.0891	4.1319
H	38			1.0940	0.9867	1.0200	1.0289	0.9598
C	39			3.8525	4.0188	4.1261	4.0592	4.2521
C	40			3.8764	3.9260	4.1095	4.1932	4.1137
H	41			1.0795	0.9819	1.0311	1.0140	1.0107
H	42			1.0637	0.9817	1.0303	1.0134	1.0085
H	43			1.0814	0.9796	1.0303	1.0143	1.0063
C	44			3.8831	3.9275	4.1074	4.1892	4.1121
H	45			1.0775	0.9807	1.0300	1.0142	1.0070
H	46			1.0788	0.9833	1.0308	1.0133	1.0120
H	47			1.0771	0.9813	1.0302	1.0141	1.0082
C	48			3.7574	3.9763	4.1487	4.1056	4.2326
C	49			4.0309	3.9883	4.1298	4.1230	4.1960
H	50			1.0675	0.9843	1.0263	1.0354	0.9652
C	51			3.9754	3.9863	4.1519	4.1381	4.2185
H	52			1.0401	0.9803	1.0242	1.0350	0.9590
C	53			3.9600	3.9860	4.1544	4.1467	4.2258
H	54			1.0423	0.9811	1.0270	1.0369	0.9645
C	55			3.9626	3.9926	4.1505	4.1444	4.2009
H	56			1.0346	0.9872	1.0262	1.0344	0.9685
C	57			4.0455	4.0205	4.1439	4.1312	4.1869
C	58			4.0919	4.0058	4.1624	4.1537	4.1715
C	59			3.9517	3.9893	4.1358	4.1358	4.1228
H	60			1.0481	0.9842	1.0262	1.0351	0.9661
C	61			3.8885	4.0119	4.1411	4.1201	4.1941
C	62			3.8984	4.0196	4.1394	4.1333	4.1557
C	63			3.9959	3.9644	4.1426	4.1132	4.1281
H	64			1.0767	0.9793	1.0265	1.0404	0.9429
C	65			3.9122	3.9611	4.1192	4.1399	4.1309
H	66			1.0851	0.9796	1.0245	1.0272	0.9747
H	67			1.0865	0.9810	1.0248	1.0267	0.9779
C	68			3.7962	3.9913	4.1059	4.0781	4.1733
H	69			1.0915	0.9878	1.0187	1.0268	0.9614
C	70			3.8639	3.9571	4.0998	4.1168	4.1345
H	71			1.1045	0.9823	1.0223	1.0236	0.9781
H	72			1.0776	0.9836	1.0231	1.0244	0.9791
C	73			3.7983	3.9901	4.1034	4.0891	4.1323
H	74			1.0937	0.9869	1.0201	1.0289	0.9602
C	75			3.8517	4.0188	4.1261	4.0591	4.2520
C	76			3.8822	3.9277	4.1072	4.1892	4.1124
H	77			1.0772	0.9808	1.0300	1.0141	1.0073
H	78			1.0785	0.9833	1.0308	1.0133	1.0121
H	79			1.0767	0.9814	1.0302	1.0140	1.0084
C	80			3.8770	3.9261	4.1095	4.1932	4.1139
H	81			1.0789	0.9820	1.0312	1.0140	1.0109
H	82			1.0640	0.9815	1.0302	1.0133	1.0082
H	83			1.0814	0.9798	1.0303	1.0143	1.0066
C	84			3.3718	3.6233	3.9383	3.8701	3.9045
C	85			3.3289	3.5974	3.8993	3.8463	3.8492
C	86			3.3593	3.6078	3.9059	3.8470	3.8671
C	87			3.3663	3.6219	3.9348	3.8667	3.9021

(*) Values from:
- Mayer bond-order analysis
- Gophinatan-Jug bond order analysis

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     - Nalewajski-Mrozek bond order analysis
       a) N-M (1) - bond-orders calculated from two-electron valence indices
                    based on partitioning of tr(Delta_P^2] (3-index set)
       b) N-M (2) - bond-orders calculated from two-electron valence indices
                    based on partitioning of tr(Delta_P^2] (4-index set)
       c) N-M (3) - bond-orders calculated from valence indices
                    based on partitioning of tr(P*Delta_P]
      A. Michalak, R.L. DeKock, T. Ziegler, J. Comp. Chem., subm.
      and original articles by Nalewajski et al. )


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=== CALCULATE ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ===
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                  This Analytical Second Derivatives Progam
                           was written for ADF by

                               Stephen K. Wolff

                         Scientific Computing & Modelling

                                Vrije University
                              Theoretical Chemistry
                                De Boelelaan 1083
                                1081 HV Amsterdam
                                 The Netherlands

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                               Date last modified:
                                    JUNE 2006


                                   References:
                                   ===========

                   Attila Berces, Ross M. Dickson, Liangyou Fan
                   Heiko Jacobsen, David Swerhone, Tom Ziegler,
                   Computer Physics Communications 100 (1997) 247.

                   Heiko Jacobsen, Attila Berces
                   David Swerhone, Tom Ziegler,
                   Computer Physics Communications 100 (1997) 263.

                   Stephen K. Wolff
                   Int. J. Quantum Chem. 104 (2005) 645.

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                  SECOND DERIVATIVES INFORMATION:
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                  === PRINT

                    EIGS,  lprint_eigbas =  F
                    U1,    lprint_u1     =  F
                    PARTS, lprint_parts  =  F

                  === DEBUG

                    ALL        =  F
                    B1         =  F
                    DENSITIES  =  F
                    FIT        =  F
                    HESSIAN    =  F
                    NUMBERS    =  F
                    SYMMETRY   =  F
                    U1         =  F

                  === CPKS

                    MAX_CPKS_ITERATIONS    =    20
                    U1_ACCURACY PARAMETER  =     5.00
                    U1 ACCURACY            =     0.0000100

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 Number of elements of the density matrix on this node (used, total):    206153    832695

 List of All Frequencies:


 Intensities
 ===========

               Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                 cm-1           1e-40 esu2 cm2          km/mole
              ----------          ----------          ----------
               -9.272264            0.000000            0.000000
               12.164459            0.000000            0.000000
               17.532110            0.000000            0.000000
               24.274624          108.392399            0.659522
               28.804192            1.632693            0.011788
               35.365897           30.023477            0.266148
               37.963216            8.233034            0.078343
               51.243134           13.111242            0.168406
               54.756002            0.457504            0.006279
               62.113122            1.287994            0.020053
               67.884133            7.757413            0.131997
               75.920034            0.956821            0.018208
               78.344004            1.171745            0.023010
               83.436249            6.342024            0.132636
               85.450414           20.733222            0.444078
               87.727787            8.893759            0.195569
               90.237522           10.275593            0.232419
               90.789190           17.595774            0.400424
               98.066845            7.912135            0.194489
              104.941899            8.932078            0.234952
              111.918667           16.961989            0.475836
              127.931160            3.328152            0.106723
              131.430961           83.288462            2.743851
```

156.349597	22.199570	0.870000
162.834441	27.257053	1.112508
165.142497	1.833323	0.075888
174.736823	2.119925	0.092850
176.429159	3.010730	0.133144
177.726233	9.088202	0.404863
183.134807	110.708611	5.081950
183.926007	113.641914	5.239137
187.027525	8.105708	0.379992
200.523273	122.097600	6.136913
202.107642	20.159852	1.021288
212.200326	74.523724	3.963863
213.145745	140.431928	7.502752
229.239432	6.397654	0.367611
236.279868	1.095557	0.064884
240.362836	10.392106	0.626108
244.522075	82.225687	5.039688
250.636005	20.238886	1.271476
252.454744	57.514266	3.639462
266.508878	1.333630	0.089089
269.560203	3.382056	0.228515
294.143993	28.443640	2.097120
295.565901	41.990696	3.110896
335.734043	1.357204	0.114214
336.349742	4.660517	0.392919
352.158737	158.065710	13.952570
356.198218	6.270603	0.559860
358.091785	24.933163	2.237947
377.388959	2.728498	0.258102
377.477514	2.264688	0.214278
396.424087	0.623372	0.061942
397.304805	0.280087	0.027893
405.827822	25.840315	2.628559
406.240542	44.138312	4.494455
433.032094	85.853725	9.318742
434.779625	28.036466	3.055417
436.189087	17.931028	1.960460
441.088400	17.800629	1.968063
454.078801	507.754568	57.791389
454.816648	47.208816	5.381924
465.931928	44.561001	5.204218
469.225872	6.249614	0.735044
472.638721	26.761135	3.170384
479.964698	203.433495	24.474274
484.853311	15.826242	1.923385
485.110178	30.691232	3.731924
492.533490	20.836743	2.572431
497.494781	2.384204	0.297310
500.454097	30.736682	3.855665
502.879927	68.676183	8.656623
517.386648	25.366844	3.289726
518.669600	12.719219	1.653596
524.107363	124.107212	16.304044
529.566391	29.098467	3.862501
545.862048	23.400437	3.201732
547.058478	7.653876	1.049526
583.064540	35.831048	5.236658
587.638425	66.474847	9.791418
592.112775	43.742201	6.492069
595.341153	69.022585	10.299952
615.796651	21.655385	3.342576
616.857520	20.267830	3.133792
622.915828	54.695000	8.539945
623.707729	120.456812	18.831745
632.113247	9.853051	1.561147
632.626654	14.929617	2.367414
648.153498	0.691743	0.112383
648.235024	16.254696	2.641128
652.356970	13.751369	2.248585
652.838082	37.747821	6.176969
714.047390	223.696528	40.037260
714.965974	75.950502	13.611127
721.610903	15.779954	2.854216
721.652609	77.305544	13.983532
722.878947	28.675867	5.195893
723.479486	28.799386	5.222609
756.607444	43.283510	8.208639
756.998739	21.463221	4.072566
766.651781	23.149749	4.448591
766.994083	33.782884	6.494815
801.632967	0.765147	0.153744
801.984335	0.387491	0.077894
829.657744	13.910816	2.892875
829.822656	10.164879	2.114295
837.052163	0.983464	0.206343
837.351421	3.532785	0.741486
839.708910	10.491734	2.208280
840.273228	12.566474	2.646745
855.411733	10.779762	2.311333
856.440821	11.185452	2.401204
887.973514	21.519080	4.789628
888.313704	15.260846	3.397997
899.315397	64.075873	14.443905
900.494361	6.485493	1.463868
902.121224	151.396152	34.234013
914.873160	0.491946	0.112812
916.016161	1.208944	0.277580
919.587015	22.036400	5.079390
920.447584	1.446717	0.333780
922.091105	30.589889	7.070169
924.373453	40.071790	9.284623
933.108149	27.766483	6.494279
933.197211	14.223568	3.327056
938.735386	9.162915	2.156031
939.356215	9.078213	2.137513
951.675712	0.059637	0.014226
953.401033	0.088165	0.021069
984.086876	1.014654	0.250282
985.084230	0.943327	0.232924
1008.437587	136.792377	34.577134
1008.755623	61.996140	15.675763
1016.484348	87.518281	22.298597
1016.523469	9.200593	2.344290
1018.038886	25.596262	6.531591
1018.139086	3.107672	0.793086
1025.027037	27.376350	7.033783

1026.113550	31.724280	8.159532
1051.438067	18.765346	4.945593
1053.028968	21.799301	5.753882
1064.486485	22.557190	6.018707
1064.588692	5.180483	1.382389
1085.887218	36.628916	9.969809
1086.233963	20.098615	5.472271
1111.807739	13.470285	3.753916
1112.025013	22.500076	6.271575
1114.713722	41.196125	11.510595
1114.957972	17.302404	4.835518
1137.188694	18.037743	5.141535
1137.600893	10.783350	3.074834
1158.058318	4.000612	1.161275
1158.524611	5.372726	1.560192
1164.413703	18.726652	5.465696
1164.572698	18.355128	5.357992
1179.157841	9.277415	2.742060
1179.334665	10.349515	3.059392
1184.403329	35.567388	10.559167
1184.730561	29.046540	8.625655
1201.811942	10.715710	3.228015
1201.989975	10.626534	3.201626
1207.486902	15.109505	4.573100
1207.649448	11.152492	3.375910
1228.913073	17.617380	5.426759
1229.874558	17.171798	5.293643
1243.671292	9.318460	2.904877
1244.441167	9.869175	3.078458
1250.562961	29.104913	9.123258
1250.645349	4.897862	1.535390
1259.773589	13.414798	4.235988
1259.974102	12.971656	4.096709
1275.032446	44.356646	14.176140
1275.911448	18.960157	6.063739
1288.778526	33.933897	10.962008
1289.727227	19.190574	6.203887
1296.762338	3.036646	0.987035
1297.608110	2.919521	0.949584
1307.518982	8.202293	2.688199
1308.347376	6.691357	2.194398
1326.647100	5.325274	1.770824
1326.733414	4.431122	1.473586
1353.626156	8.133696	2.759718
1354.333350	8.438969	2.864792
1372.320464	48.497910	16.682327
1372.925294	47.475520	16.337842
1387.545522	47.468344	16.509328
1387.683313	119.145671	41.442572
1417.895384	36.961489	13.136259
1420.600294	41.690649	14.845288
1422.287841	12.194692	4.347468
1422.328128	37.015836	13.196703
1434.650459	4.043408	1.454024
1434.929901	3.000091	1.079054
1437.779987	10.823620	3.900705
1439.094435	7.593579	2.739138
1440.645757	10.019428	3.618080
1441.207421	12.683799	4.581987
1449.047362	4.878808	1.772044
1449.278439	4.103449	1.490661
1461.821637	12.259410	4.492023
1462.061655	12.106225	4.436623
1465.477919	10.871642	3.993489
1465.568616	8.466272	3.110115
1476.774938	262.090714	97.016146
1478.236690	202.972253	75.207079
1526.509267	20.791344	7.955364
1528.048592	19.837870	7.598192
1546.779082	34.648573	13.433578
1548.560614	33.437073	12.978800
1568.362468	79.102356	31.096673
1569.513857	105.372023	41.454200
1597.255609	108.938751	43.614900
1598.409929	92.516874	37.066979
1937.394432	1194.395908	580.021944
1943.276848	1638.728041	798.214536
1999.026989	1753.803358	878.774862
2003.791102	827.605398	415.674926
2940.214017	21.803353	16.068683
2940.383706	20.807765	15.335838
2942.170534	26.601489	19.617870
2943.876268	24.251089	17.894884
2947.682863	92.394532	68.266101
2948.203716	90.368283	66.780796
2972.044348	10.649299	7.933309
2974.062547	9.346472	6.967482
2978.347238	101.597690	75.846795
2979.206845	84.132604	62.826528
2993.845713	34.363130	25.786963
2994.667502	34.304336	25.749909
2997.957456	9.608895	7.220662
2998.108074	8.618616	6.476836
3003.804359	16.684491	12.562113
3005.026730	19.114647	14.397686
3005.819624	48.137110	36.267782
3006.896458	41.644770	31.387520
3029.658511	25.029841	19.007712
3031.049850	22.907660	17.404113
3032.827747	29.703075	22.580171
3032.869708	28.825583	21.913408
3056.353472	51.904230	39.763482
3057.271164	48.722060	37.336850
3080.453377	1.325249	1.023270
3081.884568	1.666968	1.287721
3087.052130	9.987537	7.728237
3088.462658	10.442908	8.084290
3099.443415	47.585070	36.968557
3099.985759	10.017081	7.783572
3102.455814	9.306298	7.237035
3105.735994	8.165083	6.356283
3109.274187	2.547720	1.985586
3110.151327	4.101419	3.197376
3113.131995	47.937459	37.406805
3115.058341	46.805519	36.546124
3680.729947	26.598410	24.539613

```
 ============================
 Statistical Thermal Analysis  ***  ideal gas assumed  ***
 ============================

 Pressure:                 1.000000 atm.
 Temperature:            298.150000 K


 Moments of Inertia (and direction vectors)
 ==========================================

       22243.3204      51376.5618      56209.8316
 -------------------------------------------------
           0.6300          0.7761          0.0272
          -0.3538          0.2557          0.8997
          -0.6913          0.5765         -0.4357


 The rotational contribution to the molecular entropy includes
 a term, dependent on the symmetry number sigma. The results
 reported below were computed using sigma = 1, determined
 from the point group symmetry of the input geometry (NOSYM).
 If this is not the correct symmetry, please contact SCM to
 report a bug.

     Temp                                                    Transl     Rotat    Vibrat     Total
     ----                                                    ------     -----    ------     -----

     298.15   Entropy (cal/mole-K):                          46.146    39.393   173.141   258.680
              Internal Energy (Kcal/mole):                    0.889     0.889   440.084   441.861
              Constant Volume Heat Capacity (cal/mole-K):     2.981     2.981   176.822   182.784

 ********************************************************************************************


=====================================================================
*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
=====================================================================



 ============================================================
 SCAN POTENTIAL ENERGY SURFACE ALONG A RANGE OF NORMAL MODES  ***  with IR intensities  ***
 ============================================================

 RANGE OF FREQUENCIES: from  -1000.000 to      0.000


 ===================
 Vibration symmetry:  ***  A  ***
 ===================

 Total number of frequencies of this symmetry:   255
 Frequencies, cm^(-1):
      -9.272      12.164      17.532      24.275      28.804      35.366      37.963      51.243
       54.756      62.113      67.884      75.920      78.344      83.436      85.450      87.728
       90.238      90.789      98.067     104.942     111.919     127.931     131.431     156.350
      162.834     165.142     174.737     176.429     177.726     183.135     183.926     187.028
      200.523     202.108     212.200     213.146     229.239     236.280     240.363     244.522
      250.636     252.455     266.509     269.560     294.144     295.566     335.734     336.350
      352.159     356.198     358.092     377.389     377.478     396.424     397.305     405.828
      406.241     433.032     434.780     436.189     441.088     454.079     454.817     465.932
      469.226     472.639     479.965     484.853     485.110     492.533     497.495     500.454
      502.880     517.387     518.670     524.107     529.566     545.862     547.058     583.065
      587.638     592.113     595.341     615.797     616.858     622.916     623.708     632.113
      632.627     648.153     648.235     652.357     652.838     714.047     714.966     721.611
      721.653     722.879     723.479     756.607     756.999     766.652     766.994     801.633
      801.984     829.658     829.823     837.052     837.351     839.709     840.273     855.412
      856.441     887.974     888.314     899.315     900.494     902.121     914.873     916.016
      919.587     920.448     922.091     924.373     933.108     933.197     938.735     939.356
      951.676     953.401     984.087     985.084    1008.438    1008.756    1016.484    1016.523
     1018.039    1018.139    1025.027    1026.114    1051.438    1053.029    1064.486    1064.589
     1085.887    1086.234    1111.808    1112.025    1114.714    1114.958    1137.189    1137.601
     1158.058    1158.525    1164.414    1164.573    1179.158    1179.335    1184.403    1184.731
     1201.812    1201.990    1207.487    1207.649    1228.913    1229.875    1243.671    1244.441
     1250.563    1250.645    1259.774    1259.974    1275.032    1275.911    1288.779    1289.727
     1296.762    1297.608    1307.519    1308.347    1326.647    1326.733    1353.626    1354.333
     1372.320    1372.925    1387.546    1387.683    1417.895    1420.600    1422.288    1422.328
     1434.650    1434.930    1437.780    1439.094    1440.646    1441.207    1449.047    1449.278
     1461.822    1462.062    1465.478    1465.569    1476.775    1478.237    1526.509    1528.049
     1546.779    1548.561    1568.362    1569.514    1597.256    1598.410    1937.394    1943.277
     1999.027    2003.791    2940.214    2940.384    2942.171    2943.876    2947.683    2948.204
     2972.044    2974.063    2978.347    2979.207    2993.846    2994.668    2997.957    2998.108
     3003.804    3005.027    3005.820    3006.896    3029.659    3031.050    3032.828    3032.870
     3056.353    3057.271    3080.453    3081.885    3087.052    3088.463    3099.443    3099.986
     3102.456    3105.736    3109.274    3110.151    3113.132    3115.058    3680.730
 Number of frequencies in the requested range:     1
1
 ********************************************************************************************


 Scanning vibration frequency    1 A =       -9.272

 ================================================================================
 Summary of a frequency scan in the requested range:
 (One component per degenerate irreducible representations, degeneracy is not counted)
 --------------------------------------------------------------------------------
 Frequency, cm**(-1)      Dipol moment derivatives (a.u.)      IR Intensity
    Old      New              X         Y         Z             km/mole
 --------------------------------------------------------------------------------
 Vibration symmetry: A
    -9.272    16.025        -0.002    -0.003    -0.001            0.015
    12.164      not re-calculated (not in the required range)
    17.532      not re-calculated (not in the required range)
    24.275      not re-calculated (not in the required range)
```

28.804	not re-calculated (not in the required range)
35.366	not re-calculated (not in the required range)
37.963	not re-calculated (not in the required range)
51.243	not re-calculated (not in the required range)
54.756	not re-calculated (not in the required range)
62.113	not re-calculated (not in the required range)
67.884	not re-calculated (not in the required range)
75.920	not re-calculated (not in the required range)
78.344	not re-calculated (not in the required range)
83.436	not re-calculated (not in the required range)
85.450	not re-calculated (not in the required range)
87.728	not re-calculated (not in the required range)
90.238	not re-calculated (not in the required range)
90.789	not re-calculated (not in the required range)
98.067	not re-calculated (not in the required range)
104.942	not re-calculated (not in the required range)
111.919	not re-calculated (not in the required range)
127.931	not re-calculated (not in the required range)
131.431	not re-calculated (not in the required range)
156.350	not re-calculated (not in the required range)
162.834	not re-calculated (not in the required range)
165.142	not re-calculated (not in the required range)
174.737	not re-calculated (not in the required range)
176.429	not re-calculated (not in the required range)
177.726	not re-calculated (not in the required range)
183.135	not re-calculated (not in the required range)
183.926	not re-calculated (not in the required range)
187.028	not re-calculated (not in the required range)
200.523	not re-calculated (not in the required range)
202.108	not re-calculated (not in the required range)
212.200	not re-calculated (not in the required range)
213.146	not re-calculated (not in the required range)
229.239	not re-calculated (not in the required range)
236.280	not re-calculated (not in the required range)
240.363	not re-calculated (not in the required range)
244.522	not re-calculated (not in the required range)
250.636	not re-calculated (not in the required range)
252.455	not re-calculated (not in the required range)
266.509	not re-calculated (not in the required range)
269.560	not re-calculated (not in the required range)
294.144	not re-calculated (not in the required range)
295.566	not re-calculated (not in the required range)
335.734	not re-calculated (not in the required range)
336.350	not re-calculated (not in the required range)
352.159	not re-calculated (not in the required range)
356.198	not re-calculated (not in the required range)
358.092	not re-calculated (not in the required range)
377.389	not re-calculated (not in the required range)
377.478	not re-calculated (not in the required range)
396.424	not re-calculated (not in the required range)
397.305	not re-calculated (not in the required range)
405.828	not re-calculated (not in the required range)
406.241	not re-calculated (not in the required range)
433.032	not re-calculated (not in the required range)
434.780	not re-calculated (not in the required range)
436.189	not re-calculated (not in the required range)
441.088	not re-calculated (not in the required range)
454.079	not re-calculated (not in the required range)
454.817	not re-calculated (not in the required range)
465.932	not re-calculated (not in the required range)
469.226	not re-calculated (not in the required range)
472.639	not re-calculated (not in the required range)
479.965	not re-calculated (not in the required range)
484.853	not re-calculated (not in the required range)
485.110	not re-calculated (not in the required range)
492.533	not re-calculated (not in the required range)
497.495	not re-calculated (not in the required range)
500.454	not re-calculated (not in the required range)
502.880	not re-calculated (not in the required range)
517.387	not re-calculated (not in the required range)
518.670	not re-calculated (not in the required range)
524.107	not re-calculated (not in the required range)
529.566	not re-calculated (not in the required range)
545.862	not re-calculated (not in the required range)
547.058	not re-calculated (not in the required range)
583.065	not re-calculated (not in the required range)
587.638	not re-calculated (not in the required range)
592.113	not re-calculated (not in the required range)
595.341	not re-calculated (not in the required range)
615.797	not re-calculated (not in the required range)
616.858	not re-calculated (not in the required range)
622.916	not re-calculated (not in the required range)
623.708	not re-calculated (not in the required range)
632.113	not re-calculated (not in the required range)
632.627	not re-calculated (not in the required range)
648.153	not re-calculated (not in the required range)
648.235	not re-calculated (not in the required range)
652.357	not re-calculated (not in the required range)
652.838	not re-calculated (not in the required range)
714.047	not re-calculated (not in the required range)
714.966	not re-calculated (not in the required range)
721.611	not re-calculated (not in the required range)
721.653	not re-calculated (not in the required range)
722.879	not re-calculated (not in the required range)
723.479	not re-calculated (not in the required range)
756.607	not re-calculated (not in the required range)
756.999	not re-calculated (not in the required range)
766.652	not re-calculated (not in the required range)
766.994	not re-calculated (not in the required range)
801.633	not re-calculated (not in the required range)
801.984	not re-calculated (not in the required range)
829.658	not re-calculated (not in the required range)
829.823	not re-calculated (not in the required range)
837.052	not re-calculated (not in the required range)
837.351	not re-calculated (not in the required range)
839.709	not re-calculated (not in the required range)
840.273	not re-calculated (not in the required range)
855.412	not re-calculated (not in the required range)
856.441	not re-calculated (not in the required range)
887.974	not re-calculated (not in the required range)
888.314	not re-calculated (not in the required range)
899.315	not re-calculated (not in the required range)
900.494	not re-calculated (not in the required range)
902.121	not re-calculated (not in the required range)
914.873	not re-calculated (not in the required range)
916.016	not re-calculated (not in the required range)

919.587	not re-calculated (not in the required range)
920.448	not re-calculated (not in the required range)
922.091	not re-calculated (not in the required range)
924.373	not re-calculated (not in the required range)
933.108	not re-calculated (not in the required range)
933.197	not re-calculated (not in the required range)
938.735	not re-calculated (not in the required range)
939.356	not re-calculated (not in the required range)
951.676	not re-calculated (not in the required range)
953.401	not re-calculated (not in the required range)
984.087	not re-calculated (not in the required range)
985.084	not re-calculated (not in the required range)
1008.438	not re-calculated (not in the required range)
1008.756	not re-calculated (not in the required range)
1016.484	not re-calculated (not in the required range)
1016.523	not re-calculated (not in the required range)
1018.039	not re-calculated (not in the required range)
1018.139	not re-calculated (not in the required range)
1025.027	not re-calculated (not in the required range)
1026.114	not re-calculated (not in the required range)
1051.438	not re-calculated (not in the required range)
1053.029	not re-calculated (not in the required range)
1064.486	not re-calculated (not in the required range)
1064.589	not re-calculated (not in the required range)
1085.887	not re-calculated (not in the required range)
1086.234	not re-calculated (not in the required range)
1111.808	not re-calculated (not in the required range)
1112.025	not re-calculated (not in the required range)
1114.714	not re-calculated (not in the required range)
1114.958	not re-calculated (not in the required range)
1137.189	not re-calculated (not in the required range)
1137.601	not re-calculated (not in the required range)
1158.058	not re-calculated (not in the required range)
1158.525	not re-calculated (not in the required range)
1164.414	not re-calculated (not in the required range)
1164.573	not re-calculated (not in the required range)
1179.158	not re-calculated (not in the required range)
1179.335	not re-calculated (not in the required range)
1184.403	not re-calculated (not in the required range)
1184.731	not re-calculated (not in the required range)
1201.812	not re-calculated (not in the required range)
1201.990	not re-calculated (not in the required range)
1207.487	not re-calculated (not in the required range)
1207.649	not re-calculated (not in the required range)
1228.913	not re-calculated (not in the required range)
1229.875	not re-calculated (not in the required range)
1243.671	not re-calculated (not in the required range)
1244.441	not re-calculated (not in the required range)
1250.563	not re-calculated (not in the required range)
1250.645	not re-calculated (not in the required range)
1259.774	not re-calculated (not in the required range)
1259.974	not re-calculated (not in the required range)
1275.032	not re-calculated (not in the required range)
1275.911	not re-calculated (not in the required range)
1288.779	not re-calculated (not in the required range)
1289.727	not re-calculated (not in the required range)
1296.762	not re-calculated (not in the required range)
1297.608	not re-calculated (not in the required range)
1307.519	not re-calculated (not in the required range)
1308.347	not re-calculated (not in the required range)
1326.647	not re-calculated (not in the required range)
1326.733	not re-calculated (not in the required range)
1353.626	not re-calculated (not in the required range)
1354.333	not re-calculated (not in the required range)
1372.320	not re-calculated (not in the required range)
1372.925	not re-calculated (not in the required range)
1387.546	not re-calculated (not in the required range)
1387.683	not re-calculated (not in the required range)
1417.895	not re-calculated (not in the required range)
1420.600	not re-calculated (not in the required range)
1422.288	not re-calculated (not in the required range)
1422.328	not re-calculated (not in the required range)
1434.650	not re-calculated (not in the required range)
1434.930	not re-calculated (not in the required range)
1437.780	not re-calculated (not in the required range)
1439.094	not re-calculated (not in the required range)
1440.646	not re-calculated (not in the required range)
1441.207	not re-calculated (not in the required range)
1449.047	not re-calculated (not in the required range)
1449.278	not re-calculated (not in the required range)
1461.822	not re-calculated (not in the required range)
1462.062	not re-calculated (not in the required range)
1465.478	not re-calculated (not in the required range)
1465.569	not re-calculated (not in the required range)
1476.775	not re-calculated (not in the required range)
1478.237	not re-calculated (not in the required range)
1526.509	not re-calculated (not in the required range)
1528.049	not re-calculated (not in the required range)
1546.779	not re-calculated (not in the required range)
1548.561	not re-calculated (not in the required range)
1568.362	not re-calculated (not in the required range)
1569.514	not re-calculated (not in the required range)
1597.256	not re-calculated (not in the required range)
1598.410	not re-calculated (not in the required range)
1937.394	not re-calculated (not in the required range)
1943.277	not re-calculated (not in the required range)
1999.027	not re-calculated (not in the required range)
2003.791	not re-calculated (not in the required range)
2940.214	not re-calculated (not in the required range)
2940.384	not re-calculated (not in the required range)
2942.171	not re-calculated (not in the required range)
2943.876	not re-calculated (not in the required range)
2947.683	not re-calculated (not in the required range)
2948.204	not re-calculated (not in the required range)
2972.044	not re-calculated (not in the required range)
2974.063	not re-calculated (not in the required range)
2978.347	not re-calculated (not in the required range)
2979.207	not re-calculated (not in the required range)
2993.846	not re-calculated (not in the required range)
2994.668	not re-calculated (not in the required range)
2997.957	not re-calculated (not in the required range)
2998.108	not re-calculated (not in the required range)
3003.804	not re-calculated (not in the required range)
3005.027	not re-calculated (not in the required range)
3005.820	not re-calculated (not in the required range)
3006.896	not re-calculated (not in the required range)

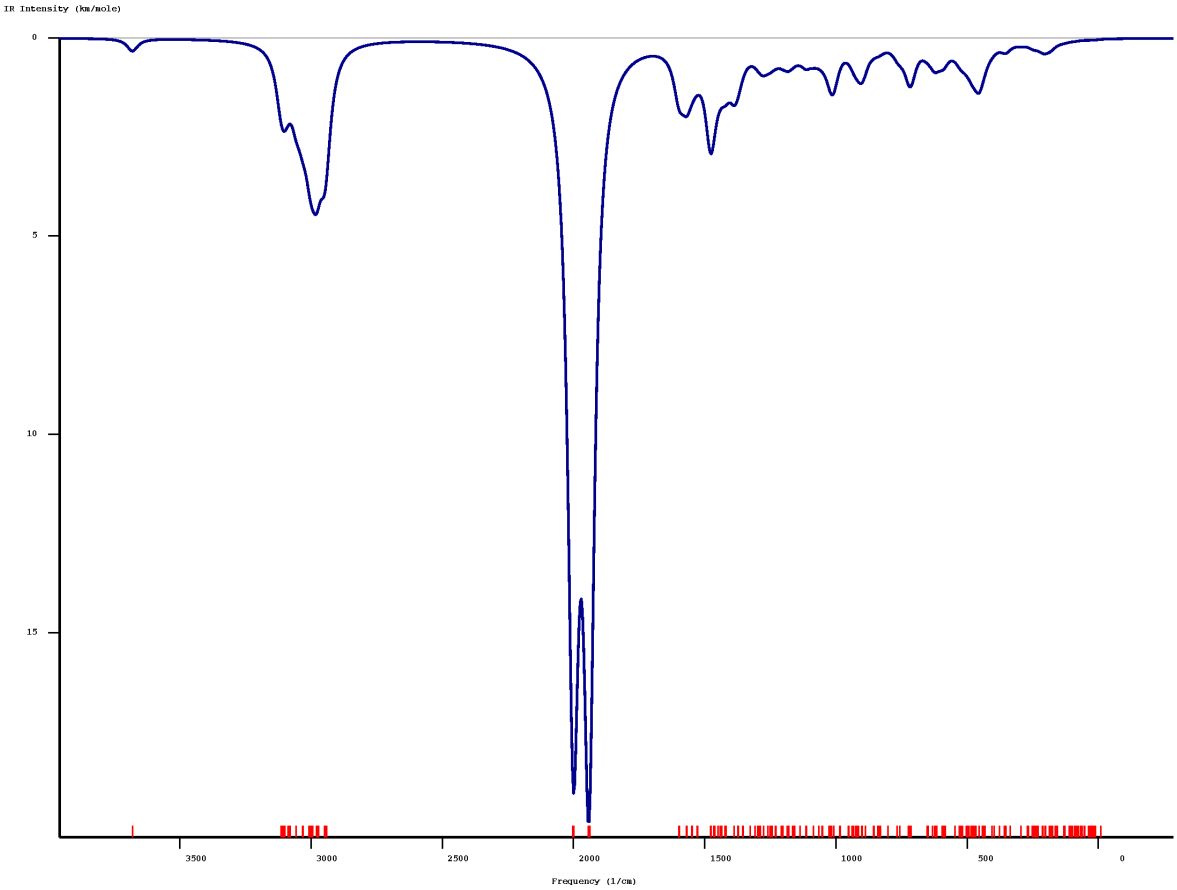
```
 3029.659      not re-calculated (not in the required range)
 3031.050      not re-calculated (not in the required range)
 3032.828      not re-calculated (not in the required range)
 3032.870      not re-calculated (not in the required range)
 3056.353      not re-calculated (not in the required range)
 3057.271      not re-calculated (not in the required range)
 3080.453      not re-calculated (not in the required range)
 3081.885      not re-calculated (not in the required range)
 3087.052      not re-calculated (not in the required range)
 3088.463      not re-calculated (not in the required range)
 3099.443      not re-calculated (not in the required range)
 3099.986      not re-calculated (not in the required range)
 3102.456      not re-calculated (not in the required range)
 3105.736      not re-calculated (not in the required range)
 3109.274      not re-calculated (not in the required range)
 3110.151      not re-calculated (not in the required range)
 3113.132      not re-calculated (not in the required range)
 3115.058      not re-calculated (not in the required range)
 3680.730      not re-calculated (not in the required range)
================================================================================


========================
No memory problems found
========================

Maximum number of active allocate calls:       10109

********************************************************************************

                            A D F   E X I T
NORMAL TERMINATION
```



b) 3b with the dispersion-corrected BP-D functional -TZP basis set with frozen core at Ru.

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2008.01   September 22, 2008  *
*  ------------------------------------                                     *
*                                          Build 200809251856               *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |               |                            *
*                              |     A D F     |                            *
*                              |               |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*************************  pentium_linux_ifc / hpmpi  ***********************

ADF 2008.01  RunTime: Oct02-2008 09:00:57

Temporary files are created in /tmp/kid_0.yMQnNA

terpRuOHax


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                        VWN
   Gradient Corrections:       Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                   Restricted
   Fragments:                  Restricted

OTHER ASPECTS
   Relativistic Corrections:   ---
   Core Treatment:             Frozen Orbital(s)

   Electric Field:             ---

   Hyperfine or Zeeman Interaction:   ---

   Empirical Dispersion Correction included with factor    1.05000

   Van der Waals Radii used in dispersion are scaled by    1.10000


Fragment File(s)
----------------
Ru:
        file : t21.Ru
        jobid: ADF 2008.01  RunTime: Oct02-2008 09:00:56
        title: Ruthenium (TZP, 3d frozen)
Cl:
        file : t21.Cl
        jobid: ADF 2008.01  RunTime: Oct02-2008 09:00:56
        title: Chlorine (TZP)
O:
        file : t21.O
        jobid: ADF 2008.01  RunTime: Oct02-2008 09:00:55
        title: Oxygen (TZP)
H:
        file : t21.H
        jobid: ADF 2008.01  RunTime: Oct02-2008 09:00:55
        title: Hydrogen (TZP)
N:
        file : t21.N
        jobid: ADF 2008.01  RunTime: Oct02-2008 09:00:55
        title: Nitrogen (TZP)
C:
        file : t21.C
        jobid: ADF 2008.01  RunTime: Oct02-2008 09:00:55
        title: Carbon (TZP)


                                  ******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ******************************************



Geometry CYCLE 73
==============

Energy gradients wrt nuclear displacements
==========================================

    Atom      Cartesian (a.u./angstrom)
                X         Y         Z
-------------------------------------
    1 Ru   -0.000270  0.000019  0.000057
```

```
     2 Ru    0.000473  0.000330 -0.000008
     3 Cl   -0.000081 -0.000050 -0.000011
     4 O     0.000238 -0.000095 -0.000275
     5 H    -0.000031  0.000105  0.000025
     6 O     0.000687 -0.000657 -0.000542
     7 O    -0.000385  0.000262  0.000014
     8 O     0.000188 -0.000092 -0.000060
     9 O     0.000000 -0.000018  0.000254
    10 N     0.000110 -0.000141  0.000081
    11 N    -0.000417  0.000014  0.000284
    12 C    -0.000093 -0.000030 -0.000133
    13 C     0.000045 -0.000014 -0.000305
    14 H    -0.000068  0.000025  0.000084
    15 C    -0.000121  0.000178  0.000033
    16 H    -0.000028  0.000024  0.000005
    17 C     0.000140 -0.000156 -0.000098
    18 H     0.000028  0.000093  0.000034
    19 C     0.000010 -0.000028  0.000007
    20 H     0.000077 -0.000029 -0.000021
    21 C    -0.000027  0.000015  0.000122
    22 C    -0.000047  0.000231 -0.000405
    23 C     0.000123 -0.000035  0.000249
    24 H     0.000058 -0.000027 -0.000007
    25 C     0.000040  0.000045 -0.000009
    26 C     0.000059 -0.000060  0.000052
    27 C    -0.000261  0.000142 -0.000048
    28 H    -0.000016 -0.000087  0.000004
    29 C     0.000041 -0.000023  0.000014
    30 H     0.000067 -0.000025 -0.000035
    31 H     0.000041 -0.000065 -0.000046
    32 C     0.000010 -0.000110  0.000001
    33 H    -0.000052  0.000013  0.000009
    34 C     0.000023 -0.000006  0.000048
    35 H     0.000019  0.000006 -0.000006
    36 H    -0.000018  0.000007 -0.000029
    37 C     0.000031 -0.000047 -0.000141
    38 H    -0.000046  0.000020  0.000031
    39 C    -0.000003  0.000027  0.000052
    40 C    -0.000042 -0.000184 -0.000011
    41 H    -0.000020  0.000022  0.000001
    42 H     0.000007  0.000028 -0.000005
    43 H    -0.000010  0.000004  0.000004
    44 C    -0.000050  0.000045 -0.000072
    45 H     0.000034 -0.000018 -0.000007
    46 H     0.000064  0.000035  0.000103
    47 H    -0.000032  0.000014  0.000018
    48 C     0.000272 -0.000007  0.000144
    49 C    -0.000055 -0.000065 -0.000049
    50 H    -0.000147 -0.000047  0.000164
    51 C    -0.000035  0.000075 -0.000049
    52 H     0.000059 -0.000028 -0.000007
    53 C     0.000038  0.000111  0.000073
    54 H    -0.000015  0.000050 -0.000115
    55 C    -0.000121 -0.000016 -0.000141
    56 H     0.000057  0.000013 -0.000056
    57 C     0.000025 -0.000046  0.000106
    58 C     0.000009 -0.000021 -0.000114
    59 C    -0.000053  0.000093 -0.000032
    60 H    -0.000024 -0.000003  0.000028
    61 C    -0.000061  0.000066 -0.000066
    62 C    -0.000150  0.000034  0.000070
    63 C     0.000256 -0.000057 -0.000115
    64 H    -0.000006 -0.000100  0.000152
    65 C    -0.000135 -0.000125 -0.000016
    66 H     0.000076  0.000264 -0.000024
    67 H    -0.000082 -0.000024 -0.000025
    68 C     0.000036  0.000000  0.000134
    69 H     0.000135 -0.000017 -0.000022
    70 C     0.000003 -0.000023 -0.000120
    71 H     0.000224 -0.000066  0.000121
    72 H    -0.000021  0.000186  0.000043
    73 C     0.000005 -0.000028  0.000010
    74 H     0.000012 -0.000056  0.000052
    75 C    -0.000100 -0.000111 -0.000038
    76 C     0.000088  0.000011 -0.000150
    77 H    -0.000107 -0.000237  0.000100
    78 H     0.000214  0.000109  0.000165
    79 H     0.000042 -0.000029  0.000000
    80 C     0.000066 -0.000112 -0.000005
    81 H     0.000025 -0.000006  0.000005
    82 H    -0.000168  0.000099 -0.000090
    83 H    -0.000034 -0.000093  0.000016
    84 C    -0.000777  0.000818  0.000967
    85 C     0.000526 -0.000216  0.000060
    86 C    -0.000479 -0.000029  0.000220
    87 C    -0.000095 -0.000071 -0.000709
 ----------------------------------------

---------------------------------------
Geometry Convergence after Step  73
---------------------------------------
current energy                                -20.65508147 Hartree
abs of energy change              0.00000253     0.00100000    T
constrained gradient max          0.00096743     0.00100000    T
constrained gradient rms          0.00017023     0.00066667    T
gradient max                      0.00096743
gradient rms                      0.00017023
cart. step max                    0.00943708     0.01000000    T
cart. step rms                    0.00298585     0.00666667    T

 Number of elements of the density matrix on this node (used, total):    103723    832695


 ====================================================
 Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
 ====================================================

 General Accuracy Parameter :                          4.50

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
```

```
    Nr. of used Symmetry Operators                    1

    Points in the Atomic Spheres                  50352
    Points in the Atomic Polyhedra               518533
    Points in the Outer Region                    40485
    ------------------------------------------------------
    Total                                        609370

    Sum of Weights                               181366.739456

 Total nr. of points:     609370
 Nr. of blocks:             4761
 Block length:               128
 Nr. of dummy points:         38


 Test of Precision of the Numerical Integration Grid
 ===================================================

 Integral of the Total Core Density:                55.99998079030989
 Relative Error:                                    -3.430E-07



 ============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

                                        hartree             eV         kcal/mol           kJ/mol
                                    ---------------     ----------     ----------     ----------

Pauli Repulsion
  Kinetic (Delta T^0):            222.271856062742586     6048.3249      139477.71      583574.68
  Delta V^Pauli Coulomb:         -111.946494475783794    -3046.2191      -70247.49     -293915.48
  Delta V^Pauli LDA-XC:           -28.591633922268176     -778.0179      -17941.52      -75067.32
  Delta V^Pauli GGA-Exchange:       1.684172307550909       45.8287        1056.83        4421.79
  Delta V^Pauli GGA-Correlation:   -0.475508393942048      -12.9392        -298.39       -1248.45
                                    ---------------     ----------     ----------     ----------
  Total Pauli Repulsion:           82.942391578299478     2256.9773       52047.14      217765.22
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  82.942391578299478     2256.9773       52047.14      217765.22
  Electrostatic Interaction:       -17.530146091982104     -477.0195      -11000.33      -46025.39
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                    ---------------     ----------     ----------     ----------
  Total Steric Interaction:         65.412245486317374     1779.9578       41046.81      171739.83
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -85.862735657089331    -2336.4439      -53879.69     -225432.58
                                    ---------------     ----------     ----------     ----------
  Total Orbital Interactions:      -85.876664828438763    -2336.8229      -53888.43     -225469.15

Alternative Decomposition Orb.Int.
  Kinetic:                        -202.912177491442890    -5521.5213     -127329.33     -532745.85
  Coulomb:                         108.043900495647335     2940.0241       67798.58      283669.22
  XC:                                8.991612167356756      244.6742        5642.32       23607.47
                                    ---------------     ----------     ----------     ----------
  Total Orbital Interactions:      -85.876664828438805    -2336.8229      -53888.43     -225469.15

  Residu (E=Steric+OrbInt+Res):     -0.000009063547154       -0.0002          -0.01          -0.02
  Dispersion Energy:                -0.190652961839779       -5.1879         -119.64         -500.56

Total Bonding Energy:               -20.655081367508320      -562.0534       -12961.26       -54229.91


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
=======================================================================================

  Electrostatic Energy:             -17.530146091982104      -477.0195       -11000.33       -46025.39
  Kinetic Energy:                    19.359678571299696       526.8037        12148.38        50828.83
  Coulomb (Steric+OrbInt) Energy:    -3.902603043683612      -106.1952        -2448.92       -10246.28
  XC Energy:                        -18.391357841302558      -500.4543       -11540.75       -48286.50
  Dispersion Energy:                 -0.190652961839779        -5.1879         -119.64         -500.56
                                    ---------------     ----------     ----------     ----------
  Total Bonding Energy:             -20.655081367508355      -562.0534       -12961.26       -54229.91


Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree):  -0.0062875884
2. Electrostatic (Fit correction):   0.0000000000


 ========================================
 F R A G M E N T   E N E R G Y   T E R M S  ***  (summed over all fragments)  ***
 ========================================
```

The energy terms below are (parts of) the Total Energy of the fragments from which the molecule is built.

Exchange and Correlation				
Exchange LDA:	-500.3051234457269 06	-13613.9951	-313946.24	-1313550.92
Exchange GGA:	-45.517734575151451	-1238.6006	-28562.81	-119506.80
Correlation LDA:	-29.628750107805942	-806.2393	-18592.32	-77790.27
Correlation GGA:	14.279219285336403	388.5573	8960.35	37490.08
Total XC:	-561.172388843347903	-15270.2777	-352141.03	-1473357.90

B O N D - O R D E R A N A L Y S I S

			DIST. [A]	BOND-ORDERS (THRESHOLD = 0.050)				
				MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
Ru	1 - Cl	3	2.5873	0.4256	0.2605	0.3407	0.5776	0.3872
Ru	1 - O	4	2.1330	0.3393	0.3182	0.4034	0.7795	0.4441
Ru	1 - O	6	3.0535	0.2047	0.2465	0.2885	0.4121	0.2843
Ru	1 - O	7	3.0515	0.2149	0.2458	0.2876	0.4160	0.2839
Ru	1 - N	10	2.1676	0.2746	0.3295	0.3723	0.4954	0.3626
Ru	1 - C	12	2.0701	0.6171	0.7406	0.8129	0.8612	0.7780
Ru	1 - C	84	1.8911	1.0880	1.0775	1.1804	1.0216	1.0822
Ru	1 - C	85	1.8905	1.0451	1.0715	1.1741	1.0170	1.0766
Ru	2 - Cl	3	2.5950	0.4195	0.2553	0.3334	0.5706	0.3791
Ru	2 - O	4	2.1295	0.3582	0.3257	0.4122	0.7861	0.4540
Ru	2 - O	8	3.0478	0.2200	0.2543	0.2972	0.4285	0.2937
Ru	2 - O	9	3.0536	0.2042	0.2448	0.2860	0.4089	0.2818
Ru	2 - N	11	2.1734	0.2679	0.3243	0.3656	0.4831	0.3556
Ru	2 - C	48	2.0705	0.6293	0.7422	0.8130	0.8591	0.7779
Ru	2 - C	86	1.8855	1.0864	1.0911	1.1924	1.0472	1.0965
Ru	2 - C	87	1.8914	1.0836	1.0708	1.1711	1.0116	1.0735
Cl	3 - C	12	4.6281	0.0535	0.1067	0.1303	0.0530	0.1580
Cl	3 - C	48	4.6400	0.0530	0.1054	0.1287	0.0535	0.1560
O	4 - H	5	0.9755	1.1174	0.8494	1.0713	1.1599	1.0580
O	4 - C	84	4.0230	0.0559	0.1260	0.1486	0.2780	0.1693
O	4 - C	87	4.0125	0.0584	0.1277	0.1506	0.2816	0.1716
O	6 - C	84	1.1623	2.0462	2.1940	2.3734	2.3838	2.4165
O	7 - C	85	1.1637	2.0119	2.1761	2.3537	2.3639	2.4006
O	8 - C	86	1.1655	1.9987	2.1589	2.3345	2.3422	2.3900
O	9 - C	87	1.1621	2.0473	2.1963	2.3758	2.3864	2.4177
N	10 - C	22	1.3645	1.2749	1.3086	1.3757	1.3927	1.4001
N	10 - C	25	2.7860	0.0360	0.0891	0.0936	0.1035	0.0962
N	10 - C	27	1.3477	1.3541	1.3799	1.4577	1.4384	1.5109
N	10 - C	85	4.0472	0.0411	0.1146	0.1193	0.1644	0.1202
N	11 - C	58	1.3626	1.2785	1.3129	1.3795	1.3985	1.3999
N	11 - C	61	2.7853	0.0361	0.0906	0.0952	0.1046	0.0977
N	11 - C	63	1.3469	1.3556	1.3843	1.4616	1.4434	1.5129
N	11 - C	86	4.0473	0.0418	0.1143	0.1189	0.1578	0.1199
C	12 - C	13	1.4027	1.4107	1.4168	1.4525	1.4208	1.5071
C	12 - C	17	2.8370	0.0427	0.0994	0.1021	0.0767	0.1061
C	12 - C	21	1.4209	1.3491	1.3206	1.3508	1.3424	1.3794
C	13 - H	14	1.0900	1.0257	0.9216	0.9603	0.9727	0.9024
C	13 - C	15	1.4003	1.3951	1.4321	1.4876	1.4494	1.5479
C	13 - C	19	2.7949	0.0611	0.1095	0.1138	0.0839	0.1185
C	15 - H	16	1.0920	1.0311	0.9277	0.9692	0.9801	0.9076
C	15 - C	17	1.4019	1.3703	1.4076	1.4646	1.4240	1.5259
C	15 - C	21	2.7958	0.0532	0.0939	0.0973	0.0908	0.0997
C	17 - H	18	1.0908	1.0322	0.9289	0.9725	0.9861	0.9140
C	17 - C	19	1.3931	1.4127	1.4631	1.5230	1.4805	1.5877
C	19 - H	20	1.0908	1.0267	0.9268	0.9634	0.9749	0.9108
C	19 - C	21	1.4093	1.3392	1.3454	1.3950	1.3835	1.4298
C	21 - C	22	1.4630	1.1681	1.0954	1.1291	1.1316	1.1170
C	22 - C	23	1.4038	1.3596	1.3479	1.3949	1.4103	1.4060
C	22 - C	26	2.7796	0.0517	0.0841	0.0864	0.0868	0.0851
C	23 - H	24	1.0894	1.0131	0.9207	0.9604	0.9751	0.9055
C	23 - C	25	1.3894	1.4254	1.4418	1.4908	1.4923	1.5175
C	23 - C	27	2.7402	0.0555	0.0944	0.0981	0.0915	0.1008
C	25 - C	26	1.4130	1.3476	1.3083	1.3433	1.3432	1.3368
C	25 - C	29	1.5194	0.9394	1.0164	1.0519	1.0527	1.0875
C	26 - C	27	1.3887	1.4266	1.4061	1.4522	1.4518	1.4586
C	26 - C	37	1.5036	0.9701	1.0156	1.0437	1.0404	1.0627
C	27 - H	28	1.0903	1.0180	0.8969	0.9357	0.9262	0.8556
C	29 - H	30	1.1022	1.0145	0.9156	0.9579	0.9876	0.9144
C	29 - H	31	1.1026	1.0094	0.9137	0.9546	0.9838	0.9126
C	29 - C	32	1.5401	0.9555	1.0076	1.0423	0.9826	1.1005
C	32 - H	33	1.1000	1.0530	0.9248	0.9536	0.9615	0.9008
C	32 - C	34	1.5580	0.9370	0.9905	1.0210	0.9649	1.0763
C	32 - C	39	1.5727	0.9056	0.9457	0.9629	0.9686	0.9720
C	34 - H	35	1.0986	1.0210	0.9342	0.9709	0.9965	0.9314
C	34 - H	36	1.0957	1.0133	0.9330	0.9709	0.9968	0.9302
C	34 - C	37	1.5673	0.9264	0.9714	1.0027	0.9443	1.0579
C	37 - H	38	1.0980	1.0528	0.9224	0.9534	0.9622	0.8982
C	37 - C	39	1.5834	0.8935	0.9263	0.9445	0.9505	0.9543
C	39 - C	40	1.5265	0.9747	1.0168	1.0525	1.0506	1.1089
C	39 - C	44	1.5325	0.9969	1.0084	1.0432	1.0420	1.0983
C	40 - H	41	1.1032	0.9782	0.9441	0.9916	1.0288	0.9744
C	40 - H	42	1.0998	0.9579	0.9430	0.9893	1.0275	0.9709
C	40 - H	43	1.1023	0.9782	0.9425	0.9915	1.0312	0.9708
C	44 - H	45	1.1017	0.9793	0.9451	0.9930	1.0311	0.9732
C	44 - H	46	1.0989	0.9531	0.9476	0.9936	1.0293	0.9773
C	44 - H	47	1.1022	0.9773	0.9448	0.9921	1.0296	0.9734
C	48 - C	49	1.4024	1.4138	1.4230	1.4586	1.4260	1.5142
C	48 - C	53	2.8347	0.0430	0.1006	0.1033	0.0786	0.1073
C	48 - C	57	1.4197	1.3486	1.3197	1.3489	1.3427	1.3747
C	49 - H	50	1.0905	1.0254	0.9225	0.9609	0.9742	0.9052
C	49 - C	51	1.4014	1.3898	1.4262	1.4818	1.4409	1.5439
C	49 - C	55	2.7931	0.0601	0.1083	0.1126	0.0817	0.1173
C	51 - H	52	1.0919	1.0309	0.9282	0.9695	0.9808	0.9088
C	51 - C	53	1.4011	1.3772	1.4136	1.4709	1.4294	1.5331
C	51 - C	57	2.7987	0.0554	0.0960	0.0995	0.0949	0.1018
C	53 - H	54	1.0909	1.0321	0.9292	0.9726	0.9862	0.9146
C	53 - C	55	1.3941	1.4052	1.4571	1.5167	1.4748	1.5807
C	55 - H	56	1.0908	1.0271	0.9267	0.9632	0.9744	0.9103
C	55 - C	57	1.4081	1.3475	1.3522	1.4014	1.3924	1.4337
C	57 - C	58	1.4632	1.1597	1.0921	1.1254	1.1262	1.1098
C	58 - C	59	1.4037	1.3611	1.3480	1.3949	1.4119	1.4032

C	58 - C	62	2.7791	0.0534	0.0852	0.0876	0.0882	0.0861
C	59 - H	60	1.0894	1.0135	0.9210	0.9604	0.9746	0.9055
C	59 - C	61	1.3891	1.4245	1.4423	1.4912	1.4927	1.5173
C	59 - C	63	2.7390	0.0560	0.0954	0.0992	0.0926	0.1019
C	61 - C	62	1.4128	1.3495	1.3099	1.3451	1.3450	1.3388
C	61 - C	65	1.5199	0.9396	1.0161	1.0516	1.0523	1.0872
C	62 - C	63	1.3895	1.4261	1.4051	1.4512	1.4508	1.4580
C	62 - C	73	1.5044	0.9707	1.0153	1.0434	1.0398	1.0625
C	63 - H	64	1.0904	1.0176	0.8979	0.9366	0.9274	0.8573
C	65 - H	66	1.1024	1.0150	0.9160	0.9581	0.9877	0.9147
C	65 - H	67	1.1028	1.0097	0.9141	0.9548	0.9838	0.9132
C	65 - C	68	1.5403	0.9560	1.0077	1.0422	0.9825	1.1004
C	68 - H	69	1.1002	1.0531	0.9250	0.9536	0.9615	0.9012
C	68 - C	70	1.5579	0.9353	0.9904	1.0207	0.9647	1.0759
C	68 - C	75	1.5727	0.9065	0.9457	0.9628	0.9685	0.9719
C	70 - H	71	1.0959	1.0134	0.9332	0.9708	0.9966	0.9306
C	70 - H	72	1.0987	1.0212	0.9342	0.9708	0.9964	0.9312
C	70 - C	73	1.5677	0.9261	0.9713	1.0024	0.9442	1.0575
C	73 - H	74	1.0981	1.0531	0.9227	0.9533	0.9621	0.8986
C	73 - C	75	1.5834	0.8926	0.9267	0.9448	0.9507	0.9546
C	75 - C	76	1.5329	0.9966	1.0084	1.0431	1.0417	1.0982
C	75 - C	80	1.5266	0.9747	1.0168	1.0524	1.0504	1.1088
C	76 - H	77	1.1020	0.9794	0.9454	0.9930	1.0309	0.9735
C	76 - H	78	1.0993	0.9533	0.9477	0.9935	1.0292	0.9773
C	76 - H	79	1.1023	0.9774	0.9450	0.9921	1.0294	0.9737
C	80 - H	81	1.1033	0.9783	0.9443	0.9916	1.0286	0.9748
C	80 - H	82	1.1000	0.9584	0.9428	0.9892	1.0276	0.9705
C	80 - H	83	1.1024	0.9783	0.9428	0.9916	1.0310	0.9712
C	84 - C	85	2.6589	0.0695	0.0715	0.0720	0.0329	0.0681
C	86 - C	87	2.6572	0.0706	0.0733	0.0737	0.0381	0.0699
Sum :				110.7739	111.5437	117.3543	117.3543	117.3543

Atomic summation :

Ru	1	4.3228	4.5018	5.0961	5.1624	4.9202
Ru	2	4.3828	4.5172	5.1034	5.1696	4.9304
Cl	3	1.0978	0.9909	1.2607	1.3534	1.4692
O	4	1.9871	1.9636	2.4479	2.6400	2.6050
H	5	1.1424	0.8824	1.1087	1.0523	1.0884
O	6	2.2883	2.5115	2.7436	2.7473	2.7900
O	7	2.2830	2.5084	2.7390	2.7457	2.7894
O	8	2.2766	2.5024	2.7325	2.7428	2.7920
O	9	2.2889	2.5124	2.7438	2.7471	2.7892
N	10	3.1845	3.4780	3.6924	3.7021	3.7750
N	11	3.1951	3.4836	3.6955	3.7023	3.7723
C	12	3.7474	3.9701	4.1458	4.1038	4.2325
C	13	4.0308	3.9878	4.1293	4.1207	4.1907
H	14	1.0687	0.9837	1.0259	1.0357	0.9629
C	15	3.9765	3.9858	4.1504	4.1366	4.2137
H	16	1.0395	0.9800	1.0238	1.0349	0.9579
C	17	3.9612	3.9859	4.1539	4.1460	4.2248
H	18	1.0425	0.9808	1.0268	1.0368	0.9639
C	19	3.9573	3.9926	4.1510	4.1453	4.2050
H	20	1.0352	0.9873	1.0263	1.0344	0.9690
C	21	4.0472	4.0187	4.1449	4.1327	4.1964
C	22	4.0910	4.0057	4.1637	4.1521	4.1822
C	23	3.9484	3.9885	4.1363	4.1373	4.1265
H	24	1.0485	0.9837	1.0262	1.0352	0.9660
C	25	3.8925	4.0115	4.1414	4.1200	4.1945
C	26	3.8938	4.0189	4.1392	4.1331	4.1542
C	27	4.0016	3.9631	4.1412	4.1107	4.1278
H	28	1.0838	0.9796	1.0266	1.0403	0.9436
C	29	3.9094	3.9610	4.1191	4.1396	4.1306
H	30	1.0857	0.9797	1.0246	1.0273	0.9750
H	31	1.0872	0.9809	1.0246	1.0266	0.9773
C	32	3.7973	3.9910	4.1062	4.0788	4.1733
H	33	1.0918	0.9877	1.0187	1.0268	0.9613
C	34	3.8636	3.9572	4.0986	4.1148	4.1324
H	35	1.0768	0.9843	1.0230	1.0242	0.9790
H	36	1.1052	0.9820	1.0219	1.0235	0.9771
C	37	3.7950	3.9897	4.1039	4.0898	4.1318
H	38	1.0939	0.9868	1.0202	1.0291	0.9599
C	39	3.8503	4.0184	4.1274	4.0610	4.2525
C	40	3.8777	3.9270	4.1094	4.1924	4.1139
H	41	1.0791	0.9821	1.0311	1.0141	1.0107
H	42	1.0631	0.9823	1.0303	1.0134	1.0090
H	43	1.0814	0.9798	1.0302	1.0144	1.0062
C	44	3.8870	3.9280	4.1078	4.1889	4.1123
H	45	1.0772	0.9809	1.0301	1.0144	1.0071
H	46	1.0782	0.9834	1.0309	1.0135	1.0120
H	47	1.0766	0.9816	1.0303	1.0142	1.0084
C	48	3.7556	3.9755	4.1476	4.1053	4.2314
C	49	4.0287	3.9885	4.1296	4.1229	4.1962
H	50	1.0681	0.9847	1.0265	1.0354	0.9658
C	51	3.9749	3.9865	4.1513	4.1377	4.2183
H	52	1.0403	0.9804	1.0241	1.0348	0.9591
C	53	3.9595	3.9862	4.1538	4.1462	4.2255
H	54	1.0423	0.9811	1.0269	1.0367	0.9645
C	55	3.9627	3.9927	4.1503	4.1442	4.2007
H	56	1.0346	0.9872	1.0261	1.0343	0.9685
C	57	4.0514	4.0204	4.1446	4.1319	4.1874
C	58	4.0920	4.0056	4.1622	4.1538	4.1706
C	59	3.9532	3.9892	4.1363	4.1363	4.1233
H	60	1.0478	0.9842	1.0263	1.0352	0.9662
C	61	3.8883	4.0118	4.1413	4.1204	4.1941
C	62	3.8950	4.0193	4.1397	4.1335	4.1554
C	63	3.9938	3.9641	4.1411	4.1120	4.1270
H	64	1.0819	0.9801	1.0268	1.0402	0.9445
C	65	3.9107	3.9613	4.1188	4.1395	4.1309
H	66	1.0854	0.9799	1.0246	1.0272	0.9752
H	67	1.0864	0.9812	1.0246	1.0265	0.9778
C	68	3.7957	3.9913	4.1059	4.0787	4.1734
H	69	1.0913	0.9880	1.0188	1.0268	0.9618
C	70	3.8602	3.9576	4.0983	4.1144	4.1321
H	71	1.1042	0.9823	1.0218	1.0233	0.9775
H	72	1.0784	0.9843	1.0229	1.0242	0.9789
C	73	3.7970	3.9901	4.1035	4.0895	4.1319
H	74	1.0929	0.9871	1.0201	1.0289	0.9603
C	75	3.8487	4.0185	4.1271	4.0608	4.2522
C	76	3.8865	3.9283	4.1074	4.1887	4.1125
H	77	1.0767	0.9811	1.0300	1.0142	1.0074
H	78	1.0780	0.9835	1.0308	1.0134	1.0120
H	79	1.0764	0.9817	1.0302	1.0141	1.0086
C	80	3.8782	3.9272	4.1093	4.1923	4.1141
H	81	1.0787	0.9824	1.0311	1.0140	1.0111

H	82	1.0634	0.9821	1.0301	1.0133	1.0085
H	83	1.0811	0.9800	1.0303	1.0143	1.0066
C	84	3.3619	3.6172	3.9320	3.8651	3.8976
C	85	3.3345	3.5988	3.8977	3.8426	3.8520
C	86	3.3629	3.6094	3.9052	3.8446	3.8706
C	87	3.3566	3.6168	3.9290	3.8634	3.8942

(*) Values from:
- Mayer bond-order analysis
- Gophinatan-Jug bond order analysis
- Nalewajski-Mrozek bond order analysis
  a) N-M (1) - bond-orders calculated from two-electron valence indices
  based on partitioning of tr(Delta_P^2] (3-index set)
  b) N-M (2) - bond-orders calculated from two-electron valence indices
  based on partitioning of tr(Delta_P^2] (4-index set)
  c) N-M (3) - bond-orders calculated from valence indices
  based on partitioning of tr(P*Delta_P]
  A. Michalak, R.L. DeKock, T. Ziegler, J. Comp. Chem., subm.
  and original articles by Nalewajski et al.)

c) ax-ax-3c

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M O D E L   P A R A M E T E R S
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DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---

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Geometry Convergence Tests
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Energy  old :        -13.26215010
        new :        -13.26215374

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy      -0.00000365     0.00100000    YES         0.28152177
gradient max           0.00082616     0.00100000    YES         0.68237568
gradient rms           0.00018868     0.00066667    YES         0.73645129
cart. step max         0.00276520     0.01000000    YES         1.08786772
cart. step rms         0.00082603     0.00666667    YES         1.04888315

prediction dE :       -0.00000416


*************************************************************************************************
                           Geometry CONVERGED
*************************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************


Coordinates (Cartesian)
=======================

    Atom                   bohr                                  angstrom                Geometric Variables
                 X           Y           Z             X           Y           Z       (0:frozen, *:LT par.)
-------------------------------------------------------------------------------------------------------------
    1 C       6.532380   -0.561811   -5.702084       3.456786   -0.297298   -3.017413      1       2       3
    2 H       2.438597   -0.149051   -5.701922       1.290450   -0.078874   -3.017327      4       5       6
    3 O       0.269403    7.637673   -4.809227       0.142562    4.041682   -2.544933      7       8       9
    4 C       4.231155    0.350128   -4.817150       2.239031    0.185280   -2.549126     10      11      12
    5 C       8.733566    0.132733   -4.415680       4.621604    0.070239   -2.336677     13      14      15
    6 Cl     -2.139865   -0.033203   -3.660535      -1.132368   -0.017571   -1.937072     16      17      18
    7 C       0.392323    5.958395   -3.400200       0.207608    3.153047   -1.799308     19      20      21
    8 N       4.060139    1.872997   -2.789244       2.148533    0.991148   -1.476004     22      23      24
    9 O       3.209952   -5.871529   -2.560260       1.698633   -3.107079   -1.354831     25      26      27
   10 C       8.557969    1.718086   -2.328391       4.528682    0.909172   -1.232132     28      29      30
   11 O      -4.488389   -7.639113   -1.904270      -2.375153   -4.042445   -1.007697     31      32      33
   12 H      10.253369    2.281055   -1.310112       5.425849    1.207082   -0.693281     34      35      36
   13 C       1.544556   -4.780231   -1.631801       0.817344   -2.529589   -0.863512     37      38      39
   14 C       6.185721    2.601927   -1.525641       3.273342    1.376880   -0.807335     40      41      42
   15 C      -3.271565   -5.957480   -1.187053      -1.731238   -3.152563   -0.628161     43      44      45
   16 Ru      0.560138    3.222467   -1.107781       0.296412    1.705256   -0.586212     46      47      48
   17 H      -6.124696    0.180615   -0.640281      -3.241050    0.095577   -0.338822     49      50      51
   18 Ru     -1.258455   -3.241123   -0.033181      -0.665946   -1.715128   -0.017558     52      53      54
   19 C       5.760682    4.334752    0.589369       3.048422    2.293852    0.311881     55      56      57
   20 C      -2.184280    4.634214    0.680284      -1.155871    2.452320    0.359991     58      59      60
   21 C       3.225596    5.063545    1.089629       1.706912    2.679512    0.576607     61      62      63
   22 C      -6.244585   -0.313233    1.356681      -3.304492   -0.165756    0.717925     64      65      66
   23 O       0.990243   -0.087895    1.175450       0.524014   -0.046512    0.622021     67      68      69
   24 H       9.699487    4.731225    1.684530       5.132747    2.503656    0.891415     70      71      72
   25 H      -9.668942    1.740466    2.118520      -5.116584    0.921015    1.121072     73      74      75
   26 C       7.755973    5.303717    2.062306       4.104284    2.806606    1.091325     76      77      78
   27 O      -3.788411    5.655394    1.786940      -2.004741    2.992706    0.945608     79      80      81
   28 N      -4.360510   -1.783698    2.228482      -2.307482   -0.943893    1.179262     82      83      84
   29 H       2.670395   -7.306004    2.561778       1.413112   -3.866171    1.355634     85      86      87
   30 C      -8.187879    0.546321    2.902674      -4.332839    0.289101    1.536029     88      89      90
   31 C       2.795764    6.799915    3.046593       1.479454    3.598360    1.612187     91      92      93
   32 H       0.882448    7.434693    3.471357       0.466972    3.934270    1.836963     94      95      96
   33 C      -0.589826   -4.976361    3.409926      -0.312122   -2.633377    1.804455     97      98      99
   34 C       7.280537    7.006621    4.011152       3.852694    3.707744    2.122610    100     101     102
   35 C       1.370876   -6.654216    4.020882       0.725436   -3.521259    2.127759    103     104     105
   36 C       4.790911    7.760307    4.494717       2.535241    4.106578    2.378502    106     107     108
   37 H       8.835848    7.749882    5.140239       4.675729    4.101061    2.720097    109     110     111
   38 C      -4.322081   -2.517261    4.702723      -2.287147   -1.332077    2.488574    112     113     114
   39 C      -8.162724   -0.146060    5.453009      -4.319527   -0.077291    2.885608    115     116     117
   40 H       4.396346    9.107323    6.007049       2.326446    4.819388    3.178794    118     119     120
   41 C      -2.239951   -4.206483    5.386042      -1.185331   -2.225975    2.850171    121     122     123
   42 C      -6.227910   -1.679271    6.351790      -3.295668   -0.888632    3.361223    124     125     126
   43 C       1.717543   -7.521074    6.494358       0.908885   -3.979981    3.436666    127     128     129
   44 H       3.265526   -8.820052    6.910465       1.728042   -4.667371    3.656860    130     131     132
   45 H      -9.648134    0.499440    6.728622      -5.105572    0.264293    3.560633    133     134     135
   46 C      -1.871387   -5.081582    7.875688      -0.990295   -2.689057    4.167635    136     137     138
   47 H      -6.191308   -2.251889    8.326153      -3.276299   -1.191648    4.406010    139     140     141
   48 C       0.098825   -6.730997    8.434325       0.052296   -3.561890    4.463252    142     143     144
   49 H      -3.128951   -4.470392    9.389800      -1.655770   -2.365630    4.968868    145     146     147
   50 H       0.374847   -7.400278   10.363572       0.198360   -3.916059    5.484166    148     149     150
   51 H      10.573433   -0.558019   -5.038838       5.595220   -0.295291   -2.666438    151     152     153
```

```
   52 H       6.581047   -1.802224   -7.343415       3.482540   -0.953696   -3.885968    154     155     156
   53 H       0.824839    0.217767    2.983280       0.436486    0.115238    1.578684    157     158     159
 ------------------------------------------------------------------------------------------------------------

 Number of elements of the density matrix on this node (used, total):    199365    396495


 ====================================================
 Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
 ====================================================

 General Accuracy Parameter :                          4.50

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
    Nr. of used Symmetry Operators                     1

    Points in the Atomic Spheres                   33332
    Points in the Atomic Polyhedra                344096
    Points in the Outer Region                     29659
    ------------------------------------------------------
    Total                                         407087

    Sum of Weights                                160406.077012

 Total nr. of points:     407087
 Nr. of blocks:             3181
 Block length:               128
 Nr. of dummy points:         81


 Test of Precision of the Numerical Integration Grid
 ====================================================

 Integral of the Total Core Density:                  55.99998029517992
 Relative Error:                                      -3.519E-07

 ============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

                                          hartree              eV          kcal/mol          kJ/mol
                                  ---------------------  -----------  ----------  -----------

Pauli Repulsion
  Kinetic (Delta T^0):             154.331086302806511     4199.5625     96844.23     405196.21
  Delta V^Pauli Coulomb:          -80.179197333956438    -2181.7870    -50313.21    -210510.45
  Delta V^Pauli LDA-XC:           -19.109076423000307     -519.9844    -11991.13     -50170.87
  Delta V^Pauli GGA-Exchange:       1.113919489302958       30.3113        699.00       2924.60
  Delta V^Pauli GGA-Correlation:   -0.311817917689307       -8.4850       -195.67       -818.68
                                  ---------------------  -----------  ----------  -----------
  Total Pauli Repulsion:           55.844914117463418     1519.6174     35043.22     146620.80
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 55.844914117463418     1519.6174     35043.22     146620.80
  Electrostatic Interaction:      -11.887072527966744     -323.4637     -7459.25     -31209.50
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  ---------------------  -----------  ----------  -----------
  Total Steric Interaction:        43.957841589496674     1196.1537     27583.96     115411.30
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                              -57.212938990762275    -1556.8433    -35901.67    -150212.55
                                  ---------------------  -----------  ----------  -----------
  Total Orbital Interactions:     -57.220005497697414    -1557.0356    -35906.10    -150231.10

Alternative Decomposition Orb.Int.
  Kinetic:                       -141.774337006106805    -3857.8760    -88964.75    -372228.47
  Coulomb:                         77.944845391469443     2120.9872     48911.13     204644.16
  XC:                               6.609486116939869      179.8533      4147.52      17353.20
                                  ---------------------  -----------  ----------  -----------
  Total Orbital Interactions:     -57.220005497697493    -1557.0356    -35906.10    -150231.10

  Residu (E=Steric+OrbInt+Res):     0.000008818684727        0.0002         0.01         0.02

Total Bonding Energy:             -13.262155089516014     -360.8816     -8322.13     -34819.78


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
================================================================================

  Electrostatic Energy:           -11.887072527966744     -323.4637     -7459.25     -31209.50
  Kinetic Energy:                  12.556749296699707      341.6865      7879.48      32967.74
  Coulomb (Steric+OrbInt) Energy:  -2.234343123802262      -60.7996     -1402.07      -5866.27
  XC Energy:                      -11.697488734446789     -318.3049     -7340.29     -30711.75
```

Total Bonding Energy:	-13.262155089516089	-360.8816	-8322.13	-34819.78

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): -0.0028811277
2. Electrostatic (Fit correction): 0.0000000000

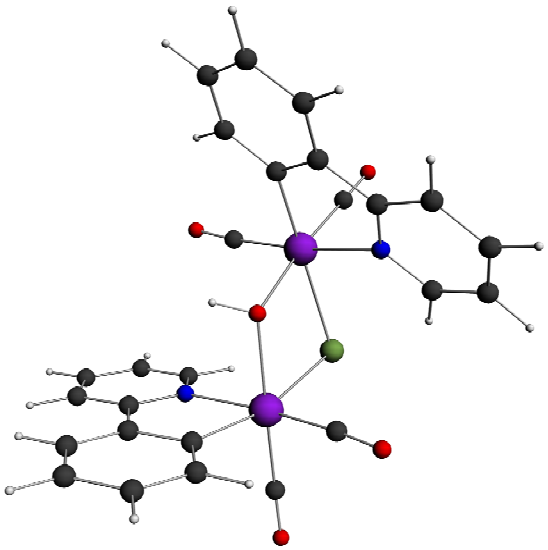


Figure 1

(1) Two points numerical differenciation frequencies

```
==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                          VWN
   Gradient Corrections:         Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                     Restricted
   Fragments:                    Restricted

OTHER ASPECTS
   Relativistic Corrections:     ---
   Core Treatment:               Frozen Orbital(s)

   Electric Field:               ---

   Hyperfine or Zeeman Interaction:   ---
```

```
 **********************************
 *  R U N   T Y P E : FREQUENCIES  *
 **********************************
```

List of All Frequencies:

Intensities
===========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
4.572761	0.000000	0.000000
17.963003	0.000000	0.000000
26.946048	154.643087	1.044489
31.127763	12.105504	0.094451
40.317049	21.469168	0.216961
56.164159	0.755760	0.010640
62.727514	0.947807	0.014902
69.072369	1.574261	0.027256
73.102035	9.678009	0.177335
79.810621	82.074872	1.641909
81.823805	66.262344	1.359016
86.843601	0.744705	0.016211
92.389847	13.129079	0.304044
93.040301	7.457387	0.173915
100.284992	26.484851	0.665751
110.229658	3.934493	0.108709
112.654989	13.078317	0.369301
122.429183	2.315971	0.071072
135.624865	71.822177	2.441608
163.093876	5.240463	0.214233
181.218018	36.020325	1.636165
183.303633	17.396865	0.799319
186.606642	39.695895	1.856739
190.209447	282.651073	13.475993
205.841230	169.050630	8.722224
219.466905	29.820088	1.640424
247.096979	122.379529	7.579740
249.907366	71.178956	4.458705
257.334070	10.456694	0.674481
263.592453	7.886087	0.521042
277.831295	50.648832	3.527189
280.189908	34.266353	2.406570
341.318145	160.061554	13.693816
362.692296	28.028415	2.548091
363.171763	25.746448	2.343729
411.684692	26.838515	2.769499
412.259359	85.861383	8.872509
420.559347	27.470153	2.895786
421.222428	3.850246	0.406516
443.043109	85.731830	9.520640
448.536964	620.512795	69.763306
462.204261	36.549547	4.234421
463.628969	24.397246	2.835237
467.453996	2.289743	0.268290
469.858924	3.527212	0.415410
473.736182	70.274301	8.344708
479.691060	103.479503	12.442110
498.633178	16.640597	2.079832
499.742169	5.168800	0.647461
517.541961	161.300236	20.924671
521.678671	52.974937	6.927102
539.301294	36.543661	4.939939
540.801395	10.188125	1.381052
553.026592	16.441617	2.279127
554.675793	5.473017	0.760929
585.561202	49.818408	7.312068
592.999069	126.685898	18.830435
622.246210	28.216699	4.400951
624.111563	66.422419	10.390944
626.200738	112.175701	17.607206
626.894018	26.501767	4.164348
641.174093	18.502552	2.973621
642.403517	21.002296	3.381838
659.209502	9.700157	1.602804
660.008577	17.145416	2.836454
711.679309	27.429099	4.892986
712.242392	20.007586	3.571911

721.219263	160.297180	28.978191
721.517404	125.974329	22.782792
739.631554	486.118292	90.122964
740.537320	169.002166	31.370200
755.904078	2.553650	0.483845
756.508331	2.789924	0.529035
780.765541	10.990208	2.150823
781.214937	20.140464	3.943829
840.034457	1.429052	0.300901
840.405383	4.965544	1.046005
861.072819	2.016098	0.435141
862.820670	3.912884	0.846244
888.574529	188.600148	42.006254
919.123219	0.276960	0.063807
919.168922	0.643741	0.148315
956.120070	3.976979	0.953112
958.661444	3.144829	0.755684
959.034465	4.215623	1.013384
960.728318	2.977850	0.717103
973.452081	2.191305	0.534682
974.807930	1.276758	0.311965
1000.608734	17.730774	4.447030
1001.811339	16.100125	4.042902
1007.599769	91.286021	23.055280
1008.162673	102.562968	25.917867
1018.227798	23.013877	5.873714
1019.008568	28.626422	7.311778
1046.929001	6.413352	1.682986
1048.335494	3.713035	0.975680
1053.706960	40.589638	10.720452
1055.950726	37.362344	9.889079
1097.661946	3.130842	0.861406
1098.570963	3.896272	1.072891
1116.276287	1.312882	0.367346
1117.427933	0.722344	0.202321
1149.994429	18.196917	5.245315
1150.652215	12.809545	3.694502
1157.881766	21.105975	6.125587
1158.036319	18.833128	5.466668
1235.410290	15.895654	4.922296
1236.169286	37.462482	11.607871
1272.348476	99.642714	31.778229
1273.164194	11.116447	3.547550
1288.169504	2.223870	0.718059
1289.515537	2.799431	0.904846
1299.808130	53.420299	17.404583
1300.409731	42.406490	13.822628
1314.699989	7.697204	2.536517
1314.993364	8.109882	2.673106
1411.007155	48.269927	17.071981
1411.121435	56.563661	20.006908
1426.330041	5.259044	1.880204
1426.461011	12.299940	4.397856
1441.162668	29.677429	10.720557
1442.800836	17.714963	6.406557
1467.787115	182.801223	67.254328
1469.164416	156.519780	57.639168
1541.415749	18.858805	7.286383
1543.040935	19.074785	7.377601
1555.988663	65.791729	25.659950
1557.501020	82.044494	32.029920
1570.634343	82.911788	32.641450
1571.923934	99.586489	39.238285
1593.510942	140.530434	56.131094
1594.278833	105.474959	42.149431
1942.577806	1097.785458	534.532316
1946.700737	1443.977142	704.591796
2002.837916	1731.305158	869.155530
2007.477491	945.299399	475.661648
3081.997041	1.245724	0.962348
3083.635854	1.678490	1.297358
3089.678543	7.287521	5.643795
3092.465397	3.611870	2.799723
3101.198066	40.645002	31.594736
3101.595084	0.264290	0.205468
3104.232288	1.895584	1.474943
3105.389604	14.183451	11.040178
3107.609894	3.892714	3.032195
3108.057753	12.854005	10.013955
3115.259685	53.672173	41.910371
3116.467748	42.906273	33.516719
3132.142497	2.006615	1.575374
3132.366893	1.168593	0.917517
3137.603894	22.321638	17.555057
3137.740191	1.487010	1.169524
3699.223373	24.229789	22.466647

```
============================
Statistical Thermal Analysis  ***  ideal gas assumed  ***
============================

Pressure:                 1.000000 atm.
Temperature:            298.150000 K


Moments of Inertia (and direction vectors)
==========================================

      14125.8418      22758.3625      24763.7368
-------------------------------------------------
         -0.6001          0.6142          0.5124
         -0.7196         -0.6943         -0.0107
          0.3492         -0.3752          0.8587


The rotational contribution to the molecular entropy includes
a term, dependent on the symmetry number sigma. The results
reported below were computed using sigma = 1, determined
from the point group symmetry of the input geometry (NOSYM).
If this is not the correct symmetry, please contact SCM to
report a bug.
```

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.414	37.318	122.342	205.075
	Internal Energy (Kcal/mole):	0.889	0.889	244.613	246.391
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	119.198	125.159

```
========================
No memory problems found
========================

Maximum number of active allocate calls:         160

*****************************************************************************

                            A D F   E X I T
NORMAL TERMINATION
```

(2) Computed IR spectrum

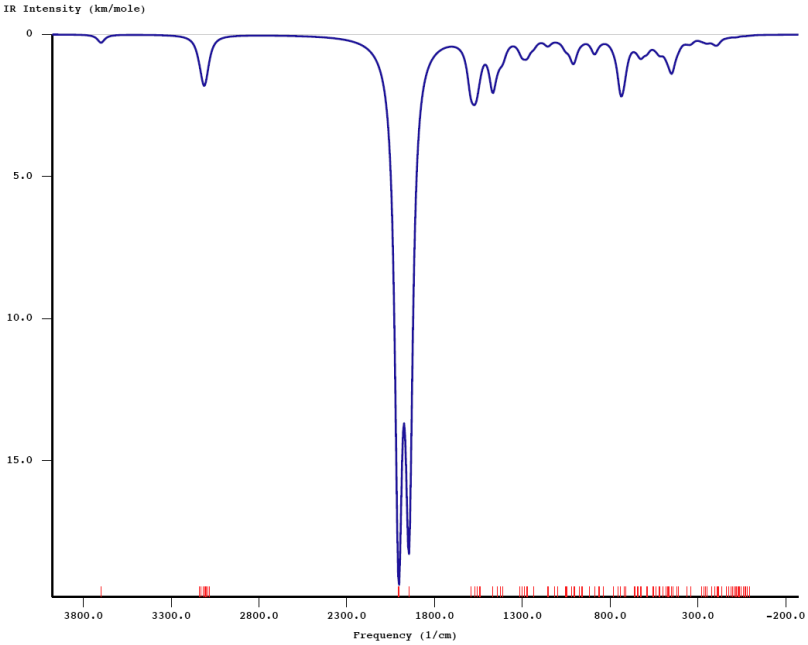
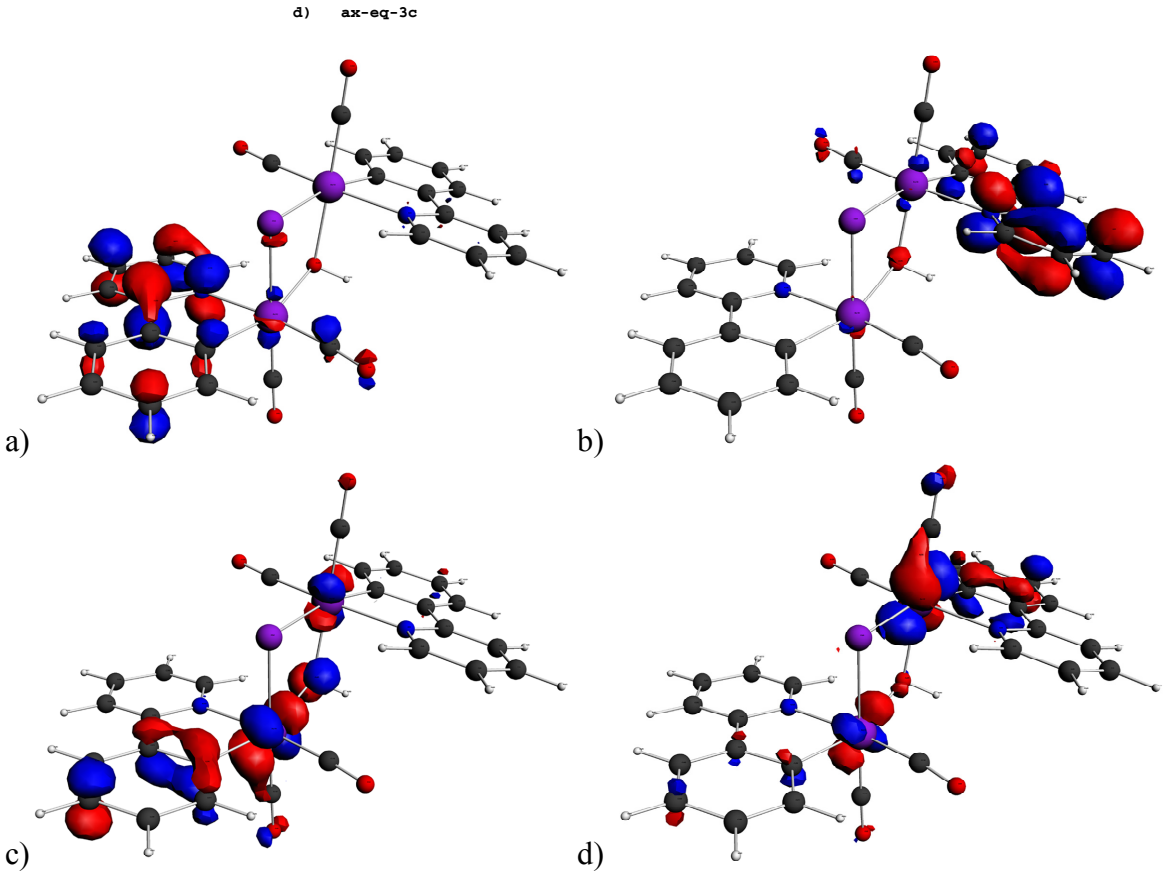


Figure 2




```
==========================
 Geometry Convergence Tests
 ==========================

 Energy  old :        -13.25708412
         new :        -13.25709926

 Convergence tests:
 (Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

       Item               Value         Criterion     Conv.        Ratio
 ------------------------------------------------------------------------
 change in energy      -0.00001515      0.00050000     YES        4.95419034
 gradient max           0.00089994      0.00100000     YES        0.80220305
 gradient rms           0.00018575      0.00066667     YES        0.88241599
 cart. step max         0.00306161      0.01000000     YES        1.07877652
 cart. step rms         0.00087077      0.00666667     YES        1.14194504

 prediction dE :       -0.00000912


 ***************************************************************************************************
                              Geometry CONVERGED
 ***************************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************


 Coordinates (Cartesian)
 =======================

     Atom                  bohr                                  angstrom                Geometric Variables
                  X           Y           Z           X           Y           Z        (0:frozen, *:LT par.)
 ------------------------------------------------------------------------------------------------------------
     1 C       6.589274   -1.762976   -6.522286    3.486894   -0.932927   -3.451445      1       2       3
     2 H       5.438880   -0.725911   -2.710644    2.878131   -0.384136   -1.434411      4       5       6
     3 C       5.152549   -0.476185   -4.736600    2.726612   -0.251986   -2.506501      7       8       9
     4 C       6.066486   -1.354402   -9.081103    3.210246   -0.716719   -4.805513     10      11      12
     5 Cl      2.334303    0.442290    1.059320    1.235260    0.234050    0.560568     13      14      15
     6 N       3.296967    1.136002   -5.381135    1.744680    0.601147   -2.847574     16      17      18
     7 O       3.331936   -6.121112   -2.587140    1.763185   -3.239153   -1.369056     19      20      21
     8 C       4.174842    0.336984   -9.752604    2.209231    0.178324   -5.160856     22      23      24
     9 O      -4.549392   -7.000396   -1.737981   -2.407435   -3.704450   -0.919700     25      26      27
    10 H       3.756579    0.691101  -11.735246    1.987896    0.365715   -6.210025     28      29      30
    11 C       1.764562   -4.821075   -1.753479    0.933766   -2.551203   -0.927901     31      32      33
    12 C       2.796845    1.610012   -7.872388    1.480027    0.851982   -4.165888     34      35      36
```

13 C	-3.142562	-5.429377	-1.113962	-1.662972	-2.873103	-0.589483	37	38	39
14 Ru	0.880336	3.154160	-2.736927	0.465854	1.669110	-1.448320	40	41	42
15 H	-5.217698	0.937384	-0.680760	-2.761087	0.496042	-0.360243	43	44	45
16 Ru	-0.805975	-2.939005	-0.153260	-0.426503	-1.555255	-0.081102	46	47	48
17 C	0.829634	3.498959	-8.327955	0.439023	1.851569	-4.406964	49	50	51
18 C	-1.443460	5.106508	-0.853379	-0.763846	2.702248	-0.451589	52	53	54
19 C	-0.313837	4.619004	-6.171067	-0.166076	2.444272	-3.265588	55	56	57
20 C	-5.366509	0.502212	1.329620	-2.839834	0.265759	0.703605	58	59	60
21 H	1.014851	3.395143	-12.433647	0.537036	1.796632	-6.579603	61	62	63
22 H	-8.560897	2.889888	2.129674	-4.530232	1.529263	1.126975	64	65	66
23 C	0.128443	4.258032	-10.785887	0.067969	2.253254	-5.707646	67	68	69
24 O	-2.873803	6.414858	0.182392	-1.520751	3.394596	0.096518	70	71	72
25 N	-3.630703	-1.137867	2.194329	-1.921285	-0.602134	1.161189	73	74	75
26 H	2.747598	-7.417365	2.421409	1.453966	-3.925101	1.281355	76	77	78
27 C	-7.188258	1.564385	2.898775	-3.803862	0.827837	1.533966	79	80	81
28 C	-2.129764	6.509220	-6.583271	-1.127023	3.444531	-3.483717	82	83	84
29 H	-3.036919	7.440731	-4.985761	-1.607068	3.937465	-2.638351	85	86	87
30 C	-0.203177	-4.722774	3.316381	-0.107516	-2.499184	1.754953	88	89	90
31 C	-1.681078	6.132657	-11.138567	-0.889588	3.245263	-5.894276	91	92	93
32 C	1.577069	-6.594738	3.902474	0.834549	-3.489785	2.065100	94	95	96
33 C	-2.807435	7.259526	-9.026113	-1.485631	3.841576	-4.776414	97	98	99
34 H	-2.201719	6.725514	-13.043083	-1.165100	3.558989	-6.902102	100	101	102
35 C	-3.609822	-1.854853	4.670572	-1.910236	-0.981546	2.471561	103	104	105
36 C	-7.185316	0.889426	5.455975	-3.802306	0.470664	2.887178	106	107	108
37 H	-4.217518	8.745080	-9.279987	-2.231814	4.627697	-4.910758	109	110	111
38 C	-1.698857	-3.744248	5.319081	-0.898997	-1.981371	2.814736	112	113	114
39 C	-5.397000	-0.818137	6.339377	-2.855969	-0.432939	3.354654	115	116	117
40 C	1.914999	-7.441536	6.386971	1.013374	-3.937891	3.379840	118	119	120
41 H	3.330276	-8.889801	6.784094	1.762306	-4.704280	3.589988	121	122	123
42 H	-8.581823	1.684687	6.747974	-4.541305	0.891498	3.570874	124	125	126
43 C	-1.343351	-4.601904	7.817099	-0.710871	-2.435223	4.136631	127	128	129
44 H	-5.388458	-1.379558	8.318320	-2.851449	-0.730031	4.401865	130	131	132
45 C	0.460346	-6.439628	8.354594	0.243605	-3.407705	4.421061	133	134	135
46 H	-2.473153	-3.822147	9.353588	-1.308736	-2.022593	4.949706	136	137	138
47 H	0.731694	-7.088085	10.292412	0.387196	-3.750853	5.446510	139	140	141
48 H	7.134322	-2.347150	-10.539543	3.775321	-1.242058	-5.577286	142	143	144
49 H	8.057706	-3.066748	-5.909851	4.263954	-1.622853	-3.127358	145	146	147
50 O	-1.745552	0.033280	-3.009709	-0.923706	0.017611	-1.592669	148	149	150
51 H	-1.697896	-0.593952	-4.739673	-0.898488	-0.314306	-2.508127	151	152	153
52 C	3.295517	5.760365	-2.347837	1.743912	3.048254	-1.242422	154	155	156
53 O	4.780583	7.354120	-2.077953	2.529776	3.891633	-1.099606	157	158	159

Number of elements of the density matrix on this node (used, total): 199365 396495

==========
Numerical Integration : Voronoi Polyhedra (Te Velde) *** (parameters, tests) ***
==========

General Accuracy Parameter : 4.50

Symmetry used in the points section: NOSYM

Summary of the Symmetry Unique Points:

Nr. of used Symmetry Operators	1
Points in the Atomic Spheres	33332
Points in the Atomic Polyhedra	337809
Points in the Outer Region	30332
Total	401473
Sum of Weights	161102.381433

Total nr. of points: 401473
Nr. of blocks: 3137
Block length: 128
Nr. of dummy points: 63

Test of Precision of the Numerical Integration Grid
==========

Integral of the Total Core Density: 55.99998621786227
Relative Error: -2.461E-07

==========
B O N D I N G E N E R G Y *** (decomposition) ***
==========

*** WARNING ***

The bond energy is computed as an energy difference between molecule and fragments. In particular when the fragments are single atoms, they are usually computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied for the true (multiplet) fragment ground state. See ref: E.J.Baerends, V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make the direct connection to that paper, where detailed explanations can be found on the meaning of the various terms.

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	154.348975084365549	4200.0493	96855.45	405243.18
Delta V^Pauli Coulomb:	-80.187944879697682	-2182.0250	-50318.70	-210533.42

Delta V^Pauli LDA-XC:	-19.116489356578601	-520.1861	-11995.78	-50190.34
Delta V^Pauli GGA-Exchange:	1.115108514121914	30.3436	699.74	2927.72
Delta V^Pauli GGA-Correlation:	-0.312320369335053	-8.4987	-195.98	-820.00
Total Pauli Repulsion:	55.847328992876129	1519.6831	35044.73	146627.14
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	55.847328992876129	1519.6831	35044.73	146627.14
Electrostatic Interaction:	-11.890772067840190	-323.5644	-7461.57	-31219.22
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	43.956556925035940	1196.1188	27583.16	115407.92
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-57.206929126019418	-1556.6797	-35897.89	-150196.77
Total Orbital Interactions:	-57.213653818249675	-1556.8627	-35902.11	-150214.43
Alternative Decomposition Orb.Int.				
Kinetic:	-141.780439776903364	-3858.0421	-88968.58	-372244.49
Coulomb:	77.953462710139746	2121.2216	48916.54	204666.79
XC:	6.613323248513936	179.9577	4149.92	17363.28
Total Orbital Interactions:	-57.213653818249682	-1556.8627	-35902.11	-150214.43
Residu (E=Steric+OrbInt+Res):	0.000008245860843	0.0002	0.01	0.02
Total Bonding Energy:	-13.257088647352891	-360.7437	-8318.95	-34806.48

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.890772067840190	-323.5644	-7461.57	-31219.22
Kinetic Energy:	12.568535307462184	342.0072	7886.88	32998.68
Coulomb (Steric+OrbInt) Energy:	-2.234473923697095	-60.8031	-1402.15	-5866.61
XC Energy:	-11.700377963277804	-318.3835	-7342.10	-30719.34
Total Bonding Energy:	-13.257088647352905	-360.7437	-8318.95	-34806.48

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): -0.0023568398
2. Electrostatic (Fit correction): 0.0000000000

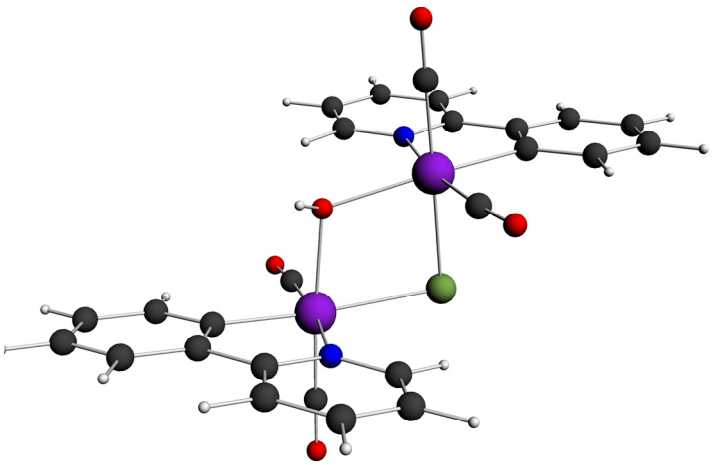
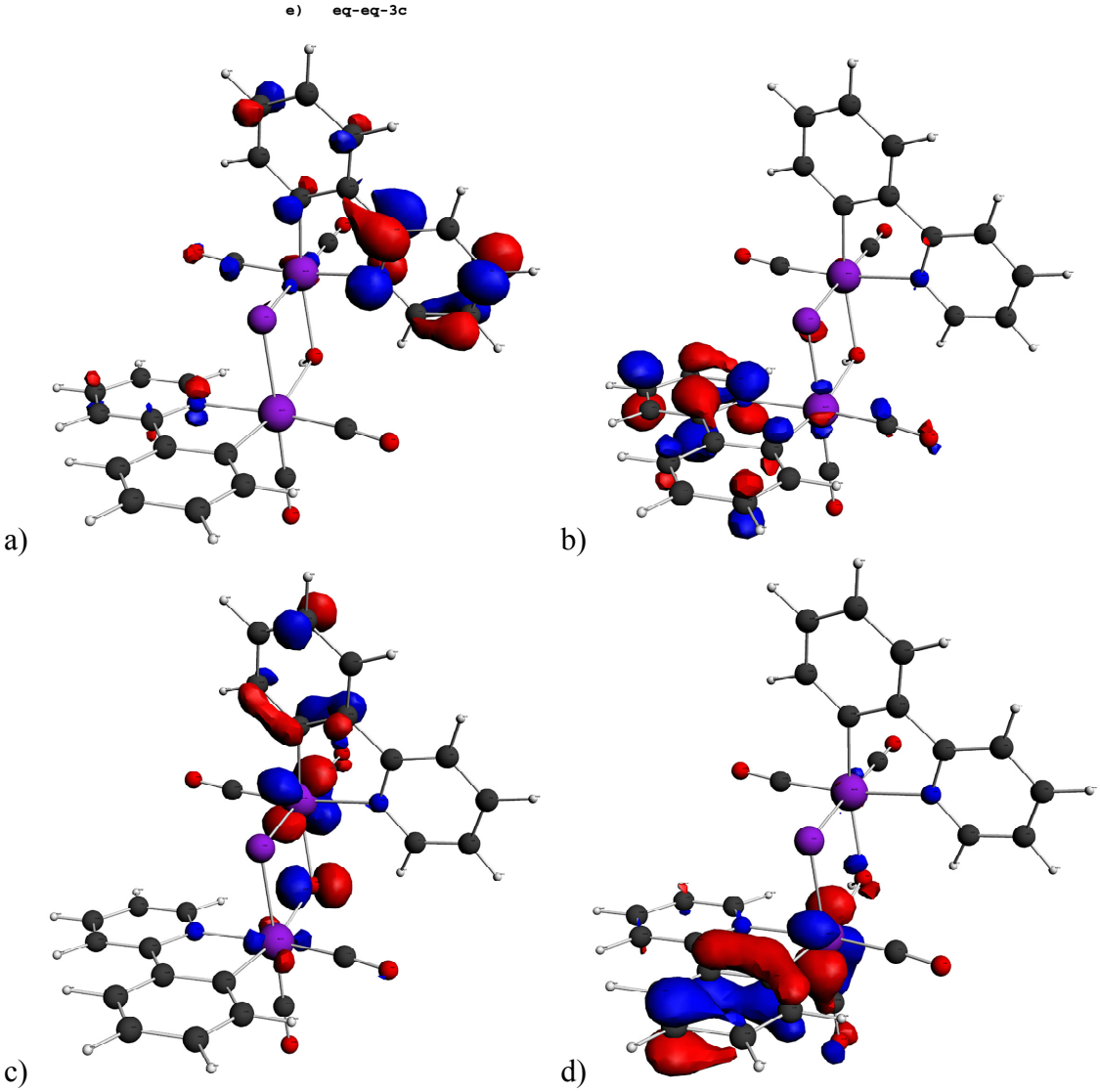


Figure 3

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 *   ------------------------------------                                    *
 *    Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007  *
 *   ------------------------------------                                    *
 *                                               Build 200708202008          *
 *                                                                           *
 *                                                                           *
 *                              =================                            *
 *                              |               |                            *
 *                              |     A D F     |                            *
 *                              |               |                            *
 *                              =================                            *
 *                                                                           *
 *                                                                           *
 *    Online information and documentation:  http://www.scm.com              *
 *    E-mail:  support@scm.com   info@scm.com                                *
 *                                                                           *
 *    Scientific publications using ADF results must be properly referenced  *
 *    See the User Manuals (or the web site) for recommended citations       *
 *    The terms and conditions of the End User License Agreement apply to    *
 *    the use of ADF, http://www.scm.com/Sales/LicAgreement.html             *
 *                                                                           *
 ******************************  macintel  *********************************

ADF 2007.01  RunTime: Jul25-2008 11:18:28
equatorial-OH


============================
A T T A C H E D   F I L E S
============================
```

```
==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                      == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
----------------
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul25-2008 11:18:26
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul25-2008 11:18:22
        title: Hydrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul25-2008 11:18:25
        title: Oxygen (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul25-2008 11:18:23
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul25-2008 11:18:24
        title: Ruthenium (TZP, 3d frozen)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jul25-2008 11:18:24
        title: Chlorine (TZP)


                                  ********************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ********************************************

==========================
Geometry Convergence Tests
==========================

Energy  old :        -13.24889219
        new :        -13.24890281

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy      -0.00001062     0.00100000    YES        2.00418792
gradient max           0.00080779     0.00100000    YES        0.65595582
gradient rms           0.00012611     0.00066667    YES        0.76766240
cart. step max         0.00479489     0.01000000    YES        0.83523059
cart. step rms         0.00147795     0.00666667    YES        0.82208823

prediction dE :       -0.00001030


*************************************************************************************************
                          Geometry CONVERGED
*************************************************************************************************


                                       ********************
                                       *  Final Geometry  *
                                       ********************


Coordinates (Cartesian)
=======================

    Atom                   bohr                                  angstrom                Geometric Variables
                  X           Y           Z             X           Y           Z       (0:frozen, *:LT par.)
-------------------------------------------------------------------------------------------------------------
    1 C       6.369117   -0.665645   -5.685543       3.370391   -0.352244   -3.008660      1       2       3
    2 H       2.263105   -0.531502   -5.205765       1.197584   -0.281259   -2.754772      4       5       6
    3 O      -0.218465    7.159612   -5.134079      -0.115607    3.788703   -2.716837      7       8       9
    4 C       4.113426    0.178575   -4.634285       2.176732    0.094498   -2.452358     10      11      12
    5 C       8.634730    0.334521   -4.759423       4.569303    0.177021   -2.518578     13      14      15
    6 O      -1.257272   -0.101801   -2.719256      -0.665320   -0.053871   -1.438968     16      17      18
    7 C       0.121980    5.657652   -3.565148       0.064549    2.993901   -1.886595     19      20      21
    8 N       4.056930    1.920057   -2.784851       2.146835    1.016050   -1.473680     22      23      24
    9 O       3.420343   -5.913892   -2.138570       1.809968   -3.129497   -1.131683     25      26      27
   10 C       8.567408    2.139412   -2.851731       4.533677    1.132128   -1.509071     28      29      30
   11 O      -4.451440   -7.137537   -2.601053      -2.355601   -3.777022   -1.376418     31      32      33
   12 H      10.313456    2.941114   -2.119832       5.457646    1.556371   -1.121767     34      35      36
   13 C       1.701283   -4.815330   -1.322410       0.900280   -2.548163   -0.699789     37      38      39
   14 C       6.235506    2.948209   -1.870660       3.299688    1.560125   -0.989911     40      41      42
   15 C      -3.215439   -5.655451   -1.547765      -1.701537   -2.992736   -0.819042     43      44      45
   16 Ru      0.635588    3.260090   -1.003264       0.336339    1.725165   -0.530904     46      47      48
   17 H      -5.814253    0.532354   -0.485635      -3.076770    0.281710   -0.256987     49      50      51
   18 Ru     -1.179587   -3.272683    0.117677      -0.624211   -1.731829    0.062272     52      53      54
   19 C       5.886932    4.884327    0.072992       3.115230    2.584674    0.038626     55      56      57
   20 C      -2.037224    4.732528    0.848665      -1.078053    2.504346    0.449094     58      59      60
   21 C       3.360488    5.540316    0.710839       1.778294    2.931809    0.376160     61      62      63
   22 C      -6.102097   -0.169609    1.427320      -3.229091   -0.089753    0.755305     64      65      66
```

23 Cl	1.425481	-0.009826	2.342444	0.754332	-0.005199	1.239568	67	68	69
24 H	9.874958	5.537286	0.811121	5.225603	2.930206	0.429227	70	71	72
25 H	-9.421254	2.066106	2.147781	-4.985513	1.093336	1.136557	73	74	75
26 C	7.940970	6.077535	1.276171	4.202181	3.216093	0.675320	76	77	78
27 O	-3.591994	5.801516	1.981393	-1.900801	3.070030	1.048508	79	80	81
28 N	-4.401705	-1.868630	2.252779	-2.329282	-0.988836	1.192119	82	83	84
29 H	2.097671	-8.025718	2.509312	1.110040	-4.247027	1.327871	85	86	87
30 C	-8.098027	0.683702	2.903814	-4.285292	0.361799	1.536632	88	89	90
31 C	2.999875	7.454945	2.507439	1.587465	3.944987	1.326880	91	92	93
32 H	1.095687	8.038616	3.034557	0.579812	4.253852	1.605819	94	95	96
33 C	-0.997680	-5.482616	3.365326	-0.527949	-2.901275	1.780854	97	98	99
34 C	7.530541	7.944644	3.083342	3.984991	4.204125	1.631634	100	101	102
35 C	0.743412	-7.400660	3.930012	0.393397	-3.916260	2.079673	103	104	105
36 C	5.049316	8.641097	3.685759	2.671983	4.572671	1.950420	106	107	108
37 H	9.127203	8.852211	4.017939	4.829908	4.684388	2.126202	109	110	111
38 C	-4.612623	-2.851302	4.630372	-2.440895	-1.508844	2.450288	112	113	114
39 C	-8.319111	-0.261723	5.363352	-4.402284	-0.138498	2.838164	115	116	117
40 H	4.704574	10.111619	5.091203	2.489553	5.350839	2.694149	118	119	120
41 C	-2.740404	-4.775346	5.280884	-1.450160	-2.527004	2.794524	121	122	123
42 C	-6.576128	-2.026065	6.221383	-3.479937	-1.072147	3.292214	124	125	126
43 C	0.812658	-8.537427	6.316090	0.430040	-4.517812	3.342331	127	128	129
44 H	2.203255	-10.011867	6.701890	1.165912	-5.298052	3.546487	130	131	132
45 H	-9.846029	0.371408	6.595026	-5.210294	0.196540	3.489938	133	134	135
46 C	-2.651275	-5.918469	7.685618	-1.402994	-3.131919	4.067054	136	137	138
47 H	-6.729686	-2.792654	8.122458	-3.561196	-1.477809	4.298220	139	140	141
48 C	-0.877501	-7.787324	8.210380	-0.464353	-4.120874	4.344746	142	143	144
49 H	-3.965542	-5.339603	9.163951	-2.098474	-2.825596	4.849354	145	146	147
50 H	-0.809240	-8.657376	10.077128	-0.428231	-4.581286	5.332587	148	149	150
51 H	10.443824	-0.290589	-5.525648	5.526634	-0.153773	-2.924047	151	152	153
52 H	6.341482	-2.084488	-7.175879	3.355768	-1.103064	-3.797312	154	155	156
53 H	-2.932914	0.242976	-3.385036	-1.552031	0.128577	-1.791284	157	158	159

Number of elements of the density matrix on this node (used, total): 199365 396495

==========
Numerical Integration : Voronoi Polyhedra (Te Velde) *** (parameters, tests) ***
==========

General Accuracy Parameter : 4.50

Symmetry used in the points section: NOSYM

Summary of the Symmetry Unique Points:

Nr. of used Symmetry Operators	1
Points in the Atomic Spheres	33332
Points in the Atomic Polyhedra	349674
Points in the Outer Region	26941
Total	409947
Sum of Weights	160384.242351

Total nr. of points: 409947
Nr. of blocks: 3203
Block length: 128
Nr. of dummy points: 37

Test of Precision of the Numerical Integration Grid
==========

Integral of the Total Core Density: 55.99998785758984
Relative Error: -2.168E-07

==========
B O N D I N G E N E R G Y *** (decomposition) ***
==========

*** WARNING ***

The bond energy is computed as an energy difference between molecule and fragments. In particular when the fragments are single atoms, they are usually computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied for the true (multiplet) fragment ground state. See ref: E.J.Baerends, V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make the direct connection to that paper, where detailed explanations can be found on the meaning of the various terms.

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	154.399220195618767	4201.4166	96886.98	405375.10
Delta V^Pauli Coulomb:	-80.216719556269538	-2182.8080	-50336.76	-210608.97
Delta V^Pauli LDA-XC:	-19.113582529498611	-520.1070	-11993.96	-50182.70
Delta V^Pauli GGA-Exchange:	1.113794427836140	30.3079	698.92	2924.27
Delta V^Pauli GGA-Correlation:	-0.311815720113016	-8.4849	-195.67	-818.67
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	55.870896817573744	1520.3245	35059.52	146689.02
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	55.870896817573744	1520.3245	35059.52	146689.02
Electrostatic Interaction: (Electrostatic Interaction =	-11.894794954510189	-323.6738	-7464.10	-31229.78

```
  Delta V_elstat in the BB paper)
                                 --------------------     -----------      ----------      -----------
  Total Steric Interaction:          43.976101863063555       1196.6506        27595.42        115459.24
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -57.218333794956862      -1556.9901       -35905.05       -150226.71
                                 --------------------     -----------      ----------      -----------
  Total Orbital Interactions:      -57.225007166023019      -1557.1717       -35909.24       -150244.24

Alternative Decomposition Orb.Int.
  Kinetic:                        -141.842428243326282      -3859.7289       -89007.48       -372407.24
  Coulomb:                          78.002352872951008       2122.5520        48947.22        204795.15
  XC:                                6.615068204352172        180.0052         4151.02         17367.86
                                 --------------------     -----------      ----------      -----------
  Total Orbital Interactions:      -57.225007166023104      -1557.1717       -35909.24       -150244.24

  Residu (E=Steric+OrbInt+Res):     -0.000011803947140         -0.0003           -0.01           -0.03

Total Bonding Energy:              -13.248917106906605       -360.5214        -8313.82        -34785.03


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
================================================================================

  Electrostatic Energy:            -11.894794954510189       -323.6738        -7464.10        -31229.78
  Kinetic Energy:                   12.556791952292485        341.6877         7879.51         32967.85
  Coulomb (Steric+OrbInt) Energy:   -2.214378487265677        -60.2563        -1389.54         -5813.85
  XC Energy:                       -11.696535617423313       -318.2789        -7339.69        -30709.25
                                 --------------------     -----------      ----------      -----------
  Total Bonding Energy:            -13.248917106906694       -360.5214        -8313.82        -34785.03


Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree):  -0.0040950644
2. Electrostatic (Fit correction):   0.0000000000
```

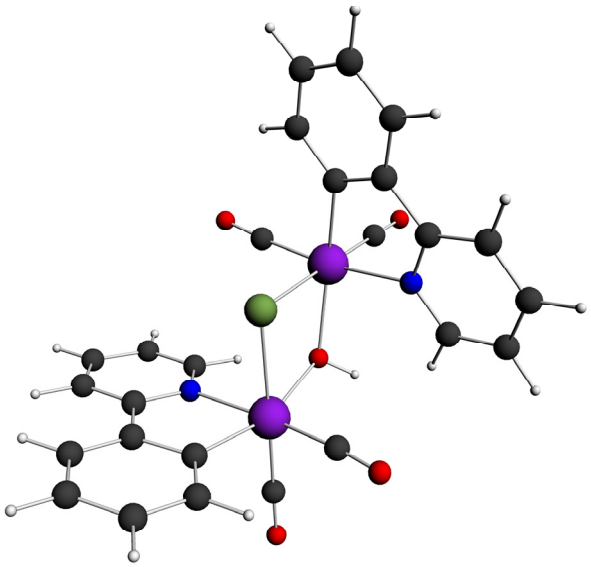

Figure 4

2. Optimized Fragments

a) ax-4

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                              Build 200708202008           *
*                                                                           *
*                                                                           *
*                               =================                           *
*                               |               |                           *
*                               |     A D F     |                           *
*                               |               |                           *
*                               =================                           *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ********************************

ADF 2007.01  RunTime: Jun24-2008 18:40:44
Ru-axOH-eqCl fragment


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                      == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
----------------
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:39
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:28
        title: Hydrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:37
        title: Oxygen (TZP)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:36
        title: Chlorine (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:33
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:34
        title: Ruthenium (TZP, 3d frozen)


                              ******************************************
                              *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                              ******************************************



==========================
Geometry Convergence Tests
==========================

Energy  old :         -6.93449968
        new :         -6.93449726

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-----------------------------------------------------------------------
change in energy       0.00000242     0.00100000    YES        1.12445169
gradient max           0.00086250     0.00100000    YES        0.85659215
gradient rms           0.00018039     0.00066667    YES        1.02364824
cart. step max         0.00087998     0.01000000    YES        0.96989319
```

```
cart. step rms          0.00037464     0.00666667    YES        1.01471645

prediction dE :        -0.00000062

*****************************************************************************************
                          Geometry CONVERGED
*****************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************


Coordinates (Cartesian)
=======================

    Atom                  bohr                                  angstrom                Geometric Variables
                  X           Y           Z           X           Y           Z       (0:frozen, *:LT par.)
-----------------------------------------------------------------------------------------------------------
    1 C       6.470443   -0.916087   -5.426807    3.424011   -0.484772   -2.871742      1       2       3
    2 H       2.337088   -0.509363   -5.312794    1.236734   -0.269543   -2.811410      4       5       6
    3 O       0.104897    7.646394   -4.776976    0.055509    4.046298   -2.527867      7       8       9
    4 C       4.180609    0.053471   -4.557680    2.212283    0.028296   -2.411820     10      11      12
    5 C       8.705673   -0.078231   -4.289662    4.606844   -0.041398   -2.269991     13      14      15
    6 Cl     -2.045607    0.399540   -4.072395   -1.082489    0.211428   -2.155019     16      17      18
    7 C       0.273788    5.927587   -3.395781    0.144883    3.136744   -1.796970     19      20      21
    8 N       4.060143    1.760127   -2.685068    2.148535    0.931419   -1.420877     22      23      24
    9 C       8.572828    1.671600   -2.333419    4.536545    0.884572   -1.234792     25      26      27
   10 H      10.291860    2.329470   -1.413143    5.446218    1.232703   -0.747803     28      29      30
   11 C       6.206590    2.583275   -1.528631    3.284386    1.367010   -0.808917     31      32      33
   12 Ru      0.527594    3.201850   -1.050745    0.279191    1.694346   -0.556030     34      35      36
   13 C       5.804809    4.402652    0.520410    3.071773    2.329783    0.275389     37      38      39
   14 C      -2.222479    4.402918    0.815766   -1.176085    2.329924    0.431685     40      41      42
   15 C       3.246650    5.035129    1.103508    1.718053    2.664476    0.583951     43      44      45
   16 O       0.804282    0.086558    1.364930    0.425608    0.045805    0.722290     46      47      48
   17 H       9.782117    4.990843    1.380879    5.176474    2.641040    0.730730     49      50      51
   18 C       7.837259    5.492533    1.855867    4.147299    2.906523    0.982082     52      53      54
   19 O      -3.882828    5.168958    2.058638   -2.054704    2.735295    1.089384     55      56      57
   20 C       2.883477    6.791551    3.077199    1.525871    3.593934    1.628384     58      59      60
   21 H       0.966019    7.341661    3.601489    0.511195    3.885040    1.905826     61      62      63
   22 C       7.403614    7.221154    3.792246    3.917824    3.821270    2.006770     64      65      66
   23 C       4.903732    7.865326    4.399676    2.594943    4.162151    2.328209     67      68      69
   24 H       8.986418    8.058538    4.817072    4.755407    4.264395    2.549085     70      71      72
   25 H       4.531797    9.218187    5.916773    2.398124    4.878055    3.131021     73      74      75
   26 H      10.537955   -0.792403   -4.917973    5.576446   -0.419321   -2.602479     76      77      78
   27 H       6.487602   -2.300804   -6.952415    3.433091   -1.217533   -3.679060     79      80      81
   28 H       1.664980    0.697147    2.877330    0.881070    0.368914    1.522618     82      83      84
-----------------------------------------------------------------------------------------------------------

Number of elements of the density matrix on this node (used, total):     55440    111628


=====================================================
Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
=====================================================

General Accuracy Parameter :                          4.50

Symmetry used in the points section:  NOSYM


Summary of the Symmetry Unique Points:
--------------------------------------
   Nr. of used Symmetry Operators                     1

   Points in the Atomic Spheres                   17756
   Points in the Atomic Polyhedra                174455
   Points in the Outer Region                     21432
   ------------------------------------------------------
   Total                                         213643

   Sum of Weights                                129774.850094

Total nr. of points:     213643
Nr. of blocks:             1670
Block length:               128
Nr. of dummy points:        117


Test of Precision of the Numerical Integration Grid
===================================================

Integral of the Total Core Density:                  27.99999361421903
Relative Error:                                      -2.281E-07


============================
B O N D I N G   E N E R G Y  ***  (decomposition)  ***
============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	78.012195225461952	2122.8198	48953.40	204820.99
Delta V^Pauli Coulomb:	-40.675041822245653	-1106.8242	-25523.98	-106792.31
Delta V^Pauli LDA-XC:	-9.649056020242478	-262.5642	-6054.87	-25333.59
Delta V^Pauli GGA-Exchange:	0.562664875695791	15.3109	353.08	1477.28
Delta V^Pauli GGA-Correlation:	-0.157410669760677	-4.2834	-98.78	-413.28
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	28.093351588908934	764.4590	17628.85	73759.08
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	28.093351588908934	764.4590	17628.85	73759.08
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-5.982436459880714	-162.7904	-3754.04	-15706.88
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	22.110915129028221	601.6686	13874.81	58052.20
Orbital Interactions				
A:	-29.043658181131701	-790.3182	-18225.17	-76254.11
Total Orbital Interactions:	-29.045414642223932	-790.3659	-18226.27	-76258.73
Alternative Decomposition Orb.Int.				
Kinetic:	-71.474184449118042	-1944.9115	-44850.73	-187655.44
Coulomb:	39.440996494662556	1073.2441	24749.60	103552.32
XC:	2.987773312231604	81.3014	1874.86	7844.40
Total Orbital Interactions:	-29.045414642223882	-790.3659	-18226.27	-76258.73
Residu (E=Steric+OrbInt+Res):	0.000003555391648	0.0001	0.00	0.01
Total Bonding Energy:	-6.934495957804062	-188.6972	-4351.46	-18206.52

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.982436459880714	-162.7904	-3754.04	-15706.88
Kinetic Energy:	6.538010776343910	177.9083	4102.66	17165.54
Coulomb (Steric+OrbInt) Energy:	-1.234041772191446	-33.5800	-774.37	-3239.98
XC Energy:	-6.256028502075759	-170.2352	-3925.72	-16425.20
Total Bonding Energy:	-6.934495957804010	-188.6972	-4351.46	-18206.52

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): -0.0034219536
2. Electrostatic (Fit correction): 0.0000000000

b) *eq-4*

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                              Build 200708202008           *
*                                                                           *
*                                                                           *
*                               =================                           *
*                               |               |                           *
*                               |     A D F     |                           *
*                               |               |                           *
*                               =================                           *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ************************************

ADF 2007.01  RunTime: Jun24-2008 18:40:16
Ru-eq-OH-ax-Cl fragment


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
----------------
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:14
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:09
        title: Hydrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:13
        title: Oxygen (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:11
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:12
        title: Ruthenium (TZP, 3d frozen)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jun24-2008 18:40:12
        title: Chlorine (TZP)



                                  ******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ******************************************


==========================
Geometry Convergence Tests
==========================

Energy  old :         -6.92960910
        new :         -6.92960337

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item              Value         Criterion    Conv.        Ratio
-----------------------------------------------------------------------------
change in energy       0.00000573     0.00100000    YES       39.73551671
gradient max           0.00099997     0.00100000    YES        0.64943898
gradient rms           0.00022866     0.00066667    YES        0.84324810
cart. step max         0.00283066     0.01000000    YES        0.70745666
cart. step rms         0.00078070     0.00666667    YES        0.72035081

prediction dE :       -0.00000252
```

```
*****************************************************************************************************
                            Geometry CONVERGED
*****************************************************************************************************


                                          ********************
                                          *  Final Geometry  *
                                          ********************


Coordinates (Cartesian)
=======================
```

Atom		bohr			angstrom			Geometric Variables		
	X	Y	Z	X	Y	Z	(0:frozen, *:LT par.)		
1	C	6.387238	-0.979756	-5.349970	3.379981	-0.518464	-2.831082	1	2	3
2	H	2.221457	-0.663143	-4.928822	1.175545	-0.350920	-2.608220	4	5	6
3	O	-0.136317	7.454149	-4.931640	-0.072136	3.944566	-2.609711	7	8	9
4	C	4.126872	-0.030698	-4.393688	2.183846	-0.016245	-2.325039	10	11	12
5	C	8.660424	0.044476	-4.462386	4.582899	0.023536	-2.361393	13	14	15
6	O	-1.227188	0.501074	-3.495287	-0.649400	0.265157	-1.849626	16	17	18
7	C	0.193244	5.833202	-3.457565	0.102260	3.086797	-1.829665	19	20	21
8	N	4.090137	1.827693	-2.664649	2.164407	0.967173	-1.410071	22	23	24
9	C	8.601838	1.949009	-2.649143	4.551897	1.031371	-1.401866	25	26	27
10	H	10.354509	2.746888	-1.925685	5.479370	1.453591	-1.019028	28	29	30
11	C	6.264509	2.833747	-1.736782	3.315035	1.499554	-0.919066	31	32	33
12	Ru	0.595691	3.257744	-1.059049	0.315226	1.723924	-0.560424	34	35	36
13	C	5.905685	4.799024	0.182379	3.125154	2.539534	0.096511	37	38	39
14	C	-2.145700	4.451711	0.838695	-1.135456	2.355744	0.443818	40	41	42
15	C	3.360263	5.355379	0.884563	1.778175	2.833945	0.468090	43	44	45
16	Cl	0.986773	-0.177106	2.121165	0.522178	-0.093721	1.122472	46	47	48
17	H	9.898472	5.630551	0.717698	5.238046	2.979559	0.379789	49	50	51
18	C	7.964584	6.082895	1.281053	4.214676	3.218929	0.677904	52	53	54
19	O	-3.799608	5.240050	2.079928	-2.010666	2.772915	1.100651	55	56	57
20	C	3.035782	7.257115	2.723521	1.606467	3.840300	1.441225	58	59	60
21	H	1.129689	7.755865	3.334230	0.597806	4.104227	1.764399	61	62	63
22	C	7.566059	7.947843	3.096690	4.003786	4.205817	1.638698	64	65	66
23	C	5.078169	8.526707	3.814934	2.687251	4.512139	2.018776	67	68	69
24	H	9.164842	8.938697	3.943989	4.849825	4.730155	2.087069	70	71	72
25	H	4.736958	9.982149	5.242766	2.506690	5.282326	2.774352	73	74	75
26	H	10.470924	-0.649259	-5.171093	5.540974	-0.343573	-2.736425	76	77	78
27	H	6.363095	-2.493707	-6.748879	3.367205	-1.319613	-3.571353	79	80	81
28	H	-2.496522	1.393468	-4.483495	-1.321102	0.737391	-2.372563	82	83	84

```
Number of elements of the density matrix on this node (used, total):     55440    111628


=====================================================
Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
=====================================================

General Accuracy Parameter :                          4.50

Symmetry used in the points section:  NOSYM


Summary of the Symmetry Unique Points:
--------------------------------------
   Nr. of used Symmetry Operators                     1

   Points in the Atomic Spheres                   17756
   Points in the Atomic Polyhedra                176229
   Points in the Outer Region                     22419
   ---------------------------------------------------
   Total                                         216404

   Sum of Weights                                129472.837888

Total nr. of points:     216404
Nr. of blocks:             1691
Block length:               128
Nr. of dummy points:         44


Test of Precision of the Numerical Integration Grid
===================================================

Integral of the Total Core Density:                  27.99999421004810
Relative Error:                                      -2.068E-07


============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

                                          hartree              eV         kcal/mol          kJ/mol
```

```
                                   --------------------     -----------      ----------      -----------

Pauli Repulsion
  Kinetic (Delta T^0):               78.090927388899843       2124.9623        49002.80        205027.70
  Delta V^Pauli Coulomb:            -40.740246704831449      -1108.5985       -25564.89       -106963.50
  Delta V^Pauli LDA-XC:              -9.656663342387995       -262.7712        -6059.65        -25353.57
  Delta V^Pauli GGA-Exchange:         0.563139034376853         15.3238          353.38          1478.52
  Delta V^Pauli GGA-Correlation:     -0.157447556337659         -4.2844          -98.80          -413.38
                                   --------------------     -----------      ----------      -----------
  Total Pauli Repulsion:             28.099708819719595       764.6320        17632.84        73775.78
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  28.099708819719595       764.6320        17632.84        73775.78
  Electrostatic Interaction:        -5.989879800056546      -162.9929        -3758.71       -15726.43
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                   --------------------     -----------      ----------      -----------
  Total Steric Interaction:          22.109829019663049       601.6391        13874.13        58049.35
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                                -29.037362663871956      -790.1468       -18221.22       -76237.58
                                   --------------------     -----------      ----------      -----------
  Total Orbital Interactions:       -29.039431224818436      -790.2031       -18222.52       -76243.02

Alternative Decomposition Orb.Int.
  Kinetic:                          -71.541387040589029     -1946.7402       -44892.90      -187831.89
  Coulomb:                           39.509469368763966      1075.1074        24792.57       103732.10
  XC:                                 2.992486447006710        81.4297         1877.81         7856.77
                                   --------------------     -----------      ----------      -----------
  Total Orbital Interactions:       -29.039431224818351      -790.2031       -18222.52       -76243.02

  Residu (E=Steric+OrbInt+Res):       0.000019593111755         0.0005            0.01            0.05

Total Bonding Energy:                -6.929582612043632      -188.5635        -4348.38        -18193.62


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
================================================================================

  Electrostatic Energy:              -5.989879800056546      -162.9929        -3758.71        -15726.43
  Kinetic Energy:                     6.549540348310813       178.2221         4109.90         17195.82
  Coulomb (Steric+OrbInt) Energy:    -1.230757742955731       -33.4906         -772.31         -3231.35
  XC Energy:                         -6.258485417342092      -170.3021        -3927.26        -16431.65
                                   --------------------     -----------      ----------      -----------
  Total Bonding Energy:              -6.929582612043555      -188.5635        -4348.38        -18193.62


Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree):  -0.0037568124
2. Electrostatic (Fit correction):   0.0000000000
```

c) Optimized fragment 5

```
 ***************************************************************************
 *                                                                         *
 *  ------------------------------------                                   *
 *   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007  *
 *  ------------------------------------                                   *
 *                                              Build 200708202008         *
 *                                                                         *
 *                                                                         *
 *                              =================                          *
 *                              |               |                          *
 *                              |     A D F     |                          *
 *                              |               |                          *
 *                              =================                          *
 *                                                                         *
 *                                                                         *
 *   Online information and documentation:  http://www.scm.com             *
 *   E-mail:  support@scm.com   info@scm.com                               *
 *                                                                         *
 *   Scientific publications using ADF results must be properly referenced *
 *   See the User Manuals (or the web site) for recommended citations      *
 *   The terms and conditions of the End User License Agreement apply to   *
 *   the use of ADF, http://www.scm.com/Sales/LicAgreement.html            *
 *                                                                         *
 ********************************  macintel  ********************************

 ADF 2007.01  RunTime: Jul24-2008 13:27:34
 RuCO2 fragment


 ============================
 A T T A C H E D   F I L E S
 ============================



 ==============================
 M O D E L   P A R A M E T E R S
 ==============================

 DENSITY FUNCTIONAL POTENTIAL (scf)
    LDA:                          VWN
    Gradient Corrections:         Becke88 Perdew86                    == Not Default ==

 SPIN  (restricted / unrestr.)
    Molecule:                     Restricted
    Fragments:                    Restricted

 OTHER ASPECTS
    Relativistic Corrections:     ---
    Core Treatment:               Frozen Orbital(s)

    Electric Field:               ---
```

```
   Hyperfine or Zeeman Interaction:   ---

Fragment File(s)
----------------
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul24-2008 13:27:31
        title: Oxygen (TZP)
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul24-2008 13:27:30
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul24-2008 13:27:21
        title: Hydrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul24-2008 13:27:29
        title: Ruthenium (TZP, 3d frozen)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul24-2008 13:27:28
        title: Nitrogen (TZP)


                                  *******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  *******************************************


==========================
Geometry Convergence Tests
==========================

Energy  old :         -6.09826808
        new :         -6.09829594

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy      -0.00002786     0.00100000    YES        1.22114636
gradient max           0.00098790     0.00100000    YES        0.25000621
gradient rms           0.00029690     0.00066667    YES        0.19603908
cart. step max         0.00102369     0.01000000    YES        0.65514899
cart. step rms         0.00035518     0.00666667    YES        0.63003253

prediction dE :       -0.00000068


*********************************************************************************************
                           Geometry CONVERGED
*********************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************


Coordinates (Cartesian)
=======================

    Atom                  bohr                                  angstrom                Geometric Variables
                  X           Y           Z             X           Y           Z       (0:frozen, *:LT par.)
-------------------------------------------------------------------------------------------------------------
    1 O       3.432588   -5.326613   -2.655948       1.816447   -2.818722   -1.405467      1       2       3
    2 O      -4.270665   -7.762778   -1.975246      -2.259939   -4.107885   -1.045255      4       5       6
    3 C       1.653840   -4.588469   -1.645057       0.875174   -2.428113   -0.870527      7       8       9
    4 C      -3.147188   -6.047599   -1.230986      -1.665420   -3.200251   -0.651410     10      11      12
    5 H      -6.180124    0.064570   -0.759304      -3.270381    0.034169   -0.401807     13      14      15
    6 Ru     -1.341316   -3.346244    0.053137      -0.709794   -1.770756    0.028119     16      17      18
    7 C      -6.227486   -0.325704    1.263379      -3.295444   -0.172355    0.668552     19      20      21
    8 H      -9.536442    1.908919    2.010048      -5.046468    1.010156    1.063672     22      23      24
    9 N      -4.396042   -1.850240    2.174604      -2.326285   -0.979105    1.150751     25      26      27
   10 H       2.385159   -7.631134    2.386298       1.262172   -4.038222    1.262775     28      29      30
   11 C      -8.085734    0.691815    2.813040      -4.278786    0.366093    1.488596     31      32      33
   12 C      -0.683669   -5.104385    3.397040      -0.361782   -2.701124    1.797636     34      35      36
   13 C       1.224543   -6.850310    3.895970       0.648000   -3.625028    2.061659     37      38      39
   14 C      -4.326629   -2.473878    4.679979      -2.289554   -1.309120    2.476538     40      41      42
   15 C      -8.033783    0.096247    5.388567      -4.251295    0.050932    2.851507     43      44      45
   16 C      -2.266848   -4.195688    5.362854      -1.199564   -2.220262    2.837900     46      47      48
   17 C      -6.151260   -1.489204    6.323224      -3.255106   -0.788053    3.346106     49      50      51
   18 C       1.672279   -7.614009    6.394972       0.884932   -4.029160    3.384073     52      53      54
   19 H       3.186695   -8.955598    6.783885       1.686326   -4.739098    3.589877     55      56      57
   20 H      -9.463900    0.859815    6.660226      -5.008080    0.454994    3.524440     58      59      60
   21 C      -1.774183   -4.982154    7.850751      -0.938857   -2.636442    4.154439     61      62      63
   22 H      -6.099732   -1.969978    8.321340      -3.227839   -1.042468    4.403464     64      65      66
   23 C       0.182376   -6.674613    8.362383       0.096509   -3.532053    4.425183     67      68      69
   24 H      -2.925826   -4.270006    9.402585      -1.548281   -2.259590    4.975634     70      71      72
   25 H       0.532460   -7.277951   10.299866       0.281765   -3.851326    5.450454     73      74      75
-------------------------------------------------------------------------------------------------------------

Number of elements of the density matrix on this node (used, total):     43660     87571


====================================================
Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
====================================================

General Accuracy Parameter :                          4.50

Symmetry used in the points section:  NOSYM


Summary of the Symmetry Unique Points:
--------------------------------------
```

```
    Nr. of used Symmetry Operators                    1

    Points in the Atomic Spheres                  15772
    Points in the Atomic Polyhedra               147049
    Points in the Outer Region                    23937
    ------------------------------------------------------
    Total                                        186758

    Sum of Weights                               129334.420264

 Total nr. of points:     186758
 Nr. of blocks:             1460
 Block length:               128
 Nr. of dummy points:        122


 Test of Precision of the Numerical Integration Grid
 ===================================================

 Integral of the Total Core Density:                 27.99998586994408
 Relative Error:                                     -5.046E-07


 ===========================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ===========================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

                                          hartree            eV        kcal/mol          kJ/mol
                                  ------------------    ----------    ----------    ----------

Pauli Repulsion
  Kinetic (Delta T^0):             73.332841400617227     1995.4881      46017.06      192535.35
  Delta V^Pauli Coulomb:          -37.438322354316227    -1018.7486     -23492.90      -98294.30
  Delta V^Pauli LDA-XC:            -9.009424462378178     -245.1589      -5653.50      -23654.24
  Delta V^Pauli GGA-Exchange:       0.498283894453412       13.5590         312.68        1308.24
  Delta V^Pauli GGA-Correlation:   -0.132704111812965       -3.6111         -83.27         -348.41
                                  ------------------    ----------    ----------    ----------
  Total Pauli Repulsion:           27.250674366563267      741.5286      17100.06      71546.64
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 27.250674366563267      741.5286      17100.06      71546.64
  Electrostatic Interaction:       -5.761726294126650     -156.7845      -3615.54      -15127.41
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  ------------------    ----------    ----------    ----------
  Total Steric Interaction:        21.488948072436617      584.7440      13484.52      56419.23
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                              -27.580082041074277     -750.4922     -17306.76     -72411.50
                                  ------------------    ----------    ----------    ----------
  Total Orbital Interactions:     -27.587232614393123     -750.6868     -17311.25     -72430.27

Alternative Decomposition Orb.Int.
  Kinetic:                        -67.577791473534973    -1838.8853     -42405.71    -177425.47
  Coulomb:                         36.703290752354015      998.7474      23031.67      96364.48
  XC:                               3.287268106787864       89.4511       2062.79       8630.72
                                  ------------------    ----------    ----------    ----------
  Total Orbital Interactions:     -27.587232614393095     -750.6868     -17311.25     -72430.27

  Residu (E=Steric+OrbInt+Res):    -0.000010418539284       -0.0003         -0.01         -0.03

Total Bonding Energy:               -6.098294960495790     -165.9430      -3826.74      -16011.07


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
======================================================================================

  Electrostatic Energy:             -5.761726294126650     -156.7845      -3615.54      -15127.41
  Kinetic Energy:                    5.755049927082254      156.6029       3611.35       15109.88
  Coulomb (Steric+OrbInt) Energy:   -0.735042020501496      -20.0015       -461.25       -1929.85
  XC Energy:                        -5.356576572949868     -145.7599      -3361.30      -14063.69
                                  ------------------    ----------    ----------    ----------
  Total Bonding Energy:             -6.098294960495759     -165.9430      -3826.74      -16011.07


Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree):   0.0011431250
2. Electrostatic (Fit correction):   0.0000000000
```

d) Strict geometry optimization for fragment 5

```
*******************************************************************************
*                                                                             *
*  ------------------------------------                                       *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007     *
*  ------------------------------------                                       *
*                                              Build 200708202008             *
*                                                                             *
*                                                                             *
*                              =================                              *
*                              |               |                              *
*                              |     A D F     |                              *
*                              |               |                              *
*                              =================                              *
*                                                                             *
*                                                                             *
*   Online information and documentation:  http://www.scm.com                 *
*   E-mail:  support@scm.com   info@scm.com                                   *
*                                                                             *
*   Scientific publications using ADF results must be properly referenced     *
*   See the User Manuals (or the web site) for recommended citations          *
*   The terms and conditions of the End User License Agreement apply to       *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html                *
*                                                                             *
******************************  macintel  *************************************

ADF 2007.01  RunTime: Jun16-2008 09:15:58
RuCO2 fragment


===========================
A T T A C H E D   F I L E S
===========================



===============================
M O D E L   P A R A M E T E R S
===============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                           VWN
   Gradient Corrections:          Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                      Restricted
   Fragments:                     Restricted

OTHER ASPECTS
   Relativistic Corrections:      ---
   Core Treatment:                Frozen Orbital(s)

   Electric Field:                ---

   Hyperfine or Zeeman Interaction:   ---


Fragment File(s)
----------------
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jun16-2008 09:15:50
        title: Oxygen (TZP)
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jun16-2008 09:15:48
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jun16-2008 09:15:31
        title: Hydrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jun16-2008 09:15:47
        title: Ruthenium (TZP, 3d frozen)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jun16-2008 09:15:45
        title: Nitrogen (TZP)


                                  ********************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ********************************************


Energy gradients wrt nuclear displacements
==========================================

    Atom      Cartesian (a.u./angstrom)
                X         Y         Z
-----------------------------------------
    1 O     0.000017 -0.000010 -0.000020
    2 O    -0.000034 -0.000045 -0.000025
    3 C     0.000071 -0.000019 -0.000011
    4 C     0.000030  0.000057  0.000027
    5 H     0.000002 -0.000001  0.000000
    6 Ru   -0.000087  0.000004  0.000034
    7 C    -0.000011 -0.000013 -0.000011
    8 H     0.000007  0.000008 -0.000002
    9 N    -0.000003  0.000017  0.000017
   10 H     0.000015  0.000000 -0.000003
   11 C     0.000005  0.000016  0.000013
   12 C     0.000031 -0.000001 -0.000027
   13 C    -0.000006  0.000003  0.000011
   14 C    -0.000016 -0.000023 -0.000007
   15 C    -0.000006 -0.000015 -0.000010
   16 C    -0.000009 -0.000008  0.000061
```

```
    17 C    -0.000011  0.000019 -0.000003
    18 C    -0.000005  0.000005 -0.000004
    19 H    -0.000005 -0.000010 -0.000010
    20 H    -0.000006 -0.000010 -0.000002
    21 C    -0.000011  0.000016 -0.000026
    22 H     0.000013  0.000010  0.000001
    23 C     0.000020 -0.000004  0.000002
    24 H     0.000005  0.000005 -0.000003
    25 H    -0.000005  0.000000 -0.000003
 ----------------------------------------
current energy                          -6.09829774 Hartree
abs of energy change              0.00000039     0.00100000    T
constrained gradient max          0.00008736     0.00010000    T
constrained gradient rms          0.00002166     0.00006667    T
gradient max                      0.00008736
gradient rms                      0.00002166
cart. step max                    0.00152354     0.01000000    T
cart. step rms                    0.00039146     0.00666667    T

 Number of elements of the density matrix on this node (used, total):     43660     87571


 ======================================================
 Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
 ======================================================

 General Accuracy Parameter :                          6.00

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
    Nr. of used Symmetry Operators                     1

    Points in the Atomic Spheres                   27088
    Points in the Atomic Polyhedra                279001
    Points in the Outer Region                     41010
    ----------------------------------------------------
    Total                                         347099

    Sum of Weights                               164038.368546

 Total nr. of points:     347099
 Nr. of blocks:             2712
 Block length:               128
 Nr. of dummy points:         37


 Test of Precision of the Numerical Integration Grid
 ======================================================

 Integral of the Total Core Density:                  27.99999959697438
 Relative Error:                                      -1.439E-08



 ============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

                                        hartree             eV         kcal/mol          kJ/mol
                                  ---------------     ----------     ----------     ----------

Pauli Repulsion
  Kinetic (Delta T^0):             73.404510087599604     1997.4383       46062.03       192723.51
  Delta V^Pauli Coulomb:          -37.465673001850391    -1019.4928      -23510.07       -98366.11
  Delta V^Pauli LDA-XC:            -9.016105574933075     -245.3407       -5657.69       -23671.78
  Delta V^Pauli GGA-Exchange:       0.498326797969398       13.5602         312.70         1308.36
  Delta V^Pauli GGA-Correlation:   -0.132515758677335       -3.6059         -83.15         -347.92
                                  ---------------     ----------     ----------     ----------
  Total Pauli Repulsion:           27.288542550108197      742.5590       17123.82        71646.06
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  27.288542550108197      742.5590       17123.82        71646.06
  Electrostatic Interaction:        -5.769530285126825     -156.9969       -3620.44       -15147.90
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  ---------------     ----------     ----------     ----------
  Total Steric Interaction:         21.519012264981370      585.5621       13503.39        56498.16
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -27.610623670532583     -751.3233      -17325.93       -72491.68
                                  ---------------     ----------     ----------     ----------
  Total Orbital Interactions:      -27.617317596370683     -751.5054      -17330.13       -72509.26

Alternative Decomposition Orb.Int.
  Kinetic:                         -67.627405684926501    -1840.2353      -42436.84      -177555.73
```

Coulomb:	36.723639962072056	999.3011	23044.43	96417.90
XC:	3.286448126483814	89.4288	2062.28	8628.57
Total Orbital Interactions:	-27.617317596370633	-751.5054	-17330.13	-72509.26
Residu (E=Steric+OrbInt+Res):	0.000007593366699	0.0002	0.00	0.02
Total Bonding Energy:	-6.098297738022613	-165.9431	-3826.74	-16011.08

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-5.769530285126825	-156.9969	-3620.44	-15147.90
Kinetic Energy:	5.777104402673103	157.2030	3625.19	15167.79
Coulomb (Steric+OrbInt) Energy:	-0.742025446411638	-20.1915	-465.63	-1948.19
XC Energy:	-5.363846409157198	-145.9577	-3365.86	-14082.78
Total Bonding Energy:	-6.098297738022558	-165.9431	-3826.74	-16011.08

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): 0.0009139915
2. Electrostatic (Fit correction): 0.0000000000

3. Geometry optimizations taking into account solvation (COSMO procedure) by tetrahydrofuran.

a) ax-ax-3c

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                             Build 200711141748            *
*                                                                           *
*                                                                           *
*                               =================                           *
*                               |               |                           *
*                               |     A D F     |                           *
*                               |               |                           *
*                               =================                           *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  pentium64_linux  *****************************

ADF 2007.01  RunTime: Jul23-2008 14:55:14
axial-OH-THF


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                          VWN
   Gradient Corrections:         Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                     Restricted
   Fragments:                    Restricted

OTHER ASPECTS
   Relativistic Corrections:     ---
   Core Treatment:               Frozen Orbital(s)

   Electric Field:               ---

   Hyperfine or Zeeman Interaction:   ---

SOLVATION
-------------------------------------------

  The Solvent-Excluding surface is calculated

       Division Level for Surface Triangles (NDIV)              3
       Final Division Level for Triangles (NFDIV)               1
       Radius of the Solvent (RSOL)                    3.18000 angstr
       Minimum Radius for new sphere (RMINSOLV)        0.50000 angstr
       Overlapping Factor (OFAC)                       0.80000
       New spheres will be assigned to the initials using ASSG1

  Dielectric Constant (EPSL)                           7.58000

       COSMO equation is solved iteratively-          conjugate-gradient

       Maximun of Iterations for Charges (NCIX)            300
       Criterion for Charge convergence (CCNV)         1.0E-06

  Disk size scaled by                                  0.10000

  Max order of Legendre Polynomial in Disk Potential        4

  Potential expansion cutoff tolerance                 0.10000

  Geometry-dependent empirical factor                  0.00000

  COSMO charges included variationally in SCF

       COSMO included at every SCF cycle

  C-Matrix calculated in cspmtx

  In cspmtx, C-Matrix calculated using fitted potential

-------------------------------------------


 Fragment File(s)
 ----------------
 C:
         file : t21.C
         jobid: ADF 2007.01  RunTime: Jul23-2008 14:55:12
         title: Carbon (TZP)
 H:
         file : t21.H
         jobid: ADF 2007.01  RunTime: Jul23-2008 14:55:08
         title: Hydrogen (TZP)
 O:
         file : t21.O
         jobid: ADF 2007.01  RunTime: Jul23-2008 14:55:11
```

```
        title: Oxygen (TZP)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jul23-2008 14:55:10
        title: Chlorine (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul23-2008 14:55:08
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul23-2008 14:55:09
        title: Ruthenium (TZP, 3d frozen)


                                  ******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ******************************************


==========================
Geometry Convergence Tests
==========================

Energy  old :        -13.28882507
        new :        -13.28879786

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy       0.00002721     0.00100000    YES        0.52001337
gradient max           0.00081031     0.00100000    YES        0.50272335
gradient rms           0.00018144     0.00066667    YES        0.68170168
cart. step max         0.00241952     0.01000000    YES        0.56846243
cart. step rms         0.00058947     0.00666667    YES        0.45694838

prediction dE :       -0.00000496


*************************************************************************************************
                            Geometry CONVERGED
*************************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************


Coordinates (Cartesian)
=======================

    Atom                 bohr                                  angstrom                 Geometric Variables
                  X           Y           Z           X           Y           Z       (0:frozen, *:LT par.)
-----------------------------------------------------------------------------------------------------------
    1 C       6.563477   -0.510361   -5.736903    3.473243   -0.270071   -3.035839      1       2       3
    2 H       2.477071   -0.097916   -5.767412    1.310809   -0.051815   -3.051983      4       5       6
    3 O       0.302786    7.637985   -4.829826    0.160228    4.041847   -2.555834      7       8       9
    4 C       4.255705    0.386899   -4.852651    2.252022    0.204738   -2.567913     10      11      12
    5 C       8.759157    0.162785   -4.428740    4.635147    0.086142   -2.343588     13      14      15
    6 Cl     -2.152106   -0.036710   -3.692752   -1.138846   -0.019426   -1.954120     16      17      18
    7 C       0.415784    5.961056   -3.411858    0.220023    3.154455   -1.805477     19      20      21
    8 N       4.071890    1.881310   -2.801449    2.154751    0.995546   -1.482463     22      23      24
    9 O       3.212709   -5.857577   -2.553465    1.700092   -3.099696   -1.351235     25      26      27
   10 C       8.572783    1.724348   -2.320264    4.536521    0.912486   -1.227831     28      29      30
   11 O      -4.522600   -7.629512   -1.868980   -2.393257   -4.037364   -0.989022     31      32      33
   12 H      10.263829    2.274716   -1.290373    5.431385    1.203728   -0.682836     34      35      36
   13 C       1.540609   -4.774778   -1.627358    0.815255   -2.526704   -0.861161     37      38      39
   14 C       6.196386    2.598383   -1.526820    3.278986    1.375005   -0.807958     40      41      42
   15 C      -3.282936   -5.956585   -1.161157   -1.737255   -3.152089   -0.614458     43      44      45
   16 Ru      0.571226    3.228370   -1.126616    0.302280    1.708380   -0.596180     46      47      48
   17 H      -6.183874    0.150424   -0.624775   -3.272365    0.079601   -0.330617     49      50      51
   18 Ru     -1.268942   -3.243901   -0.025919   -0.671495   -1.716598   -0.013716     52      53      54
   19 C       5.761658    4.322289    0.599501    3.048938    2.287257    0.317242     55      56      57
   20 C      -2.190894    4.635527    0.649647   -1.159371    2.453015    0.343778     58      59      60
   21 C       3.226268    5.058234    1.091920    1.707267    2.676702    0.577819     61      62      63
   22 C      -6.271392   -0.333855    1.373441   -3.318677   -0.176668    0.726794     64      65      66
   23 O       0.973478   -0.074281    1.199546    0.515143   -0.039308    0.634772     67      68      69
   24 H       9.696707    4.706663    1.712896    5.131276    2.490659    0.906426     70      71      72
   25 H      -9.710034    1.689000    2.145477   -5.138328    0.893781    1.135337     73      74      75
   26 C       7.754217    5.279247    2.087220    4.103355    2.793657    1.104509     76      77      78
   27 O      -3.806571    5.648082    1.745151   -2.014351    2.988836    0.923494     79      80      81
   28 N      -4.369025   -1.788216    2.240680   -2.311989   -0.946283    1.185717     82      83      84
   29 H       2.668590   -7.320509    2.559453    1.412157   -3.873847    1.354404     85      86      87
   30 C      -8.211539    0.517609    2.928476   -4.345359    0.273907    1.549683     88      89      90
   31 C       2.785789    6.783967    3.057110    1.474176    3.589921    1.617753     91      92      93
   32 H       0.873425    7.422629    3.479073    0.462197    3.927886    1.841046     94      95      96
   33 C      -0.586660   -4.979065    3.418066   -0.310447   -2.634808    1.808763     97      98      99
   34 C       7.269958    6.973389    4.047157    3.847096    3.690158    2.141663    100     101     102
   35 C       1.374577   -6.661072    4.019791    0.727395   -3.524887    2.127182    103     104     105
   36 C       4.778323    7.731248    4.525288    2.528579    4.091200    2.394679    106     107     108
   37 H       8.821970    7.705856    5.186618    4.668385    4.077763    2.744640    109     110     111
   38 C      -4.320953   -2.512585    4.718492   -2.286550   -1.329603    2.496918    112     113     114
   39 C      -8.165975   -0.157900    5.483453   -4.321248   -0.083557    2.901718    115     116     117
   40 H       4.377674    9.067755    6.044030    2.316565    4.798449    3.198363    118     119     120
   41 C      -2.232091   -4.203946    5.396265   -1.181172   -2.224632    2.855581    121     122     123
   42 C      -6.214792   -1.677919    6.378494   -3.288727   -0.887916    3.375354    124     125     126
   43 C       1.728077   -7.529390    6.497102    0.914459   -3.984382    3.438118    127     128     129
   44 H       3.274009   -8.831138    6.908068    1.732531   -4.673237    3.655592    130     131     132
   45 H      -9.645454    0.484203    6.764168   -5.104154    0.256229    3.579444    133     134     135
   46 C      -1.860089   -5.079652    7.886430   -0.984317   -2.688036    4.173319    136     137     138
   47 H      -6.166313   -2.240214    8.354366   -3.263072   -1.185470    4.420940    139     140     141
   48 C       0.112716   -6.734804    8.440343    0.059647   -3.563905    4.466437    142     143     144
   49 H      -3.114898   -4.468061    9.400651   -1.648333   -2.364396    4.974610    145     146     147
   50 H       0.388901   -7.404874   10.368578    0.205798   -3.918490    5.486815    148     149     150
   51 H      10.600852   -0.517179   -5.051103    5.609729   -0.273679   -2.672928    151     152     153
   52 H       6.621768   -1.716911   -7.401858    3.504089   -0.908550   -3.916894    154     155     156
   53 H       0.609010    0.286879    2.967991    0.322274    0.151810    1.570593    157     158     159
-----------------------------------------------------------------------------------------------------------
```

```
 About initial set of coordinates
 --------------------------------
 Number of spheres               =      53
 Number of TOTAL coord.          =      53

 about final set of coordinates
 ------------------------------
 ncor,nptsaf,npsurf=     260      60    2189


 ---------------------------------------------
  COSMO surface
  Area            =         1600.711
  Volume          =         3743.151
  Number of Points =        2189
 ---------------------------------------------

 Number of elements of the density matrix on this node (used, total):     97079    396495


 ====================================================
 Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
 ====================================================

 General Accuracy Parameter :                          5.00

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
    Nr. of used Symmetry Operators                     1

    Points in the Atomic Spheres                   39550
    Points in the Atomic Polyhedra                454287
    Points in the Outer Region                     36028
    ---------------------------------------------------
    Total                                         529865

    Sum of Weights                                172322.805878

 Total nr. of points:     529865
 Nr. of blocks:             4140
 Block length:               128
 Nr. of dummy points:         55


 Test of Precision of the Numerical Integration Grid
 ===================================================

 Integral of the Total Core Density:                  55.99999208038639
 Relative Error:                                      -1.414E-07


 ============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	154.053401221526912	4192.0063	96669.98	404467.15
Delta V^Pauli Coulomb:	-80.039243614995200	-2177.9786	-50225.39	-210143.00
Delta V^Pauli LDA-XC:	-19.079129749497781	-519.1695	-11972.34	-50092.25
Delta V^Pauli GGA-Exchange:	1.112167940966742	30.2636	697.90	2920.00
Delta V^Pauli GGA-Correlation:	-0.311076391612604	-8.4648	-195.20	-816.73
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	55.736119406388070	1516.6570	34974.95	146335.16
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	55.736119406388070	1516.6570	34974.95	146335.16
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-11.861686721142723	-322.7729	-7443.32	-31142.85
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	43.874432685245345	1193.8841	27531.63	115192.31
Orbital Interactions				
A:	-57.126000636582091	-1554.4776	-35847.11	-149984.29
Total Orbital Interactions:	-57.132884285706723	-1554.6649	-35851.43	-150002.37
Alternative Decomposition Orb.Int.				
Kinetic:	-141.455760105592049	-3849.2071	-88764.84	-371392.05
Coulomb:	77.748609320675598	2115.6473	48787.99	204128.94
XC:	6.574266499209576	178.8949	4125.41	17260.73

Total Orbital Interactions:	-57.132884285706872	-1554.6649	-35851.43	-150002.37
Residu (E=Steric+OrbInt+Res):	0.000000699438322	0.0000	0.00	0.00
Solvation Energy (el):	-0.030349551206372	-0.8259	-19.04	-79.68
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.006021711976085	0.1639	3.78	15.81
Total Bonding Energy:	-13.282778740253343	-361.4428	-8335.07	-34873.93

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.861686721142723	-322.7729	-7443.32	-31142.85
Kinetic Energy:	12.597641115934863	342.7993	7905.14	33075.10
Coulomb (Steric+OrbInt) Energy:	-2.290633594881285	-62.3313	-1437.39	-6014.06
XC Energy:	-11.703771700934066	-318.4758	-7344.23	-30728.25
Solvation:	-0.024327839230287	-0.6620	-15.27	-63.87
Total Bonding Energy:	-13.282778740253498	-361.4428	-8335.07	-34873.93

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): -0.0030697956
2. Electrostatic (Fit correction): 0.0000000000

b) ax-eq-3c

```
*******************************************************************************
*                                                                             *
*  ------------------------------------                                       *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007     *
*  ------------------------------------                                       *
*                                              Build 200711141748             *
*                                                                             *
*                                                                             *
*                               =================                             *
*                               |               |                             *
*                               |     A D F     |                             *
*                               |               |                             *
*                               =================                             *
*                                                                             *
*                                                                             *
*   Online information and documentation:  http://www.scm.com                 *
*   E-mail:  support@scm.com   info@scm.com                                   *
*                                                                             *
*   Scientific publications using ADF results must be properly referenced     *
*   See the User Manuals (or the web site) for recommended citations          *
*   The terms and conditions of the End User License Agreement apply to       *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html                *
*                                                                             *
*****************************  pentium64_linux  *******************************

ADF 2007.01  RunTime: Jul23-2008 14:58:38
equatorial-parallel-OH


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                      == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---

SOLVATION
-------------------------------------------

 The Solvent-Excluding surface is calculated

      Division Level for Surface Triangles (NDIV)                3
      Final Division Level for Triangles (NFDIV)                 1
      Radius of the Solvent (RSOL)                         3.18000 angstr
      Minimum Radius for new sphere (RMINSOLV)             0.50000 angstr
      Overlapping Factor (OFAC)                            0.80000
      New spheres will be assigned to the initials using ASSG1

 Dielectric Constant (EPSL)                                7.58000

      COSMO equation is solved iteratively-              conjugate-gradient

      Maximun of Iterations for Charges (NCIX)                 300
      Criterion for Charge convergence (CCNV)              1.0E-06

 Disk size scaled by                                       0.10000

 Max order of Legendre Polynomial in Disk Potential           4

 Potential expansion cutoff tolerance                      0.10000

 Geometry-dependent empirical factor                       0.00000

 COSMO charges included variationally in SCF

      COSMO included at every SCF cycle

 C-Matrix calculated in cspmtx

 In cspmtx, C-Matrix calculated using fitted potential

-------------------------------------------


 Fragment File(s)
 ----------------
 C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul23-2008 14:57:11
        title: Carbon (TZP)
 H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul23-2008 14:57:08
        title: Hydrogen (TZP)
 Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jul23-2008 14:57:10
        title: Chlorine (TZP)
 N:
```

```
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul23-2008 14:57:08
        title: Nitrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul23-2008 14:57:09
        title: Oxygen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul23-2008 14:57:08
        title: Ruthenium (TZP, 3d frozen)


                                  ******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ******************************************


============================
G E O M E T R Y   U P D A T E  ***  17  ***
============================

*** Using NEW gradient routines ***

Energy gradients wrt nuclear displacements
==========================================

    Atom      Cartesian (a.u./angstrom)
                X         Y         Z
----------------------------------------
    1 C    -0.000117 -0.000102  0.000033
    2 H    -0.000154 -0.000143  0.000022
    3 C    -0.000072 -0.000137  0.000036
    4 C     0.000001 -0.000119  0.000024
    5 Cl    0.000277 -0.000158 -0.000239
    6 N    -0.000197 -0.000374 -0.000191
    7 O     0.000239  0.000223  0.000349
    8 C    -0.000007  0.000024 -0.000009
    9 O     0.000030 -0.000259 -0.000069
   10 H     0.000083 -0.000002  0.000032
   11 C    -0.000888 -0.000027 -0.000240
   12 C     0.000012 -0.000130 -0.000008
   13 C     0.000285  0.000516  0.000129
   14 Ru    0.000202  0.000891  0.000107
   15 H    -0.000063  0.000003 -0.000011
   16 Ru    0.000099 -0.000624  0.000061
   17 C     0.000057  0.000029  0.000032
   18 C     0.000997 -0.000709 -0.000392
   19 C     0.000216  0.000065 -0.000228
   20 C    -0.000083  0.000092 -0.000023
   21 H     0.000183  0.000109 -0.000010
   22 H    -0.000035 -0.000003  0.000027
   23 C     0.000077  0.000013 -0.000067
   24 O    -0.000597 -0.000158 -0.000244
   25 N    -0.000106 -0.000101  0.000070
   26 H     0.000031  0.000050  0.000015
   27 C    -0.000023 -0.000026  0.000007
   28 C     0.000005  0.000068  0.000041
   29 H     0.000089  0.000061 -0.000069
   30 C    -0.000177  0.000090  0.000062
   31 C     0.000213  0.000133 -0.000095
   32 C    -0.000013  0.000038 -0.000074
   33 C     0.000134  0.000133 -0.000019
   34 H     0.000260  0.000167 -0.000021
   35 C    -0.000063  0.000087  0.000019
   36 C    -0.000076  0.000045  0.000015
   37 H     0.000190  0.000137 -0.000065
   38 C     0.000041  0.000080  0.000017
   39 C     0.000006 -0.000072  0.000037
   40 C     0.000088  0.000016  0.000032
   41 H     0.000032  0.000095  0.000008
   42 H    -0.000005 -0.000033 -0.000008
   43 C    -0.000052 -0.000033  0.000062
   44 H    -0.000018  0.000005  0.000004
   45 C     0.000030  0.000080  0.000036
   46 H     0.000024  0.000050  0.000001
   47 H     0.000057  0.000081  0.000003
   48 H    -0.000055 -0.000109  0.000043
   49 H    -0.000126 -0.000185  0.000003
   50 O    -0.000501  0.000116  0.000072
   51 H    -0.000222  0.000080  0.000186
   52 C    -0.000031 -0.000282  0.000175
   53 O    -0.000276  0.000210  0.000323
----------------------------------------


=========================
Geometry Convergence Tests
=========================

Energy  old :        -13.28516158
        new :        -13.28518595

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value          Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy      -0.00002437     0.00050000    YES        0.76342064
gradient max           0.00096606     0.00100000    YES        0.68513242
gradient rms           0.00020439     0.00066667    YES        0.81808943
cart. step max         0.00713196     0.01000000    YES        2.20408168
cart. step rms         0.00230590     0.00666667    YES        3.08484563

prediction dE :       -0.00002482


*****************************************************************************************************
                              Geometry CONVERGED
*****************************************************************************************************
```

```
                    ********************
                    *  Final Geometry  *
                    ********************


Coordinates (Cartesian)
=======================

    Atom                 bohr                                angstrom                Geometric Variables
                  X           Y           Z           X           Y           Z       (0:frozen, *:LT par.)
-------------------------------------------------------------------------------------------------------------
    1 C       6.647777   -1.702077   -6.534872    3.517852   -0.900700   -3.458105      1       2       3
    2 H       5.537448   -0.652863   -2.723094    2.930291   -0.345480   -1.440999      4       5       6
    3 C       5.212616   -0.423688   -4.742253    2.758397   -0.224206   -2.509492      7       8       9
    4 C       6.094488   -1.325051   -9.091941    3.225064   -0.701187   -4.811248     10      11      12
    5 Cl      2.363147    0.449107    1.110294    1.250524    0.237657    0.587542     13      14      15
    6 N       3.324934    1.161264   -5.383725    1.759479    0.614514   -2.848944     16      17      18
    7 O       3.311051   -6.126451   -2.625705    1.752133   -3.241978   -1.389463     19      20      21
    8 C       4.168047    0.336051   -9.760355    2.205635    0.177830   -5.164957     22      23      24
    9 O      -4.563469   -6.959740   -1.746890   -2.414884   -3.682936   -0.924415     25      26      27
   10 H       3.729237    0.665337  -11.740652    1.973427    0.352081   -6.212885     28      29      30
   11 C       1.761967   -4.822673   -1.765169    0.932393   -2.552048   -0.934087     31      32      33
   12 C       2.797961    1.601683   -7.873443    1.480617    0.847574   -4.166446     34      35      36
   13 C      -3.139159   -5.402854   -1.123045   -1.661172   -2.859067   -0.594290     37      38      39
   14 Ru      0.907414    3.171178   -2.743265    0.480183    1.678115   -1.451673     40      41      42
   15 H      -5.230512    0.942453   -0.686583   -2.767868    0.498725   -0.363324     43      44      45
   16 Ru     -0.804630   -2.945089   -0.141865   -0.425792   -1.558474   -0.075072     46      47      48
   17 C       0.804162    3.472421   -8.327184    0.425544    1.837526   -4.406556     49      50      51
   18 C      -1.408570    5.117142   -0.835108   -0.745383    2.707875   -0.441920     52      53      54
   19 C      -0.324982    4.610478   -6.170546   -0.171973    2.439760   -3.265312     55      56      57
   20 C      -5.369630    0.506622    1.321922   -2.841486    0.268093    0.699531     58      59      60
   21 H       0.931927    3.319019  -12.431307    0.493154    1.756349   -6.578365     61      62      63
   22 H      -8.570127    2.886344    2.114563   -4.535116    1.527388    1.118978     64      65      66
   23 C       0.062384    4.195811  -10.783166    0.033012    2.220327   -5.706206     67      68      69
   24 O      -2.806513    6.431537    0.236763   -1.485143    3.403423    0.125289     70      71      72
   25 N      -3.632040   -1.136309    2.192069   -1.921993   -0.601309    1.159993     73      74      75
   26 H       2.692360   -7.481023    2.427222    1.424736   -3.958787    1.284431     76      77      78
   27 C      -7.193118    1.568934    2.889258   -3.806434    0.830244    1.528929     79      80      81
   28 C      -2.159566    6.484624   -6.571675   -1.142793    3.431515   -3.477581     82      83      84
   29 H      -3.053109    7.429598   -4.974539   -1.615636    3.931574   -2.632413     85      86      87
   30 C      -0.230085   -4.748151    3.319340   -0.121756   -2.512613    1.756519     88      89      90
   31 C      -1.771694    6.053936  -11.132581   -0.937540    3.203605   -5.891108     91      92      93
   32 C       1.528606   -6.644366    3.906906    0.808904   -3.516047    2.067445     94      95      96
   33 C      -2.879287    7.201936   -9.017812   -1.523653    3.811100   -4.772020     97      98      99
   34 H      -2.324591    6.615160  -13.036233   -1.230121    3.500592   -6.898477    100     101     102
   35 C      -3.627821   -1.852406    4.668318   -1.919760   -0.980251    2.470367    103     104     105
   36 C      -7.196532    0.899334    5.447539   -3.808241    0.475907    2.882714    106     107     108
   37 H      -4.304929    8.670766   -9.269297   -2.278070    4.588372   -4.905101    109     110     111
   38 C      -1.725665   -3.759713    5.323638   -0.913183   -1.989555    2.817148    112     113     114
   39 C      -5.410165   -0.814844    6.337896   -2.862936   -0.431197    3.353870    115     116     117
   40 C       1.851321   -7.503322    6.392433    0.979677   -3.970587    3.382730    118     119     120
   41 H       3.245259   -8.970288    6.790683    1.717317   -4.746872    3.593475    121     122     123
   42 H      -8.593167    1.695194    6.735254   -4.547308    0.897058    3.564143    124     125     126
   43 C      -1.387467   -4.625881    7.820323   -0.734216   -2.447911    4.138337    127     128     129
   44 H      -5.409351   -1.372147    8.315865   -2.862505   -0.726109    4.400566    130     131     132
   45 C       0.398832   -6.486750    8.359583    0.211053   -3.432640    4.423701    133     134     135
   46 H      -2.517560   -3.841543    9.353219   -1.332235   -2.032857    4.949510    136     137     138
   47 H       0.654188   -7.144444   10.295017    0.346181   -3.780677    5.447888    139     140     141
   48 H       7.163522   -2.308561  -10.552020    3.790772   -1.221638   -5.583888    142     143     144
   49 H       8.149818   -2.969583   -5.928150    4.312698   -1.571436   -3.137042    145     146     147
   50 O      -1.681848    0.021088   -3.030215   -0.889996    0.011160   -1.603521    148     149     150
   51 H      -1.502242   -0.667526   -4.729973   -0.794952   -0.353240   -2.502994    151     152     153
   52 C       3.292869    5.799315   -2.390895    1.742511    3.068865   -1.265207    154     155     156
   53 O       4.764315    7.415905   -2.158916    2.521167    3.924328   -1.142449    157     158     159
-------------------------------------------------------------------------------------------------------------

About initial set of coordinates
--------------------------------
Number of spheres               =      53
Number of TOTAL coord.          =      53

about final set of coordinates
------------------------------
ncor,nptsaf,npsurf=     253      60    2289


-------------------------------------------
 COSMO surface
 Area             =         1598.633
 Volume           =         3659.296
 Number of Points =         2289
-------------------------------------------

Number of elements of the density matrix on this node (used, total):     97079    396495


=====================================================
Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
=====================================================

General Accuracy Parameter :                          5.00

Symmetry used in the points section:  NOSYM


Summary of the Symmetry Unique Points:
--------------------------------------
   Nr. of used Symmetry Operators                     1

   Points in the Atomic Spheres                   39354
   Points in the Atomic Polyhedra                438379
   Points in the Outer Region                     36207
   ------------------------------------------------------
   Total                                         513940

   Sum of Weights                                172949.589972

Total nr. of points:     513940
Nr. of blocks:             4016
Block length:               128
Nr. of dummy points:        108


Test of Precision of the Numerical Integration Grid
```

```
 ====================================================

 Integral of the Total Core Density:                 55.99999322447157
 Relative Error:                                     -1.210E-07


 ============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	154.089284374563420	4192.9828	96692.50	404561.36
Delta V^Pauli Coulomb:	-80.071921640863096	-2178.8678	-50245.89	-210228.80
Delta V^Pauli LDA-XC:	-19.086262960286252	-519.3636	-11976.81	-50110.98
Delta V^Pauli GGA-Exchange:	1.113407381969616	30.2974	698.67	2923.25
Delta V^Pauli GGA-Correlation:	-0.311652367355379	-8.4805	-195.56	-818.24
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	55.732854788028312	1516.5681	34972.90	146326.59
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	55.732854788028312	1516.5681	34972.90	146326.59
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-11.866284430473929	-322.8980	-7446.21	-31154.93
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	43.866570357554380	1193.6701	27526.69	115171.66
Orbital Interactions				
A:	-57.112917156174930	-1554.1216	-35838.90	-149949.94
Total Orbital Interactions:	-57.119519785880428	-1554.3012	-35843.04	-149967.28
Alternative Decomposition Orb.Int.				
Kinetic:	-141.484582367181673	-3849.9914	-88782.93	-371467.72
Coulomb:	77.787327294447323	2116.7009	48812.29	204230.60
XC:	6.577735286853827	178.9893	4127.59	17269.84
Total Orbital Interactions:	-57.119519785880520	-1554.3012	-35843.04	-149967.28
Residu (E=Steric+OrbInt+Res):	-0.000000069578914	0.0000	0.00	0.00
Solvation Energy (el):	-0.032211807386534	-0.8765	-20.21	-84.57
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.006016267306523	0.1637	3.78	15.80
Total Bonding Energy:	-13.279145037984975	-361.3439	-8332.79	-34864.39

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.866284430473929	-322.8980	-7446.21	-31154.93
Kinetic Energy:	12.604702007381746	342.9914	7909.57	33093.64
Coulomb (Steric+OrbInt) Energy:	-2.284594415994690	-62.1670	-1433.60	-5998.20
XC Energy:	-11.706772658818185	-318.5575	-7346.11	-30736.13
Solvation:	-0.026195540080011	-0.7128	-16.44	-68.78
Total Bonding Energy:	-13.279145037985067	-361.3439	-8332.79	-34864.39

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): -0.0026188294
2. Electrostatic (Fit correction):   0.0000000000

c) eq-eq-3c

```
*******************************************************************************
*                                                                             *
*  ------------------------------------                                       *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007     *
*  ------------------------------------                                       *
*                                              Build 200711141748             *
*                                                                             *
*                                                                             *
*                              =================                              *
*                              |               |                              *
*                              |     A D F     |                              *
*                              |               |                              *
*                              =================                              *
*                                                                             *
*                                                                             *
*   Online information and documentation:  http://www.scm.com                 *
*   E-mail:  support@scm.com   info@scm.com                                   *
*                                                                             *
*   Scientific publications using ADF results must be properly referenced     *
*   See the User Manuals (or the web site) for recommended citations          *
*   The terms and conditions of the End User License Agreement apply to       *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html                *
*                                                                             *
*****************************  pentium64_linux  *******************************

ADF 2007.01  RunTime: Jul24-2008 16:58:59
equatorial-OH


===========================
A T T A C H E D   F I L E S
===========================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                          VWN
   Gradient Corrections:         Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                     Restricted
   Fragments:                    Restricted

OTHER ASPECTS
   Relativistic Corrections:     ---
   Core Treatment:               Frozen Orbital(s)

   Electric Field:               ---

   Hyperfine or Zeeman Interaction:   ---

SOLVATION
-------------------------------------------

  The Solvent-Excluding surface is calculated

       Division Level for Surface Triangles (NDIV)              3
       Final Division Level for Triangles (NFDIV)               1
       Radius of the Solvent (RSOL)                   3.18000 angstr
       Minimum Radius for new sphere (RMINSOLV)       0.50000 angstr
       Overlapping Factor (OFAC)                      0.80000
       New spheres will be assigned to the initials using ASSG1

  Dielectric Constant (EPSL)                          7.58000

       COSMO equation is solved iteratively-        conjugate-gradient

       Maximun of Iterations for Charges (NCIX)           300
       Criterion for Charge convergence (CCNV)        1.0E-06

  Disk size scaled by                                 0.10000

  Max order of Legendre Polynomial in Disk Potential       4

  Potential expansion cutoff tolerance                0.10000

  Geometry-dependent empirical factor                 0.00000

  COSMO charges included variationally in SCF

       COSMO included at every SCF cycle

  C-Matrix calculated in cspmtx

  In cspmtx, C-Matrix calculated using fitted potential

-------------------------------------------


Fragment File(s)
----------------
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul24-2008 16:56:05
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul24-2008 16:56:00
        title: Hydrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul24-2008 16:56:05
        title: Oxygen (TZP)
```

```
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul24-2008 16:56:01
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul24-2008 16:56:03
        title: Ruthenium (TZP, 3d frozen)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jul24-2008 16:56:02
        title: Chlorine (TZP)


                                  ********************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ********************************************


==========================
Geometry Convergence Tests
==========================

Energy  old :        -13.28076053
        new :        -13.28078884

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy      -0.00002831     0.00100000    YES         0.83160108
gradient max           0.00099916     0.00100000    YES         0.91414683
gradient rms           0.00022198     0.00066667    YES         1.01483267
cart. step max         0.00635838     0.01000000    YES         0.92664433
cart. step rms         0.00189156     0.00666667    YES         0.93195578

prediction dE :       -0.00001481

*************************************************************************************************
                           Geometry CONVERGED
*************************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************


Coordinates (Cartesian)
=======================

    Atom                  bohr                                  angstrom                  Geometric Variables
                 X           Y           Z           X           Y           Z       (0:frozen, *:LT par.)
-----------------------------------------------------------------------------------------------------------
    1 C       6.371104   -0.650122   -5.704918    3.371443   -0.344030   -3.018913     1     2     3
    2 H       2.270503   -0.509433   -5.247926    1.201498   -0.269580   -2.777083     4     5     6
    3 O      -0.221455    7.143608   -5.133864   -0.117189    3.780234   -2.716724     7     8     9
    4 C       4.113875    0.194542   -4.654339    2.176969    0.102947   -2.462970    10    11    12
    5 C       8.639641    0.335402   -4.769401    4.571901    0.177487   -2.523858    13    14    15
    6 O      -1.282012   -0.084956   -2.679073   -0.678412   -0.044957   -1.417704    16    17    18
    7 C       0.123198    5.649545   -3.555459    0.065194    2.989611   -1.881468    19    20    21
    8 N       4.058261    1.927123   -2.792790    2.147539    1.019790   -1.477881    22    23    24
    9 O       3.408463   -5.908784   -2.176831    1.803681   -3.126794   -1.151929    25    26    27
   10 C       8.574768    2.137118   -2.853143    4.537572    1.130914   -1.509818    28    29    30
   11 O      -4.443482   -7.150391   -2.578203   -2.351389   -3.783824   -1.364326    31    32    33
   12 H      10.323543    2.928469   -2.119253    5.462984    1.549679   -1.121461    34    35    36
   13 C       1.693505   -4.815396   -1.344848    0.896164   -2.548198   -0.711663    37    38    39
   14 C       6.243078    2.946391   -1.879405    3.303695    1.559163   -0.994538    40    41    42
   15 C      -3.207132   -5.654244   -1.541552   -1.697141   -2.992097   -0.815754    43    44    45
   16 Ru      0.643288    3.268130   -0.999393    0.340413    1.729420   -0.528856    46    47    48
   17 H      -5.876514    0.464549   -0.530797   -3.109717    0.245829   -0.280885    49    50    51
   18 Ru     -1.184830   -3.278798    0.118359   -0.626985   -1.735065    0.062633    52    53    54
   19 C       5.896311    4.887472    0.069935    3.120194    2.586339    0.037008    55    56    57
   20 C      -2.046912    4.739921    0.836606   -1.083179    2.508258    0.442713    58    59    60
   21 C       3.370452    5.556192    0.703989    1.783566    2.940210    0.372535    61    62    63
   22 C      -6.129283   -0.206190    1.396252   -3.243477   -0.109111    0.738865    64    65    66
   23 Cl      1.449345   -0.005098    2.393617    0.766961   -0.002698    1.266648    67    68    69
   24 H       9.885938    5.525696    0.812889    5.231413    2.924072    0.430162    70    71    72
   25 H      -9.459361    2.011848    2.106953   -5.005678    1.064624    1.114951    73    74    75
   26 C       7.954994    6.072928    1.275577    4.209602    3.213655    0.675006    76    77    78
   27 O      -3.608602    5.803787    1.962839   -1.909590    3.071232    1.038690    79    80    81
   28 N      -4.414981   -1.887002    2.239359   -2.336307   -0.998558    1.185018    82    83    84
   29 H       2.074565   -8.064783    2.502672    1.097812   -4.267699    1.324357    85    86    87
   30 C      -8.120323    0.654301    2.877622   -4.297090    0.346241    1.522772    88    89    90
   31 C       3.011788    7.478815    2.495777    1.593770    3.957619    1.320708    91    92    93
   32 H       1.109684    8.076732    3.014698    0.587220    4.274022    1.595310    94    95    96
   33 C      -1.007917   -5.501273    3.363125   -0.533367   -2.911148    1.779689    97    98    99
   34 C       7.546537    7.948414    3.081509    3.993456    4.206120    1.630664   100   101   102
   35 C       0.730808   -7.424400    3.926715    0.386727   -3.928823    2.077928   103   104   105
   36 C       5.066614    8.661073    3.678702    2.681137    4.583243    1.946685   106   107   108
   37 H       9.146407    8.849929    4.014993    4.840070    4.683181    2.124643   109   110   111
   38 C      -4.622612   -2.849611    4.625782   -2.446181   -1.507949    2.447858   112   113   114
   39 C      -8.326638   -0.260489    5.349516   -4.406267   -0.137845    2.830842   115   116   117
   40 H       4.725290   10.137074    5.078102    2.500516    5.364309    2.687216   118   119   120
   41 C      -2.743722   -4.777669    5.281116   -1.451915   -2.528234    2.794646   121   122   123
   42 C      -6.575264   -2.017535    6.219983   -3.479480   -1.067634    3.291473   124   125   126
   43 C       0.806699   -8.553447    6.321854    0.426887   -4.526289    3.345381   127   128   129
   44 H       2.192105  -10.031558    6.707994    1.160012   -5.308472    3.549718   130   131   132
   45 H      -9.848624    0.380481    6.579849   -5.211667    0.201342    3.481906   133   134   135
   46 C      -2.649984   -5.909722    7.691724   -1.402311   -3.127290    4.070285   136   137   138
   47 H      -6.725526   -2.765340    8.127856   -3.558995   -1.463355    4.301076   139   140   141
   48 C      -0.876055   -7.785612    8.217731   -0.463588   -4.119968    4.348636   142   143   144
   49 H      -3.959356   -5.323023    9.169122   -2.095201   -2.816822    4.852090   145   146   147
   50 H      -0.807284   -8.647122   10.087651   -0.427197   -4.575860    5.338155   148   149   150
   51 H      10.446292   -0.291770   -5.533984    5.527940   -0.154398   -2.928458   151   152   153
   52 H       6.341767   -2.053809   -7.208626    3.355919   -1.086829   -3.814640   154   155   156
   53 H      -3.006759    0.311727   -3.176735   -1.591109    0.164959   -1.681056   157   158   159
-----------------------------------------------------------------------------------------------------------

About initial set of coordinates
```

```
 --------------------------------
 Number of spheres               =      53
 Number of TOTAL coord.          =      53

 about final set of coordinates
 ------------------------------
 ncor,nptsaf,npsurf=     243      60    2187


 ---------------------------------------------
  COSMO surface
  Area             =         1604.053
  Volume           =         3652.291
  Number of Points =         2187
 ---------------------------------------------

 Number of elements of the density matrix on this node (used, total):     97079    396495


 ====================================================
 Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
 ====================================================

 General Accuracy Parameter :                          5.00

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
    Nr. of used Symmetry Operators                    1

    Points in the Atomic Spheres                  39354
    Points in the Atomic Polyhedra               449697
    Points in the Outer Region                    33895
    ---------------------------------------------------
    Total                                        522946

    Sum of Weights                               171674.991338

 Total nr. of points:     522946
 Nr. of blocks:             4086
 Block length:               128
 Nr. of dummy points:         62


 Test of Precision of the Numerical Integration Grid
 ===================================================

 Integral of the Total Core Density:                 55.99999462599539
 Relative Error:                                     -9.596E-08


 ============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	154.170323450376799	4195.1880	96743.35	404774.13
Delta V^Pauli Coulomb:	-80.117549475107040	-2180.1094	-50274.53	-210348.60
Delta V^Pauli LDA-XC:	-19.089247172079013	-519.4448	-11978.68	-50118.81
Delta V^Pauli GGA-Exchange:	1.112161860450094	30.2635	697.89	2919.98
Delta V^Pauli GGA-Correlation:	-0.311151896881990	-8.4669	-195.25	-816.93
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	55.764536766758852	1517.4303	34992.78	146409.77
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	55.764536766758852	1517.4303	34992.78	146409.77
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-11.871052327636569	-323.0278	-7449.20	-31167.44
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	43.893484439122282	1194.4025	27543.58	115242.33
Orbital Interactions				
A:	-57.131382660048118	-1554.6240	-35850.49	-149998.42
Total Orbital Interactions:	-57.137724883654926	-1554.7966	-35854.47	-150015.08
Alternative Decomposition Orb.Int.				
Kinetic:	-141.576909207918106	-3852.5037	-88840.86	-371710.12
Coulomb:	77.855448954229203	2118.5546	48855.04	204409.45
XC:	6.583735370034140	179.1526	4131.36	17285.59
Total Orbital Interactions:	-57.137724883654762	-1554.7966	-35854.47	-150015.08

Residu (E=Steric+OrbInt+Res):	-0.000007109234254	-0.0002	0.00	-0.02
Solvation Energy (el):	-0.036522957779945	-0.9938	-22.92	-95.89
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.006030467681630	0.1641	3.78	15.83
Total Bonding Energy:	-13.274740043865211	-361.2241	-8330.03	-34852.83

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.871052327636569	-323.0278	-7449.20	-31167.44
Kinetic Energy:	12.593414242458692	342.6842	7902.49	33064.00
Coulomb (Steric+OrbInt) Energy:	-2.262107630112084	-61.5551	-1419.49	-5939.16
XC Energy:	-11.704501838476768	-318.4957	-7344.69	-30730.17
Solvation:	-0.030492490098315	-0.8297	-19.13	-80.06
Total Bonding Energy:	-13.274740043865043	-361.2241	-8330.03	-34852.83

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): -0.0045485245
2. Electrostatic (Fit correction): 0.0000000000

4. Single Point calculations on fragments from gas-phase optimized geometries.

a) From *ax-ax*-3c

***(1)* ax-4**

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                              Build 200708202008           *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |               |                            *
*                              |     A D F     |                            *
*                              |               |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ************************************

ADF 2007.01  RunTime: Jul22-2008 18:47:23
axOHeqCl fragment


===========================
A T T A C H E D   F I L E S
===========================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
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Cl:
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        jobid: ADF 2007.01  RunTime: Jul22-2008 18:47:19
        title: Chlorine (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul22-2008 18:47:18
        title: Oxygen (TZP)
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul22-2008 18:47:17
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul22-2008 18:47:14
        title: Hydrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul22-2008 18:47:16
        title: Ruthenium (TZP, 3d frozen)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul22-2008 18:47:15
        title: Nitrogen (TZP)


                                    ************************************
                                    *  R U N   T Y P E : SINGLE POINT  *
                                    ************************************



===============
G E O M E T R Y  ***  3D  Molecule  ***
===============


ATOMS
=====                              X Y Z                    CHARGE
                                 (Angstrom)               Nucl      +Core       At.Mass
                          -------------------------    ----------------       -------
   1  Cl             -1.1324   -0.0176   -1.9371      17.00      17.00       34.9689
   2  O               1.6986   -3.1071   -1.3548       8.00       8.00       15.9949
   3  O              -2.3752   -4.0424   -1.0077       8.00       8.00       15.9949
```

```
   4  C              0.8173   -2.5296   -0.8635      6.00      6.00       12.0000
   5  C             -1.7312   -3.1526   -0.6282      6.00      6.00       12.0000
   6  H             -3.2410    0.0956   -0.3388      1.00      1.00        1.0078
   7  Ru            -0.6659   -1.7151   -0.0176     44.00     16.00      101.9043
   8  C             -3.3045   -0.1658    0.7179      6.00      6.00       12.0000
   9  O              0.5240   -0.0465    0.6220      8.00      8.00       15.9949
  10  H             -5.1166    0.9210    1.1211      1.00      1.00        1.0078
  11  N             -2.3075   -0.9439    1.1793      7.00      7.00       14.0031
  12  H              1.4131   -3.8662    1.3556      1.00      1.00        1.0078
  13  C             -4.3328    0.2891    1.5360      6.00      6.00       12.0000
  14  C             -0.3121   -2.6334    1.8045      6.00      6.00       12.0000
  15  C              0.7254   -3.5213    2.1278      6.00      6.00       12.0000
  16  C             -2.2871   -1.3321    2.4886      6.00      6.00       12.0000
  17  C             -4.3195   -0.0773    2.8856      6.00      6.00       12.0000
  18  C             -1.1853   -2.2260    2.8502      6.00      6.00       12.0000
  19  C             -3.2957   -0.8886    3.3612      6.00      6.00       12.0000
  20  C              0.9089   -3.9800    3.4367      6.00      6.00       12.0000
  21  H              1.7280   -4.6674    3.6569      1.00      1.00        1.0078
  22  H             -5.1056    0.2643    3.5606      1.00      1.00        1.0078
  23  C             -0.9903   -2.6891    4.1676      6.00      6.00       12.0000
  24  H             -3.2763   -1.1916    4.4060      1.00      1.00        1.0078
  25  C              0.0523   -3.5619    4.4633      6.00      6.00       12.0000
  26  H             -1.6558   -2.3656    4.9689      1.00      1.00        1.0078
  27  H              0.1984   -3.9161    5.4842      1.00      1.00        1.0078
  28  H              0.4365    0.1152    1.5787      1.00      1.00        1.0078


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 <Jul22-2008> <18:47:23>  RunType   : SINGLE POINT
 <Jul22-2008> <18:47:25>  Net Charge: -1 (Nuclei minus Electrons)
 <Jul22-2008> <18:47:25>  Symmetry  : NOSYM
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 <Jul22-2008> <18:47:25>  >>>> CORORT
 <Jul22-2008> <18:47:26>  >>>> FITINT
 <Jul22-2008> <18:47:36>  >>>> CLSMAT
 <Jul22-2008> <18:47:37>  >>>> ORTHON
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 <Jul22-2008> <18:49:35>    3  ErrMat   1.04664709  MaxEl  0.14215918
 <Jul22-2008> <18:50:01>    4  ErrMat   5.02727116  MaxEl -1.23038236
 <Jul22-2008> <18:50:27>    5  ErrMat   1.13234306  MaxEl -0.23070991
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 <Jul22-2008> <18:51:18>    7  ErrMat   0.25578820  MaxEl -0.05183249
 <Jul22-2008> <18:51:43>    8  ErrMat   0.10662979  MaxEl -0.02243907
 <Jul22-2008> <18:52:09>    9  ErrMat   0.04678236  MaxEl -0.00741751
 <Jul22-2008> <18:52:35>   10  ErrMat   0.01999900  MaxEl -0.00489166
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 <Jul22-2008> <18:57:14>  >>>> TOTEN
 <Jul22-2008> <19:00:40>  >>>> POPAN
 <Jul22-2008> <19:00:40>  >>>> DEBYE
 <Jul22-2008> <19:00:41>  >>>> AMETS
 <Jul22-2008> <19:00:46>   Bond Energy LDA      -7.54819466 a.u.
 <Jul22-2008> <19:00:46>   Bond Energy LDA    -205.39682736 eV
 <Jul22-2008> <19:00:46>            + GGA-X      -6.47185612 a.u.
 <Jul22-2008> <19:00:46>            + GGA-X    -176.10816539 eV
 <Jul22-2008> <19:00:46>           + GGA-XC      -6.92541455 a.u.
 <Jul22-2008> <19:00:46>           + GGA-XC    -188.45011820 eV
 <Jul22-2008> <19:00:46>  >>>> POPUL
 <Jul22-2008> <19:00:48>  NORMAL TERMINATION
 <Jul22-2008> <19:00:48>  END
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*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                              Build 200708202008           *
*                                                                           *
*                                                                           *
*                               =================                           *
*                               |               |                           *
*                               |     A D F     |                           *
*                               |               |                           *
*                               =================                           *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ************************************

ADF 2007.01  RunTime: Jul22-2008 18:37:05
RuCO2 fragment


===========================
A T T A C H E D   F I L E S
===========================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
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C:
        file : t21.C
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        title: Carbon (TZP)
H:
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        jobid: ADF 2007.01  RunTime: Jul22-2008 18:36:57
        title: Hydrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul22-2008 18:37:02
        title: Oxygen (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul22-2008 18:37:01
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul22-2008 18:37:01
        title: Ruthenium (TZP, 3d frozen)


                                    ************************************
                                    *  R U N   T Y P E : SINGLE POINT  *
                                    ************************************



===============
G E O M E T R Y  ***  3D  Molecule  ***
===============


ATOMS
=====
                              X Y Z                    CHARGE
                           (Angstrom)                Nucl     +Core       At.Mass
                      -------------------------    ----------------      -------
   1  C               3.4568   -0.2973   -3.0174      6.00      6.00       12.0000
   2  H               1.2904   -0.0789   -3.0173      1.00      1.00        1.0078
   3  O               0.1426    4.0417   -2.5449      8.00      8.00       15.9949
   4  C               2.2390    0.1853   -2.5491      6.00      6.00       12.0000
   5  C               4.6216    0.0702   -2.3367      6.00      6.00       12.0000
   6  C               0.2076    3.1530   -1.7993      6.00      6.00       12.0000
   7  N               2.1485    0.9911   -1.4760      7.00      7.00       14.0031
   8  C               4.5287    0.9092   -1.2321      6.00      6.00       12.0000
   9  H               5.4258    1.2071   -0.6933      1.00      1.00        1.0078
  10  C               3.2733    1.3769   -0.8073      6.00      6.00       12.0000
  11  Ru              0.2964    1.7053   -0.5862     44.00     16.00      101.9043
  12  C               3.0484    2.2939    0.3119      6.00      6.00       12.0000
```

```
  13  C             -1.1559    2.4523    0.3600      6.00      6.00      12.0000
  14  C              1.7069    2.6795    0.5766      6.00      6.00      12.0000
  15  H              5.1327    2.5037    0.8914      1.00      1.00       1.0078
  16  C              4.1043    2.8066    1.0913      6.00      6.00      12.0000
  17  O             -2.0047    2.9927    0.9456      8.00      8.00      15.9949
  18  C              1.4795    3.5984    1.6122      6.00      6.00      12.0000
  19  H              0.4670    3.9343    1.8370      1.00      1.00       1.0078
  20  C              3.8527    3.7077    2.1226      6.00      6.00      12.0000
  21  C              2.5352    4.1066    2.3785      6.00      6.00      12.0000
  22  H              4.6757    4.1011    2.7201      1.00      1.00       1.0078
  23  H              2.3264    4.8194    3.1788      1.00      1.00       1.0078
  24  H              5.5952   -0.2953   -2.6664      1.00      1.00       1.0078
  25  H              3.4825   -0.9537   -3.8860      1.00      1.00       1.0078

<Jul22-2008> <18:37:05>  ADF 2007.01  RunTime: Jul22-2008 18:37:05
 <Jul22-2008> <18:37:05>  RuCO2 fragment
 <Jul22-2008> <18:37:12>  RunType   : SINGLE POINT
 <Jul22-2008> <18:37:13>  Net Charge: 1 (Nuclei minus Electrons)
 <Jul22-2008> <18:37:13>  Symmetry  : NOSYM
 <Jul22-2008> <18:37:13>  >>>> FRAGM
 <Jul22-2008> <18:37:14>  >>>> CORORT
 <Jul22-2008> <18:37:14>  >>>> FITINT
 <Jul22-2008> <18:37:22>  >>>> CLSMAT
 <Jul22-2008> <18:37:22>  >>>> ORTHON
 <Jul22-2008> <18:37:24>  >>>> GENPT
 <Jul22-2008> <18:37:24>  Acc.Num.Int.=   4.500
 <Jul22-2008> <18:37:30>  Block Length= 128
 <Jul22-2008> <18:37:41>  >>>> PTBAS
 <Jul22-2008> <18:37:57>  >>>> CYCLE
 <Jul22-2008> <18:38:09>    1
 <Jul22-2008> <18:38:30>    2  ErrMat   2.41109572  MaxEl -0.31458679
 <Jul22-2008> <18:38:48>    3  ErrMat   1.15567328  MaxEl  0.23086051
 <Jul22-2008> <18:39:07>    4  ErrMat   1.59209668  MaxEl  0.23106680
 <Jul22-2008> <18:39:26>    5  ErrMat   0.51020846  MaxEl -0.07682797
 <Jul22-2008> <18:39:44>    6  ErrMat   0.25036135  MaxEl  0.04446496
 <Jul22-2008> <18:40:03>    7  ErrMat   0.13290771  MaxEl -0.01950336
 <Jul22-2008> <18:40:22>    8  ErrMat   0.04732809  MaxEl -0.01003323
 <Jul22-2008> <18:40:40>    9  ErrMat   0.01696897  MaxEl  0.00346477
 <Jul22-2008> <18:40:59>   10  ErrMat   0.00808345  MaxEl -0.00229756
 <Jul22-2008> <18:41:17>   11  ErrMat   0.00322267  MaxEl -0.00044221
 <Jul22-2008> <18:41:36>   12  ErrMat   0.00116742  MaxEl -0.00014848
 <Jul22-2008> <18:41:55>   13  ErrMat   0.00062640  MaxEl  0.00013985
 <Jul22-2008> <18:42:14>   14  ErrMat   0.00027690  MaxEl  0.00004580
 <Jul22-2008> <18:42:33>   15  ErrMat   0.00009569  MaxEl  0.00002755
 <Jul22-2008> <18:42:51>   16  ErrMat   0.00011690  MaxEl  0.00001921
 <Jul22-2008> <18:43:10>   17  ErrMat   0.00003467  MaxEl  0.00000892
 <Jul22-2008> <18:43:29>   18  ErrMat   0.00002110  MaxEl -0.00000281
 <Jul22-2008> <18:43:47>   19  ErrMat   0.00001070  MaxEl  0.00000183
 <Jul22-2008> <18:44:06>   20  ErrMat   0.00000197  MaxEl -0.00000033
 <Jul22-2008> <18:44:07>  SCF converged
 <Jul22-2008> <18:44:25>   21  ErrMat   0.00000129  MaxEl  0.00000016
 <Jul22-2008> <18:44:27>  >>>> COREPS
 <Jul22-2008> <18:44:37>  >>>> TOTEN
 <Jul22-2008> <18:46:51>  >>>> POPAN
 <Jul22-2008> <18:46:52>  >>>> DEBYE
 <Jul22-2008> <18:46:53>  >>>> AMETS
 <Jul22-2008> <18:46:59>   Bond Energy LDA      -6.65773791 a.u.
 <Jul22-2008> <18:46:59>   Bond Energy LDA    -181.16626622 eV
 <Jul22-2008> <18:46:59>           + GGA-X      -5.66454795 a.u.
 <Jul22-2008> <18:46:59>           + GGA-X    -154.14019246 eV
 <Jul22-2008> <18:46:59>          + GGA-XC      -6.09319314 a.u.
 <Jul22-2008> <18:46:59>          + GGA-XC    -165.80422149 eV
 <Jul22-2008> <18:46:59>  >>>> POPUL
 <Jul22-2008> <18:47:00>  NORMAL TERMINATION
 <Jul22-2008> <18:47:00>  END
```

b) From *ax-eq-3c*

(1) ax-4

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                              Build 200708202008           *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |               |                            *
*                              |     A D F     |                            *
*                              |               |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ************************************

ADF 2007.01  RunTime: Jul22-2008 19:45:25
axOHeqCl fragment


===========================
A T T A C H E D   F I L E S
===========================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
----------------
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:45:22
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:45:10
        title: Hydrogen (TZP)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:45:20
        title: Chlorine (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:45:15
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:45:18
        title: Ruthenium (TZP, 3d frozen)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:45:16
        title: Oxygen (TZP)


                                    ************************************
                                    *  R U N   T Y P E : SINGLE POINT  *
                                    ************************************



===============
G E O M E T R Y  ***  3D  Molecule  ***
===============


ATOMS
=====                            X Y Z                  CHARGE
                                (Angstrom)             Nucl     +Core       At.Mass
                          -------------------------    ----------------     -------
   1  C                  3.4869   -0.9329   -3.4514      6.00      6.00       12.0000
   2  H                  2.8781   -0.3841   -1.4344      1.00      1.00        1.0078
   3  C                  2.7266   -0.2520   -2.5065      6.00      6.00       12.0000
```

```
    4  C              3.2102   -0.7167   -4.8055      6.00      6.00       12.0000
    5  Cl             1.2353    0.2340    0.5606     17.00     17.00       34.9689
    6  N              1.7447    0.6011   -2.8476      7.00      7.00       14.0031
    7  C              2.2092    0.1783   -5.1609      6.00      6.00       12.0000
    8  H              1.9879    0.3657   -6.2100      1.00      1.00        1.0078
    9  C              1.4800    0.8520   -4.1659      6.00      6.00       12.0000
   10  Ru             0.4659    1.6691   -1.4483     44.00     16.00      101.9043
   11  C              0.4390    1.8516   -4.4070      6.00      6.00       12.0000
   12  C             -0.7638    2.7022   -0.4516      6.00      6.00       12.0000
   13  C             -0.1661    2.4443   -3.2656      6.00      6.00       12.0000
   14  H              0.5370    1.7966   -6.5796      1.00      1.00        1.0078
   15  C              0.0680    2.2533   -5.7076      6.00      6.00       12.0000
   16  O             -1.5208    3.3946    0.0965      8.00      8.00       15.9949
   17  C             -1.1270    3.4445   -3.4837      6.00      6.00       12.0000
   18  H             -1.6071    3.9375   -2.6384      1.00      1.00        1.0078
   19  C             -0.8896    3.2453   -5.8943      6.00      6.00       12.0000
   20  C             -1.4856    3.8416   -4.7764      6.00      6.00       12.0000
   21  H             -1.1651    3.5590   -6.9021      1.00      1.00        1.0078
   22  H             -2.2318    4.6277   -4.9108      1.00      1.00        1.0078
   23  H              3.7753   -1.2421   -5.5773      1.00      1.00        1.0078
   24  H              4.2640   -1.6229   -3.1274      1.00      1.00        1.0078
   25  O             -0.9237    0.0176   -1.5927      8.00      8.00       15.9949
   26  H             -0.8985   -0.3143   -2.5081      1.00      1.00        1.0078
   27  C              1.7439    3.0483   -1.2424      6.00      6.00       12.0000
   28  O              2.5298    3.8916   -1.0996      8.00      8.00       15.9949

<Jul22-2008> <19:45:25>  ADF 2007.01  RunTime: Jul22-2008 19:45:25
 <Jul22-2008> <19:45:25>  axOHeqCl fragment
 <Jul22-2008> <19:45:33>  RunType   : SINGLE POINT
 <Jul22-2008> <19:45:36>  Net Charge: -1 (Nuclei minus Electrons)
 <Jul22-2008> <19:45:36>  Symmetry  : NOSYM
 <Jul22-2008> <19:45:36>  >>>> FRAGM
 <Jul22-2008> <19:45:37>  >>>> CORORT
 <Jul22-2008> <19:45:37>  >>>> FITINT
 <Jul22-2008> <19:45:49>  >>>> CLSMAT
 <Jul22-2008> <19:45:50>  >>>> ORTHON
 <Jul22-2008> <19:45:54>  >>>> GENPT
 <Jul22-2008> <19:45:54>  Acc.Num.Int.=   4.500
 <Jul22-2008> <19:46:07>  Block Length= 128
 <Jul22-2008> <19:46:20>  >>>> PTBAS
 <Jul22-2008> <19:46:44>  >>>> CYCLE
 <Jul22-2008> <19:47:37>    1
 <Jul22-2008> <19:49:53>    2  ErrMat   2.30698227  MaxEl -0.32609371
 <Jul22-2008> <19:51:44>    3  ErrMat   1.05034319  MaxEl  0.13109624
 <Jul22-2008> <19:52:31>    4  ErrMat   5.01194581  MaxEl -1.14584707
 <Jul22-2008> <19:53:50>    5  ErrMat   1.12474165  MaxEl -0.22437715
 <Jul22-2008> <19:56:29>    6  ErrMat   0.38740556  MaxEl -0.06963710
 <Jul22-2008> <19:59:06>    7  ErrMat   0.24708869  MaxEl  0.05132524
 <Jul22-2008> <20:00:41>    8  ErrMat   0.10496913  MaxEl -0.02170051
 <Jul22-2008> <20:01:50>    9  ErrMat   0.04603166  MaxEl -0.00693248
 <Jul22-2008> <20:04:20>   10  ErrMat   0.01968045  MaxEl -0.00453438
 <Jul22-2008> <20:06:53>   11  ErrMat   0.01173080  MaxEl -0.00213570
 <Jul22-2008> <20:08:32>   12  ErrMat   0.00333585  MaxEl  0.00063773
 <Jul22-2008> <20:09:17>   13  ErrMat   0.00151323  MaxEl -0.00033329
 <Jul22-2008> <20:11:05>   14  ErrMat   0.00034980  MaxEl  0.00005699
 <Jul22-2008> <20:14:25>   15  ErrMat   0.00015370  MaxEl -0.00002681
 <Jul22-2008> <20:17:06>   16  ErrMat   0.00009069  MaxEl -0.00001287
 <Jul22-2008> <20:18:45>   17  ErrMat   0.00003283  MaxEl  0.00000503
 <Jul22-2008> <20:19:27>   18  ErrMat   0.00000865  MaxEl  0.00000114
 <Jul22-2008> <20:21:28>   19  ErrMat   0.00000560  MaxEl  0.00000070
 <Jul22-2008> <20:22:55>  SCF converged
 <Jul22-2008> <20:24:19>   20  ErrMat   0.00000137  MaxEl -0.00000021
 <Jul22-2008> <20:25:19>  >>>> COREPS
 <Jul22-2008> <20:26:01>  >>>> TOTEN
 <Jul22-2008> <20:32:18>  >>>> POPAN
 <Jul22-2008> <20:32:24>  >>>> DEBYE
 <Jul22-2008> <20:32:31>  >>>> AMETS
 <Jul22-2008> <20:33:29>   Bond Energy LDA      -7.54820720 a.u.
 <Jul22-2008> <20:33:29>   Bond Energy LDA    -205.39716854 eV
 <Jul22-2008> <20:33:29>           + GGA-X      -6.47198572 a.u.
 <Jul22-2008> <20:33:29>           + GGA-X    -176.11169213 eV
 <Jul22-2008> <20:33:29>          + GGA-XC      -6.92555322 a.u.
 <Jul22-2008> <20:33:29>          + GGA-XC    -188.45389185 eV
 <Jul22-2008> <20:33:29>  >>>> POPUL
 <Jul22-2008> <20:33:39>  NORMAL TERMINATION
 <Jul22-2008> <20:33:43>  END
```

(2) 5

```
*****************************************************************************
*                                                                           *
*  ---------------------------------------                                  *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007   *
*  ---------------------------------------                                  *
*                                              Build 200708202008           *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |               |                            *
*                              |     A D F     |                            *
*                              |               |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ************************************

ADF 2007.01  RunTime: Jul22-2008 19:07:53
RuCO2 fragment


==========================
A T T A C H E D   F I L E S
==========================
```

```
==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                      == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
----------------
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:07:48
        title: Oxygen (TZP)
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:07:47
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:07:22
        title: Hydrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:07:46
        title: Ruthenium (TZP, 3d frozen)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul22-2008 19:07:44
        title: Nitrogen (TZP)


                                    ************************************
                                    *  R U N   T Y P E : SINGLE POINT  *
                                    ************************************



===============
G E O M E T R Y  ***  3D  Molecule  ***
===============

ATOMS
=====
                                X Y Z                    CHARGE
                             (Angstrom)                Nucl     +Core       At.Mass
                          -------------------------    ----------------     -------
   1  O                     1.7632   -3.2392   -1.3691      8.00      8.00      15.9949
   2  O                    -2.4074   -3.7045   -0.9197      8.00      8.00      15.9949
   3  C                     0.9338   -2.5512   -0.9279      6.00      6.00      12.0000
   4  C                    -1.6630   -2.8731   -0.5895      6.00      6.00      12.0000
   5  H                    -2.7611    0.4960   -0.3602      1.00      1.00       1.0078
   6  Ru                   -0.4265   -1.5553   -0.0811     44.00     16.00     101.9043
   7  C                    -2.8398    0.2658    0.7036      6.00      6.00      12.0000
   8  H                    -4.5302    1.5293    1.1270      1.00      1.00       1.0078
   9  N                    -1.9213   -0.6021    1.1612      7.00      7.00      14.0031
  10  H                     1.4540   -3.9251    1.2814      1.00      1.00       1.0078
  11  C                    -3.8039    0.8278    1.5340      6.00      6.00      12.0000
  12  C                    -0.1075   -2.4992    1.7550      6.00      6.00      12.0000
  13  C                     0.8345   -3.4898    2.0651      6.00      6.00      12.0000
  14  C                    -1.9102   -0.9815    2.4716      6.00      6.00      12.0000
  15  C                    -3.8023    0.4707    2.8872      6.00      6.00      12.0000
  16  C                    -0.8990   -1.9814    2.8147      6.00      6.00      12.0000
  17  C                    -2.8560   -0.4329    3.3547      6.00      6.00      12.0000
  18  C                     1.0134   -3.9379    3.3798      6.00      6.00      12.0000
  19  H                     1.7623   -4.7043    3.5900      1.00      1.00       1.0078
  20  H                    -4.5413    0.8915    3.5709      1.00      1.00       1.0078
  21  C                    -0.7109   -2.4352    4.1366      6.00      6.00      12.0000
  22  H                    -2.8514   -0.7300    4.4019      1.00      1.00       1.0078
  23  C                     0.2436   -3.4077    4.4211      6.00      6.00      12.0000
  24  H                    -1.3087   -2.0226    4.9497      1.00      1.00       1.0078
  25  H                     0.3872   -3.7509    5.4465      1.00      1.00       1.0078


<Jul22-2008> <19:07:53>  ADF 2007.01  RunTime: Jul22-2008 19:07:53
 <Jul22-2008> <19:07:53>  RuCO2 fragment
 <Jul22-2008> <19:08:00>  RunType   : SINGLE POINT
 <Jul22-2008> <19:08:14>  Net Charge: 1 (Nuclei minus Electrons)
 <Jul22-2008> <19:08:14>  Symmetry  : NOSYM
 <Jul22-2008> <19:08:14>  >>>> FRAGM
 <Jul22-2008> <19:08:16>  >>>> CORORT
 <Jul22-2008> <19:08:17>  >>>> FITINT
 <Jul22-2008> <19:08:26>  >>>> CLSMAT
 <Jul22-2008> <19:08:26>  >>>> ORTHON
 <Jul22-2008> <19:08:29>  >>>> GENPT
 <Jul22-2008> <19:08:29>  Acc.Num.Int.=   4.500
 <Jul22-2008> <19:08:38>  Block Length= 128
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 <Jul22-2008> <19:09:04>  >>>> CYCLE
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 <Jul22-2008> <19:11:00>    2  ErrMat   2.40403183  MaxEl  0.39168173
 <Jul22-2008> <19:12:32>    3  ErrMat   1.15392900  MaxEl  0.21985946
 <Jul22-2008> <19:13:09>    4  ErrMat   1.56583664  MaxEl -0.21863657
 <Jul22-2008> <19:13:43>    5  ErrMat   0.50359425  MaxEl  0.11191293
 <Jul22-2008> <19:14:37>    6  ErrMat   0.24687274  MaxEl -0.04493380
 <Jul22-2008> <19:16:19>    7  ErrMat   0.13030907  MaxEl  0.02018983
 <Jul22-2008> <19:17:37>    8  ErrMat   0.04627115  MaxEl  0.00886581
 <Jul22-2008> <19:19:09>    9  ErrMat   0.01667901  MaxEl -0.00302066
```

```
<Jul22-2008> <19:20:34>   10  ErrMat   0.00787523  MaxEl  0.00198011
<Jul22-2008> <19:21:12>   11  ErrMat   0.00314049  MaxEl -0.00042730
<Jul22-2008> <19:21:48>   12  ErrMat   0.00157941  MaxEl -0.00039118
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<Jul22-2008> <19:23:28>   14  ErrMat   0.00027989  MaxEl  0.00006512
<Jul22-2008> <19:25:28>   15  ErrMat   0.00026770  MaxEl  0.00005462
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<Jul22-2008> <19:29:02>   17  ErrMat   0.00012853  MaxEl  0.00004143
<Jul22-2008> <19:30:20>   18  ErrMat   0.00009164  MaxEl  0.00002593
<Jul22-2008> <19:30:57>   19  ErrMat   0.00007781  MaxEl  0.00002136
<Jul22-2008> <19:31:29>   20  ErrMat   0.00004763  MaxEl  0.00001420
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<Jul22-2008> <19:34:24>   22  ErrMat   0.00001610  MaxEl -0.00000620
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<Jul22-2008> <19:38:43>  SCF converged
<Jul22-2008> <19:39:33>   25  ErrMat   0.00000138  MaxEl  0.00000018
<Jul22-2008> <19:39:36>  >>>> COREPS
<Jul22-2008> <19:39:57>  >>>> TOTEN
<Jul22-2008> <19:43:37>  >>>> POPAN
<Jul22-2008> <19:43:44>  >>>> DEBYE
<Jul22-2008> <19:43:49>  >>>> AMETS
<Jul22-2008> <19:44:34>   Bond Energy LDA      -6.65747672 a.u.
<Jul22-2008> <19:44:34>   Bond Energy LDA    -181.15915902 eV
<Jul22-2008> <19:44:34>            + GGA-X     -5.66324940 a.u.
<Jul22-2008> <19:44:34>            + GGA-X    -154.10485696 eV
<Jul22-2008> <19:44:34>          + GGA-XC      -6.09237756 a.u.
<Jul22-2008> <19:44:34>          + GGA-XC    -165.78202835 eV
<Jul22-2008> <19:44:34>  >>>> POPUL
<Jul22-2008> <19:44:39>  NORMAL TERMINATION
<Jul22-2008> <19:44:42>  END
```

(3) eq-4

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*******************************************************************************
*                                                                             *
*  ---------------------------------                                          *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007     *
*  ---------------------------------                                          *
*                                              Build 200708202008             *
*                                                                             *
*                                                                             *
*                             =================                               *
*                             |               |                               *
*                             |     A D F     |                               *
*                             |               |                               *
*                             =================                               *
*                                                                             *
*                                                                             *
*   Online information and documentation:  http://www.scm.com                 *
*   E-mail:  support@scm.com   info@scm.com                                   *
*                                                                             *
*   Scientific publications using ADF results must be properly referenced     *
*   See the User Manuals (or the web site) for recommended citations          *
*   The terms and conditions of the End User License Agreement apply to       *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html                *
*                                                                             *
******************************  macintel  *************************************

ADF 2007.01  RunTime: Jul28-2008 15:18:39
ruoheqclax fragment


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                           VWN
   Gradient Corrections:          Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                      Restricted
   Fragments:                     Restricted

OTHER ASPECTS
   Relativistic Corrections:      ---
   Core Treatment:                Frozen Orbital(s)

   Electric Field:                ---

   Hyperfine or Zeeman Interaction:   ---


Fragment File(s)
----------------
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:18:35
        title: Chlorine (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:18:35
        title: Oxygen (TZP)
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:18:34
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:18:31
        title: Hydrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:18:33
```

```
        title: Ruthenium (TZP, 3d frozen)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:18:32
        title: Nitrogen (TZP)


                                     ************************************
                                     *  R U N   T Y P E : SINGLE POINT  *
                                     ************************************

 ===============
 G E O M E T R Y  ***  3D  Molecule  ***
 ===============


 ATOMS
 =====                            X Y Z                    CHARGE
                                (Angstrom)              Nucl     +Core       At.Mass
                          -------------------------    ----------------      -------
    1  C                 3.4869   -0.9329   -3.4514      6.00      6.00       12.0000
    2  H                 2.8781   -0.3841   -1.4344      1.00      1.00        1.0078
    3  C                 2.7266   -0.2520   -2.5065      6.00      6.00       12.0000
    4  C                 3.2102   -0.7167   -4.8055      6.00      6.00       12.0000
    5  N                 1.7447    0.6011   -2.8476      7.00      7.00       14.0031
    6  C                 2.2092    0.1783   -5.1609      6.00      6.00       12.0000
    7  H                 1.9879    0.3657   -6.2100      1.00      1.00        1.0078
    8  C                 1.4800    0.8520   -4.1659      6.00      6.00       12.0000
    9  Ru                0.4659    1.6691   -1.4483     44.00     16.00      101.9043
   10  C                 0.4390    1.8516   -4.4070      6.00      6.00       12.0000
   11  C                -0.7638    2.7022   -0.4516      6.00      6.00       12.0000
   12  C                -0.1661    2.4443   -3.2656      6.00      6.00       12.0000
   13  H                 0.5370    1.7966   -6.5796      1.00      1.00        1.0078
   14  C                 0.0680    2.2533   -5.7076      6.00      6.00       12.0000
   15  O                -1.5208    3.3946    0.0965      8.00      8.00       15.9949
   16  C                -1.1270    3.4445   -3.4837      6.00      6.00       12.0000
   17  H                -1.6071    3.9375   -2.6384      1.00      1.00        1.0078
   18  C                -0.8896    3.2453   -5.8943      6.00      6.00       12.0000
   19  C                -1.4856    3.8416   -4.7764      6.00      6.00       12.0000
   20  H                -1.1651    3.5590   -6.9021      1.00      1.00        1.0078
   21  H                -2.2318    4.6277   -4.9108      1.00      1.00        1.0078
   22  H                 3.7753   -1.2421   -5.5773      1.00      1.00        1.0078
   23  H                 4.2640   -1.6229   -3.1274      1.00      1.00        1.0078
   24  C                 1.7439    3.0483   -1.2424      6.00      6.00       12.0000
   25  O                 2.5298    3.8916   -1.0996      8.00      8.00       15.9949


<Jul28-2008> <15:18:39>  ADF 2007.01  RunTime: Jul28-2008 15:18:39
 <Jul28-2008> <15:18:39>  ruoheqclax fragment
 <Jul28-2008> <15:18:39>  RunType   : SINGLE POINT
 <Jul28-2008> <15:18:41>  Net Charge: -1 (Nuclei minus Electrons)
 <Jul28-2008> <15:18:41>  Symmetry  : NOSYM
 <Jul28-2008> <15:18:41>  >>>> FRAGM
 <Jul28-2008> <15:18:41>  >>>> CORORT
 <Jul28-2008> <15:18:42>  >>>> FITINT
 <Jul28-2008> <15:18:52>  >>>> CLSMAT
 <Jul28-2008> <15:18:53>  >>>> ORTHON
 <Jul28-2008> <15:18:55>  >>>> GENPT
 <Jul28-2008> <15:18:55>  Acc.Num.Int.=   4.500
 <Jul28-2008> <15:19:02>  Block Length= 128
 <Jul28-2008> <15:19:17>  >>>> PTBAS
 <Jul28-2008> <15:19:40>  >>>> CYCLE
 <Jul28-2008> <15:19:57>    1
 <Jul28-2008> <15:20:24>    2  ErrMat   2.30879054  MaxEl -0.32403438
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 <Jul28-2008> <15:22:31>    7  ErrMat   0.25439826  MaxEl -0.03907997
 <Jul28-2008> <15:22:57>    8  ErrMat   0.10480366  MaxEl  0.02367572
 <Jul28-2008> <15:23:22>    9  ErrMat   0.03954118  MaxEl -0.00539896
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 <Jul28-2008> <15:24:13>   11  ErrMat   0.00961463  MaxEl -0.00161801
 <Jul28-2008> <15:24:38>   12  ErrMat   0.00250799  MaxEl  0.00033163
 <Jul28-2008> <15:25:04>   13  ErrMat   0.00098334  MaxEl -0.00013944
 <Jul28-2008> <15:25:30>   14  ErrMat   0.00060498  MaxEl  0.00013496
 <Jul28-2008> <15:25:55>   15  ErrMat   0.00016697  MaxEl -0.00004699
 <Jul28-2008> <15:26:20>   16  ErrMat   0.00015721  MaxEl -0.00001819
 <Jul28-2008> <15:26:46>   17  ErrMat   0.00008551  MaxEl  0.00001576
 <Jul28-2008> <15:27:11>   18  ErrMat   0.00004528  MaxEl -0.00000806
 <Jul28-2008> <15:27:37>   19  ErrMat   0.00002702  MaxEl -0.00000462
 <Jul28-2008> <15:28:02>   20  ErrMat   0.00001372  MaxEl  0.00000252
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 <Jul28-2008> <15:28:29>  SCF converged
 <Jul28-2008> <15:28:55>   22  ErrMat   0.00000403  MaxEl  0.00000067
 <Jul28-2008> <15:28:57>  >>>> COREPS
 <Jul28-2008> <15:29:10>  >>>> TOTEN
 <Jul28-2008> <15:32:36>  >>>> POPAN
 <Jul28-2008> <15:32:37>  >>>> DEBYE
 <Jul28-2008> <15:32:39>  >>>> AMETS
 <Jul28-2008> <15:32:54>   Bond Energy LDA      -7.54587112 a.u.
 <Jul28-2008> <15:32:54>   Bond Energy LDA    -205.33360064 eV
 <Jul28-2008> <15:32:54>           + GGA-X      -6.46871665 a.u.
 <Jul28-2008> <15:32:54>           + GGA-X    -176.02273614 eV
 <Jul28-2008> <15:32:54>          + GGA-XC      -6.92249361 a.u.
 <Jul28-2008> <15:32:54>          + GGA-XC    -188.37063556 eV
 <Jul28-2008> <15:32:54>  >>>> POPUL
 <Jul28-2008> <15:32:56>  NORMAL TERMINATION
 <Jul28-2008> <15:32:56>  END



                                        (4)  5

 ****************************************************************************
 *                                                                          *
 *  ------------------------------------                                    *
 *   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007  *
 *  ------------------------------------                                    *
 *                                              Build 200708202008          *
 *                                                                          *
 *                                                                          *
```

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*                            |               |                              *
*                            |     A D F     |                              *
*                            |               |                              *
*                            =================                              *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ********************************

ADF 2007.01  RunTime: Jul28-2008 15:08:33
ruco2 fragment


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                      == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         ---
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
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C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:08:31
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:08:27
        title: Hydrogen (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:08:29
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:08:30
        title: Ruthenium (TZP, 3d frozen)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul28-2008 15:08:29
        title: Oxygen (TZP)


                                    ***********************************
                                    *  R U N   T Y P E : SINGLE POINT  *
                                    ***********************************


===============
G E O M E T R Y  ***  3D  Molecule  ***
===============


ATOMS
=====
                              X Y Z                    CHARGE
                           (Angstrom)                Nucl     +Core       At.Mass
                        -------------------------    ----------------     -------
   1  C                  3.4869   -0.9329   -3.4514     6.00      6.00      12.0000
   2  H                  2.8781   -0.3841   -1.4344     1.00      1.00       1.0078
   3  C                  2.7266   -0.2520   -2.5065     6.00      6.00      12.0000
   4  C                  3.2102   -0.7167   -4.8055     6.00      6.00      12.0000
   5  N                  1.7447    0.6011   -2.8476     7.00      7.00      14.0031
   6  C                  2.2092    0.1783   -5.1609     6.00      6.00      12.0000
   7  H                  1.9879    0.3657   -6.2100     1.00      1.00       1.0078
   8  C                  1.4800    0.8520   -4.1659     6.00      6.00      12.0000
   9  Ru                 0.4659    1.6691   -1.4483    44.00     16.00     101.9043
  10  C                  0.4390    1.8516   -4.4070     6.00      6.00      12.0000
  11  C                 -0.7638    2.7022   -0.4516     6.00      6.00      12.0000
  12  C                 -0.1661    2.4443   -3.2656     6.00      6.00      12.0000
  13  H                  0.5370    1.7966   -6.5796     1.00      1.00       1.0078
  14  C                  0.0680    2.2533   -5.7076     6.00      6.00      12.0000
  15  O                 -1.5208    3.3946    0.0965     8.00      8.00      15.9949
  16  C                 -1.1270    3.4445   -3.4837     6.00      6.00      12.0000
  17  H                 -1.6071    3.9375   -2.6384     1.00      1.00       1.0078
  18  C                 -0.8896    3.2453   -5.8943     6.00      6.00      12.0000
  19  C                 -1.4856    3.8416   -4.7764     6.00      6.00      12.0000
  20  H                 -1.1651    3.5590   -6.9021     1.00      1.00       1.0078
  21  H                 -2.2318    4.6277   -4.9108     1.00      1.00       1.0078
  22  H                  3.7753   -1.2421   -5.5773     1.00      1.00       1.0078
  23  H                  4.2640   -1.6229   -3.1274     1.00      1.00       1.0078
  24  C                  1.7439    3.0483   -1.2424     6.00      6.00      12.0000
  25  O                  2.5298    3.8916   -1.0996     8.00      8.00      15.9949
```

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 <Jul28-2008> <15:08:33>  ruco2 fragment
 <Jul28-2008> <15:08:34>  RunType   : SINGLE POINT
 <Jul28-2008> <15:08:35>  Net Charge: 1 (Nuclei minus Electrons)
 <Jul28-2008> <15:08:35>  Symmetry  : NOSYM
 <Jul28-2008> <15:08:35>  >>>> FRAGM
 <Jul28-2008> <15:08:36>  >>>> CORORT
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 <Jul28-2008> <15:09:57>    2  ErrMat   2.41038547  MaxEl  0.34145804
 <Jul28-2008> <15:10:16>    3  ErrMat   1.15529720  MaxEl  0.22895615
 <Jul28-2008> <15:10:34>    4  ErrMat   1.59351108  MaxEl  0.22427847
 <Jul28-2008> <15:10:53>    5  ErrMat   0.51108759  MaxEl -0.09015932
 <Jul28-2008> <15:11:11>    6  ErrMat   0.25064503  MaxEl -0.04657639
 <Jul28-2008> <15:11:30>    7  ErrMat   0.13501592  MaxEl  0.02129422
 <Jul28-2008> <15:11:48>    8  ErrMat   0.04767447  MaxEl -0.00974103
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 <Jul28-2008> <15:12:25>   10  ErrMat   0.00819228  MaxEl -0.00228357
 <Jul28-2008> <15:12:44>   11  ErrMat   0.00328548  MaxEl  0.00047365
 <Jul28-2008> <15:13:02>   12  ErrMat   0.00112232  MaxEl  0.00017590
 <Jul28-2008> <15:13:21>   13  ErrMat   0.00060710  MaxEl  0.00014188
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 <Jul28-2008> <15:13:58>   15  ErrMat   0.00008135  MaxEl  0.00001158
 <Jul28-2008> <15:14:16>   16  ErrMat   0.00008373  MaxEl  0.00001826
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 <Jul28-2008> <15:15:13>  SCF converged
 <Jul28-2008> <15:15:31>   20  ErrMat   0.00000243  MaxEl  0.00000040
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 <Jul28-2008> <15:17:56>  >>>> POPAN
 <Jul28-2008> <15:17:57>  >>>> DEBYE
 <Jul28-2008> <15:17:57>  >>>> AMETS
 <Jul28-2008> <15:18:01>   Bond Energy LDA      -6.65711912 a.u.
 <Jul28-2008> <15:18:01>   Bond Energy LDA    -181.14942818 eV
 <Jul28-2008> <15:18:01>           + GGA-X      -5.66432674 a.u.
 <Jul28-2008> <15:18:01>           + GGA-X    -154.13417299 eV
 <Jul28-2008> <15:18:01>          + GGA-XC      -6.09278470 a.u.
 <Jul28-2008> <15:18:01>          + GGA-XC    -165.79310738 eV
 <Jul28-2008> <15:18:01>  >>>> POPUL
 <Jul28-2008> <15:18:02>  NORMAL TERMINATION
 <Jul28-2008> <15:18:03>  END
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c) From *eq-eq*-3c

(1) **eq-4**

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*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                              Build 200708202008           *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |      A D F    |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ********************************

ADF 2007.01  RunTime: Jul28-2008 12:27:31
eqohaxcl fragment


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                          VWN
   Gradient Corrections:         Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                     Restricted
   Fragments:                    Restricted

OTHER ASPECTS
   Relativistic Corrections:     ---
   Core Treatment:               Frozen Orbital(s)

   Electric Field:               ---

   Hyperfine or Zeeman Interaction:   ---


Fragment File(s)
----------------
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:27:29
        title: Oxygen (TZP)
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:27:28
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:27:24
        title: Hydrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:27:27
        title: Ruthenium (TZP, 3d frozen)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:27:27
        title: Chlorine (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:27:26
        title: Nitrogen (TZP)


                                  ************************************
                                  *  R U N   T Y P E : SINGLE POINT  *
                                  ************************************



===============
G E O M E T R Y  ***  3D  Molecule  ***
===============


ATOMS
=====                            X Y Z                    CHARGE
                               (Angstrom)              Nucl     +Core       At.Mass
                          -------------------------    ----------------    -------
   1  O              -0.6653   -0.0539   -1.4390      8.00       8.00       15.9949
```

```
    2  O              1.8100   -3.1295   -1.1317      8.00      8.00      15.9949
    3  O             -2.3556   -3.7770   -1.3764      8.00      8.00      15.9949
    4  C              0.9003   -2.5482   -0.6998      6.00      6.00      12.0000
    5  C             -1.7015   -2.9927   -0.8190      6.00      6.00      12.0000
    6  H             -3.0768    0.2817   -0.2570      1.00      1.00       1.0078
    7  Ru            -0.6242   -1.7318    0.0623     44.00     16.00     101.9043
    8  C             -3.2291   -0.0898    0.7553      6.00      6.00      12.0000
    9  Cl             0.7543   -0.0052    1.2396     17.00     17.00      34.9689
   10  H             -4.9855    1.0933    1.1366      1.00      1.00       1.0078
   11  N             -2.3293   -0.9888    1.1921      7.00      7.00      14.0031
   12  H              1.1100   -4.2470    1.3279      1.00      1.00       1.0078
   13  C             -4.2853    0.3618    1.5366      6.00      6.00      12.0000
   14  C             -0.5279   -2.9013    1.7809      6.00      6.00      12.0000
   15  C              0.3934   -3.9163    2.0797      6.00      6.00      12.0000
   16  C             -2.4409   -1.5088    2.4503      6.00      6.00      12.0000
   17  C             -4.4023   -0.1385    2.8382      6.00      6.00      12.0000
   18  C             -1.4502   -2.5270    2.7945      6.00      6.00      12.0000
   19  C             -3.4799   -1.0721    3.2922      6.00      6.00      12.0000
   20  C              0.4300   -4.5178    3.3423      6.00      6.00      12.0000
   21  H              1.1659   -5.2981    3.5465      1.00      1.00       1.0078
   22  H             -5.2103    0.1965    3.4899      1.00      1.00       1.0078
   23  C             -1.4030   -3.1319    4.0671      6.00      6.00      12.0000
   24  H             -3.5612   -1.4778    4.2982      1.00      1.00       1.0078
   25  C             -0.4644   -4.1209    4.3447      6.00      6.00      12.0000
   26  H             -2.0985   -2.8256    4.8494      1.00      1.00       1.0078
   27  H             -0.4282   -4.5813    5.3326      1.00      1.00       1.0078
   28  H             -1.5520    0.1286   -1.7913      1.00      1.00       1.0078

<Jul28-2008> <12:27:31>  ADF 2007.01  RunTime: Jul28-2008 12:27:31
 <Jul28-2008> <12:27:31>  eqohaxcl fragment
 <Jul28-2008> <12:27:34>  RunType   : SINGLE POINT
 <Jul28-2008> <12:27:37>  Net Charge: -1 (Nuclei minus Electrons)
 <Jul28-2008> <12:27:37>  Symmetry  : NOSYM
 <Jul28-2008> <12:27:37>  >>>> FRAGM
 <Jul28-2008> <12:27:40>  >>>> CORORT
 <Jul28-2008> <12:27:41>  >>>> FITINT
 <Jul28-2008> <12:27:51>  >>>> CLSMAT
 <Jul28-2008> <12:27:51>  >>>> ORTHON
 <Jul28-2008> <12:27:54>  >>>> GENPT
 <Jul28-2008> <12:27:54>  Acc.Num.Int.=   4.500
 <Jul28-2008> <12:28:01>  Block Length= 128
 <Jul28-2008> <12:28:11>  >>>> PTBAS
 <Jul28-2008> <12:28:35>  >>>> CYCLE
 <Jul28-2008> <12:28:53>    1
 <Jul28-2008> <12:29:26>    2  ErrMat   2.31229919  MaxEl -0.31097613
 <Jul28-2008> <12:29:51>    3  ErrMat   1.06227361  MaxEl -0.14464013
 <Jul28-2008> <12:30:17>    4  ErrMat   4.86155027  MaxEl  1.23177560
 <Jul28-2008> <12:30:42>    5  ErrMat   1.22207690  MaxEl -0.26238412
 <Jul28-2008> <12:31:07>    6  ErrMat   0.29717815  MaxEl  0.05109957
 <Jul28-2008> <12:31:33>    7  ErrMat   0.31340377  MaxEl -0.04973100
 <Jul28-2008> <12:31:58>    8  ErrMat   0.14404034  MaxEl  0.02768747
 <Jul28-2008> <12:32:23>    9  ErrMat   0.04939118  MaxEl -0.00683842
 <Jul28-2008> <12:32:49>   10  ErrMat   0.01956687  MaxEl  0.00373522
 <Jul28-2008> <12:33:14>   11  ErrMat   0.00945570  MaxEl -0.00138230
 <Jul28-2008> <12:33:39>   12  ErrMat   0.00347485  MaxEl -0.00043366
 <Jul28-2008> <12:34:05>   13  ErrMat   0.00096242  MaxEl  0.00013165
 <Jul28-2008> <12:34:30>   14  ErrMat   0.00066131  MaxEl  0.00012096
 <Jul28-2008> <12:34:56>   15  ErrMat   0.00019758  MaxEl  0.00005123
 <Jul28-2008> <12:35:21>   16  ErrMat   0.00010005  MaxEl  0.00001534
 <Jul28-2008> <12:35:46>   17  ErrMat   0.00027252  MaxEl -0.00011233
 <Jul28-2008> <12:36:12>   18  ErrMat   0.00006392  MaxEl  0.00002662
 <Jul28-2008> <12:36:37>   19  ErrMat   0.00006161  MaxEl  0.00002008
 <Jul28-2008> <12:37:02>   20  ErrMat   0.00003373  MaxEl  0.00001516
 <Jul28-2008> <12:37:27>   21  ErrMat   0.00002754  MaxEl  0.00001277
 <Jul28-2008> <12:37:53>   22  ErrMat   0.00001964  MaxEl  0.00000882
 <Jul28-2008> <12:38:18>   23  ErrMat   0.00001103  MaxEl  0.00000499
 <Jul28-2008> <12:38:43>   24  ErrMat   0.00000663  MaxEl  0.00000310
 <Jul28-2008> <12:39:09>   25  ErrMat   0.00000062  MaxEl  0.00000007
 <Jul28-2008> <12:39:10>  SCF converged
 <Jul28-2008> <12:39:35>   26  ErrMat   0.00000064  MaxEl -0.00000027
 <Jul28-2008> <12:39:37>  >>>> COREPS
 <Jul28-2008> <12:39:50>  >>>> TOTEN
 <Jul28-2008> <12:43:15>  >>>> POPAN
 <Jul28-2008> <12:43:15>  >>>> DEBYE
 <Jul28-2008> <12:43:16>  >>>> AMETS
 <Jul28-2008> <12:43:24>   Bond Energy LDA      -7.53527499 a.u.
 <Jul28-2008> <12:43:24>   Bond Energy LDA    -205.04526537 eV
 <Jul28-2008> <12:43:24>           + GGA-X      -6.46032098 a.u.
 <Jul28-2008> <12:43:24>           + GGA-X    -175.79427839 eV
 <Jul28-2008> <12:43:24>          + GGA-XC      -6.91321234 a.u.
 <Jul28-2008> <12:43:24>          + GGA-XC    -188.11807937 eV
 <Jul28-2008> <12:43:24>  >>>> POPUL
 <Jul28-2008> <12:43:26>  NORMAL TERMINATION
 <Jul28-2008> <12:43:26>  END
```

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                              Build 200708202008           *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |      A D F    |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ********************************

ADF 2007.01  RunTime: Jul28-2008 12:43:42
ruco2 fragment


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                         VWN
   Gradient Corrections:        Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                    Restricted
   Fragments:                   Restricted

OTHER ASPECTS
   Relativistic Corrections:    ---
   Core Treatment:              Frozen Orbital(s)

   Electric Field:              ---

   Hyperfine or Zeeman Interaction:   ---


Fragment File(s)
----------------
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:43:39
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:43:35
        title: Hydrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:43:38
        title: Oxygen (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:43:36
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul28-2008 12:43:37
        title: Ruthenium (TZP, 3d frozen)


                                    ************************************
                                    *  R U N   T Y P E : SINGLE POINT  *
                                    ************************************



===============
G E O M E T R Y  ***  3D  Molecule  ***
===============


ATOMS
=====                             X Y Z                  CHARGE
                                (Angstrom)              Nucl     +Core       At.Mass
                          -------------------------    ----------------      -------
   1  C                   3.3704   -0.3522   -3.0087      6.00      6.00      12.0000
   2  H                   1.1976   -0.2813   -2.7548      1.00      1.00       1.0078
   3  O                  -0.1156    3.7887   -2.7168      8.00      8.00      15.9949
   4  C                   2.1767    0.0945   -2.4524      6.00      6.00      12.0000
   5  C                   4.5693    0.1770   -2.5186      6.00      6.00      12.0000
   6  C                   0.0645    2.9939   -1.8866      6.00      6.00      12.0000
   7  N                   2.1468    1.0161   -1.4737      7.00      7.00      14.0031
   8  C                   4.5337    1.1321   -1.5091      6.00      6.00      12.0000
   9  H                   5.4576    1.5564   -1.1218      1.00      1.00       1.0078
```

```
  10  C              3.2997    1.5601   -0.9899      6.00      6.00      12.0000
  11  Ru             0.3363    1.7252   -0.5309     44.00     16.00     101.9043
  12  C              3.1152    2.5847    0.0386      6.00      6.00      12.0000
  13  C             -1.0781    2.5043    0.4491      6.00      6.00      12.0000
  14  C              1.7783    2.9318    0.3762      6.00      6.00      12.0000
  15  H              5.2256    2.9302    0.4292      1.00      1.00       1.0078
  16  C              4.2022    3.2161    0.6753      6.00      6.00      12.0000
  17  O             -1.9008    3.0700    1.0485      8.00      8.00      15.9949
  18  C              1.5875    3.9450    1.3269      6.00      6.00      12.0000
  19  H              0.5798    4.2539    1.6058      1.00      1.00       1.0078
  20  C              3.9850    4.2041    1.6316      6.00      6.00      12.0000
  21  C              2.6720    4.5727    1.9504      6.00      6.00      12.0000
  22  H              4.8299    4.6844    2.1262      1.00      1.00       1.0078
  23  H              2.4896    5.3508    2.6941      1.00      1.00       1.0078
  24  H              5.5266   -0.1538   -2.9240      1.00      1.00       1.0078
  25  H              3.3558   -1.1031   -3.7973      1.00      1.00       1.0078


<Jul28-2008> <12:43:42>  ADF 2007.01  RunTime: Jul28-2008 12:43:42
 <Jul28-2008> <12:43:42>  ruco2 fragment
 <Jul28-2008> <12:43:43>  RunType   : SINGLE POINT
 <Jul28-2008> <12:43:44>  Net Charge: 1 (Nuclei minus Electrons)
 <Jul28-2008> <12:43:44>  Symmetry  : NOSYM
 <Jul28-2008> <12:43:44>  >>>> FRAGM
 <Jul28-2008> <12:43:44>  >>>> CORORT
 <Jul28-2008> <12:43:44>  >>>> FITINT
 <Jul28-2008> <12:43:53>  >>>> CLSMAT
 <Jul28-2008> <12:43:53>  >>>> ORTHON
 <Jul28-2008> <12:43:54>  >>>> GENPT
 <Jul28-2008> <12:43:54>  Acc.Num.Int.=   4.500
 <Jul28-2008> <12:44:00>  Block Length= 128
 <Jul28-2008> <12:44:03>  >>>> PTBAS
 <Jul28-2008> <12:44:19>  >>>> CYCLE
 <Jul28-2008> <12:44:31>    1
 <Jul28-2008> <12:44:51>    2  ErrMat   2.40253306  MaxEl -0.29635206
 <Jul28-2008> <12:45:09>    3  ErrMat   1.15187624  MaxEl  0.21703495
 <Jul28-2008> <12:45:28>    4  ErrMat   1.56740109  MaxEl  0.22765890
 <Jul28-2008> <12:45:47>    5  ErrMat   0.50547455  MaxEl -0.07671555
 <Jul28-2008> <12:46:05>    6  ErrMat   0.24748402  MaxEl  0.04488541
 <Jul28-2008> <12:46:24>    7  ErrMat   0.13022714  MaxEl -0.01958316
 <Jul28-2008> <12:46:43>    8  ErrMat   0.04641909  MaxEl -0.00972992
 <Jul28-2008> <12:47:01>    9  ErrMat   0.01658930  MaxEl  0.00332487
 <Jul28-2008> <12:47:20>   10  ErrMat   0.00788041  MaxEl -0.00218971
 <Jul28-2008> <12:47:39>   11  ErrMat   0.00309376  MaxEl -0.00041944
 <Jul28-2008> <12:47:58>   12  ErrMat   0.00109157  MaxEl -0.00013052
 <Jul28-2008> <12:48:17>   13  ErrMat   0.00058364  MaxEl  0.00012653
 <Jul28-2008> <12:48:35>   14  ErrMat   0.00027887  MaxEl -0.00005498
 <Jul28-2008> <12:48:54>   15  ErrMat   0.00009576  MaxEl  0.00002252
 <Jul28-2008> <12:49:13>   16  ErrMat   0.00009130  MaxEl  0.00001576
 <Jul28-2008> <12:49:32>   17  ErrMat   0.00002529  MaxEl  0.00000550
 <Jul28-2008> <12:49:51>   18  ErrMat   0.00001089  MaxEl  0.00000142
 <Jul28-2008> <12:50:09>   19  ErrMat   0.00000362  MaxEl -0.00000054
 <Jul28-2008> <12:50:10>  SCF converged
 <Jul28-2008> <12:50:29>   20  ErrMat   0.00000205  MaxEl -0.00000027
 <Jul28-2008> <12:50:30>  >>>> COREPS
 <Jul28-2008> <12:50:41>  >>>> TOTEN
 <Jul28-2008> <12:52:54>  >>>> POPAN
 <Jul28-2008> <12:52:54>  >>>> DEBYE
 <Jul28-2008> <12:52:55>  >>>> AMETS
 <Jul28-2008> <12:52:57>   Bond Energy LDA      -6.65793403 a.u.
 <Jul28-2008> <12:52:57>   Bond Energy LDA    -181.17160306 eV
 <Jul28-2008> <12:52:57>           + GGA-X      -5.66404838 a.u.
 <Jul28-2008> <12:52:57>           + GGA-X    -154.12659839 eV
 <Jul28-2008> <12:52:57>          + GGA-XC      -6.09302987 a.u.
 <Jul28-2008> <12:52:57>          + GGA-XC    -165.79977882 eV
 <Jul28-2008> <12:52:57>  >>>> POPUL
 <Jul28-2008> <12:52:58>  NORMAL TERMINATION
 <Jul28-2008> <12:53:01>  END
```

5. Geometry Optimizations using the BP/TZP(ZORA) method (all electron, no frozen core, scalar relativistic correction).

a) ax-ax-3c

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                              Build 200708202008           *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |      A D F    |                            *
*                              |               |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  macintel  ********************************

ADF 2007.01  RunTime: Jun25-2008 16:18:26
axial-OH


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                         VWN
   Gradient Corrections:        Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                    Restricted
   Fragments:                   Restricted

OTHER ASPECTS
   Relativistic Corrections:    scalar (ZORA,SAPA)                   *** SPECIAL ***
   Core Treatment:              Frozen Orbital(s)

   Electric Field:              ---

   Hyperfine or Zeeman Interaction:   ---


Fragment File(s)
----------------
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jun25-2008 16:18:24
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jun25-2008 16:18:17
        title: Hydrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jun25-2008 16:18:23
        title: Oxygen (TZP)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jun25-2008 16:18:22
        title: Chlorine (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jun25-2008 16:18:19
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jun25-2008 16:18:20
        title: Ruthenium (TZP, all electron)


                                  ******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ******************************************



==========================
Geometry Convergence Tests
==========================

Energy  old :        -13.29448343
        new :        -13.29452435

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-----------------------------------------------------------------------
change in energy      -0.00004092     0.00100000    YES        2.21909700
gradient max           0.00093862     0.00100000    YES        0.11750460
gradient rms           0.00019532     0.00066667    YES        0.18134203
```

```
cart. step max          0.00146043     0.01000000    YES         0.28842283
cart. step rms          0.00041231     0.00666667    YES         0.35387470

prediction dE :        -0.00000331

****************************************************************************************************
                          Geometry CONVERGED
****************************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************


Coordinates (Cartesian)
=======================
```

Atom	bohr X	bohr Y	bohr Z	angstrom X	angstrom Y	angstrom Z	Geometric Variables (0:frozen, *:LT par.)		
1 C	6.447443	-0.531322	-5.759069	3.411840	-0.281163	-3.047568	1	2	3
2 H	2.358218	-0.108261	-5.724865	1.247915	-0.057289	-3.029468	4	5	6
3 O	0.238973	7.653803	-4.748308	0.126459	4.050218	-2.512697	7	8	9
4 C	4.157464	0.381159	-4.849594	2.200035	0.201701	-2.566295	10	11	12
5 C	8.661223	0.140944	-4.482695	4.583322	0.074584	-2.372140	13	14	15
6 Cl	-2.113476	-0.040095	-3.623881	-1.118404	-0.021217	-1.917675	16	17	18
7 C	0.362341	5.962929	-3.347397	0.191743	3.155446	-1.771366	19	20	21
8 N	4.004264	1.889482	-2.803691	2.118965	0.999871	-1.483650	22	23	24
9 O	3.238977	-5.920843	-2.472278	1.713993	-3.133175	-1.308273	25	26	27
10 C	8.507942	1.706041	-2.380021	4.502209	0.902798	-1.259453	28	29	30
11 O	-4.438364	-7.652991	-1.876306	-2.348681	-4.049788	-0.992898	31	32	33
12 H	10.212694	2.249944	-1.367849	5.404325	1.190619	-0.723835	34	35	36
13 C	1.565432	-4.803020	-1.579996	0.828391	-2.541649	-0.836098	37	38	39
14 C	6.146269	2.595662	-1.551078	3.252465	1.373565	-0.820795	40	41	42
15 C	-3.224056	-5.960428	-1.167880	-1.706097	-3.154123	-0.618016	43	44	45
16 Ru	0.544850	3.232856	-1.088235	0.288322	1.710753	-0.575869	46	47	48
17 H	-6.084611	0.167588	-0.718683	-3.219837	0.088684	-0.380311	49	50	51
18 Ru	-1.226130	-3.256879	-0.035921	-0.648840	-1.723466	-0.019008	52	53	54
19 C	5.744628	4.309243	0.579542	3.039926	2.280353	0.306680	55	56	57
20 C	-2.159541	4.629632	0.719919	-1.142780	2.449896	0.380965	58	59	60
21 C	3.210790	5.038883	1.099483	1.699077	2.666462	0.581821	61	62	63
22 C	-6.216087	-0.313256	1.280007	-3.289412	-0.165768	0.677351	64	65	66
23 O	0.997543	-0.094535	1.134743	0.527877	-0.050026	0.600480	67	68	69
24 H	9.692296	4.695724	1.643427	5.128942	2.484870	0.869664	70	71	72
25 H	-9.644352	1.746006	2.000814	-5.103571	0.923947	1.058785	73	74	75
26 C	7.753054	5.268008	2.040950	4.102739	2.787710	1.080024	76	77	78
27 O	-3.743264	5.666094	1.850307	-1.980850	2.998368	0.979140	79	80	81
28 N	-4.332206	-1.777742	2.175329	-2.292505	-0.940740	1.151135	82	83	84
29 H	2.687232	-7.298173	2.603141	1.422022	-3.862027	1.377523	85	86	87
30 C	-8.169361	0.558173	2.804695	-4.323040	0.295373	1.484181	88	89	90
31 C	2.801808	6.767215	3.076261	1.482653	3.581056	1.627887	91	92	93
32 H	0.893085	7.403807	3.520326	0.472600	3.917926	1.862876	94	95	96
33 C	-0.578627	-4.953009	3.407354	-0.306196	-2.621019	1.803094	97	98	99
34 C	7.295563	6.960285	4.002181	3.860646	3.683224	2.117863	100	101	102
35 C	1.374894	-6.638117	4.047547	0.727563	-3.512740	2.141870	103	104	105
36 C	4.810401	7.714412	4.511232	2.545555	4.082291	2.387241	106	107	108
37 H	8.860789	7.696894	5.121415	4.688928	4.073021	2.710136	109	110	111
38 C	-4.315185	-2.488017	4.658348	-2.283498	-1.316602	2.465092	112	113	114
39 C	-8.160186	-0.108280	5.361608	-4.318185	-0.057299	2.837241	115	116	117
40 H	4.431194	9.054223	6.033255	2.344887	4.791288	3.192661	118	119	120
41 C	-2.244060	-4.173360	5.370180	-1.187505	-2.208447	2.841777	121	122	123
42 C	-6.232090	-1.632494	6.285948	-3.297880	-0.863879	3.326380	124	125	126
43 C	1.688204	-7.502277	6.524736	0.893359	-3.970034	3.452742	127	128	129
44 H	3.224658	-8.808011	6.959990	1.706416	-4.660999	3.683068	130	131	132
45 H	-9.652793	0.550189	6.621625	-5.108038	0.291147	3.504013	133	134	135
46 C	-1.906500	-5.047799	7.864215	-1.008876	-2.671180	4.161563	136	137	138
47 H	-6.207116	-2.185968	8.265347	-3.284664	-1.156764	4.373833	139	140	141
48 C	0.049967	-6.704383	8.445861	0.026442	-3.547807	4.469357	142	143	144
49 H	-3.178773	-4.430883	9.363147	-1.682134	-2.344722	4.954764	145	146	147
50 H	0.300572	-7.375427	10.377590	0.159056	-3.902908	5.491584	148	149	150
51 H	10.492977	-0.552956	-5.124925	5.552644	-0.292612	-2.711993	151	152	153
52 H	6.478467	-1.757891	-7.410754	3.428257	-0.930236	-3.921602	154	155	156
53 H	0.887871	0.192114	2.954605	0.469841	0.101662	1.563510	157	158	159

```
Number of elements of the density matrix on this node (used, total):    219716    436645


=====================================================
Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
=====================================================

General Accuracy Parameter :                          4.50

Symmetry used in the points section:  NOSYM


Summary of the Symmetry Unique Points:
---------------------------------------
   Nr. of used Symmetry Operators                     1

   Points in the Atomic Spheres                   34100
   Points in the Atomic Polyhedra                348628
   Points in the Outer Region                     29764
   ------------------------------------------------------
   Total                                         412492

   Sum of Weights                                160167.237290

Total nr. of points:     412492
Nr. of blocks:             3223
Block length:               128
Nr. of dummy points:         52


Test of Precision of the Numerical Integration Grid
===================================================

Integral of the Total Core Density:                   0.00000000000000
```

```
 ============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.
```

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	155.557007744150241	4232.9216	97613.51	408414.87
Delta V^Pauli Coulomb:	-81.098440078174690	-2206.8008	-50890.04	-212923.92
Delta V^Pauli LDA-XC:	-19.207658116836846	-522.6670	-12052.99	-50429.70
Delta V^Pauli GGA-Exchange:	1.115283271728579	30.3484	699.85	2928.18
Delta V^Pauli GGA-Correlation:	-0.312524211671960	-8.5042	-196.11	-820.53
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	56.053668609195327	1525.2979	35174.21	147168.89
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	56.053668609195327	1525.2979	35174.21	147168.89
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-11.929644924816984	-324.6222	-7485.97	-31321.28
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	44.124023684378344	1200.6758	27688.25	115847.61
Orbital Interactions				
A:	-57.413155836783410	-1562.2915	-36027.30	-150738.22
Total Orbital Interactions:	-57.418555668335266	-1562.4384	-36030.69	-150752.40
Alternative Decomposition Orb.Int.				
Kinetic:	-142.952114418546699	-3889.9250	-89703.82	-375320.72
Coulomb:	78.799581080777116	2144.2457	49447.49	206888.27
XC:	6.733977669434484	183.2409	4225.64	17680.06
Total Orbital Interactions:	-57.418555668335102	-1562.4384	-36030.69	-150752.40
Residu (E=Steric+OrbInt+Res):	0.000007390452793	0.0002	0.00	0.02
Total Bonding Energy:	-13.294524593504130	-361.7624	-8342.44	-34904.77

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.929644924816984	-324.6222	-7485.97	-31321.28
Kinetic Energy:	12.604893325603541	342.9966	7909.69	33094.14
Coulomb (Steric+OrbInt) Energy:	-2.298851606944780	-62.5549	-1442.55	-6035.63
XC Energy:	-11.670921387345743	-317.5819	-7323.61	-30642.00
Total Bonding Energy:	-13.294524593503965	-361.7624	-8342.44	-34904.77

```
Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree):  -0.0133455155
2. Electrostatic (Fit correction):   0.0000000000

Scaled ZORA energy correction, not included in bonding energy (hartree):          -0.0009478079
 WARNING: This scaled ZORA energy correction should only be used to compare two calculations
 in which the only difference in the calculation is the electron configuration.
 Then the difference in energy of this term should be added to the difference in energy of
 the two electron configurations.
 This term should not be used otherwise.
 In practice it is useful only for core excitation energy calculations.
```

(1) Bond Order Analysis

		DIST. [A]	BOND-ORDERS (THRESHOLD = 0.050)				
			MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
C	1 - C 4	1.3904	1.4250	1.4339	1.4916	1.4816	1.5295
C	1 - C 5	1.3983	1.3579	1.4012	1.4598	1.4247	1.5171
C	1 - C 14	2.7789	0.0596	0.0939	0.0972	0.1248	0.0977
C	1 - H 52	1.0888	1.0290	0.9226	0.9701	0.9854	0.9043
H	2 - C 4	1.0900	1.0156	0.8980	0.9387	0.9257	0.8546
O	3 - C 7	1.1638	2.0400	2.1882	2.3656	2.3764	2.4081
O	3 - Ru 16	3.0415	0.2177	0.2501	0.2905	0.4152	0.2863
C	4 - N 8	1.3475	1.3762	1.3958	1.4723	1.4588	1.5194
C	4 - C 10	2.7385	0.0637	0.1079	0.1122	0.1088	0.1149

C	5 - N	8	2.7782	0.0382	0.0940	0.0993	0.0694	0.1038
C	5 - C	10	1.3895	1.4126	1.4674	1.5277	1.4948	1.5852
C	5 - H	51	1.0908	1.0271	0.9236	0.9687	0.9750	0.8982
Cl	6 - Ru	16	2.6037	0.4318	0.2567	0.3314	0.5688	0.3756
Cl	6 - Ru	18	2.5929	0.4373	0.2629	0.3399	0.5765	0.3851
Cl	6 - C	21	4.6270	0.0538	0.1062	0.1288	0.0582	0.1555
Cl	6 - C	33	4.6112	0.0540	0.1073	0.1302	0.0570	0.1573
C	7 - Ru	16	1.8777	1.0946	1.0924	1.1869	1.0249	1.0878
C	7 - C	20	2.6289	0.0895	0.0748	0.0752	0.0386	0.0713
C	7 - O	23	4.0017	0.0586	0.1314	0.1552	0.2860	0.1770
N	8 - C	14	1.3652	1.2915	1.3082	1.3725	1.3922	1.3899
N	8 - Ru	16	2.1635	0.2462	0.3291	0.3685	0.4824	0.3580
N	8 - C	20	4.0272	0.0436	0.1185	0.1231	0.1615	0.1239
O	9 - C	13	1.1650	2.0089	2.1780	2.3578	2.3689	2.4031
O	9 - Ru	18	3.0385	0.2271	0.2514	0.2926	0.4222	0.2889
C	10 - H	12	1.0879	1.0174	0.9217	0.9638	0.9771	0.9030
C	10 - C	14	1.4057	1.3708	1.3455	1.3910	1.4084	1.3968
O	11 - C	15	1.1643	2.0384	2.1862	2.3634	2.3741	2.4065
O	11 - Ru	18	3.0413	0.2188	0.2524	0.2936	0.4188	0.2894
C	13 - C	15	2.6165	0.0918	0.0740	0.0745	0.0337	0.0704
C	13 - Ru	18	1.8760	1.0673	1.0907	1.1875	1.0235	1.0876
C	13 - N	28	4.0314	0.0429	0.1185	0.1233	0.1682	0.1239
C	14 - C	19	1.4624	1.1703	1.0997	1.1326	1.1341	1.1168
C	15 - Ru	18	1.8771	1.0976	1.0987	1.1956	1.0335	1.0957
C	15 - O	23	4.0138	0.0555	0.1294	0.1528	0.2833	0.1743
Ru	16 - C	20	1.8735	1.1026	1.1066	1.2019	1.0512	1.1042
Ru	16 - C	21	2.0601	0.6435	0.7555	0.8223	0.8648	0.7861
Ru	16 - O	23	2.1311	0.3609	0.3272	0.4126	0.7930	0.4550
Ru	16 - O	27	3.0373	0.2297	0.2582	0.3003	0.4329	0.2968
H	17 - C	22	1.0901	1.0149	0.8968	0.9375	0.9242	0.8529
Ru	18 - O	23	2.1375	0.3324	0.3178	0.4013	0.7836	0.4424
Ru	18 - N	28	2.1641	0.2595	0.3317	0.3722	0.4915	0.3621
Ru	18 - C	33	2.0599	0.6370	0.7529	0.8211	0.8666	0.7854
C	19 - C	21	1.4222	1.3382	1.3157	1.3447	1.3380	1.3703
C	19 - C	26	1.4089	1.3443	1.3462	1.3951	1.3853	1.4278
C	19 - C	36	2.7964	0.0536	0.0933	0.0967	0.0912	0.0989
C	20 - O	27	1.1666	1.9992	2.1613	2.3393	2.3477	2.3937
C	21 - C	31	1.4063	1.4090	1.4148	1.4495	1.4188	1.5034
C	21 - C	34	2.8400	0.0415	0.0993	0.1019	0.0787	0.1057
C	22 - N	28	1.3487	1.3732	1.3921	1.4695	1.4550	1.5184
C	22 - C	30	1.3900	1.4257	1.4350	1.4927	1.4828	1.5303
C	22 - C	42	2.7395	0.0637	0.1073	0.1115	0.1080	0.1142
O	23 - H	53	0.9766	1.1245	0.8493	1.0732	1.1620	1.0606
H	24 - C	26	1.0904	1.0260	0.9265	0.9632	0.9741	0.9093
H	25 - C	30	1.0887	1.0287	0.9220	0.9699	0.9850	0.9033
C	26 - C	31	2.7918	0.0601	0.1087	0.1130	0.0829	0.1176
C	26 - C	34	1.3920	1.4097	1.4627	1.5223	1.4816	1.5857
N	28 - C	38	1.3667	1.2858	1.3057	1.3708	1.3894	1.3916
N	28 - C	39	2.7797	0.0380	0.0930	0.0983	0.0671	0.1029
H	29 - C	35	1.0902	1.0248	0.9217	0.9608	0.9731	0.9021
C	30 - C	38	2.7786	0.0579	0.0931	0.0963	0.1220	0.0969
C	30 - C	39	1.3983	1.3571	1.4003	1.4589	1.4242	1.5158
C	31 - H	32	1.0904	1.0242	0.9227	0.9613	0.9745	0.9048
C	31 - C	36	1.3991	1.3958	1.4334	1.4888	1.4494	1.5500
C	33 - C	35	1.4066	1.4054	1.4091	1.4440	1.4136	1.4973
C	33 - C	41	1.4233	1.3398	1.3171	1.3469	1.3384	1.3753
C	33 - C	48	2.8423	0.0412	0.0982	0.1008	0.0767	0.1047
C	34 - C	36	1.4005	1.3695	1.4070	1.4640	1.4242	1.5247
C	34 - H	37	1.0903	1.0320	0.9285	0.9723	0.9858	0.9133
C	35 - C	43	1.3982	1.4017	1.4387	1.4940	1.4568	1.5537
C	35 - C	46	2.7933	0.0609	0.1097	0.1139	0.0846	0.1186
C	36 - H	40	1.0916	1.0305	0.9273	0.9690	0.9796	0.9068
C	38 - C	41	1.4624	1.1759	1.1021	1.1353	1.1383	1.1222
C	38 - C	42	1.4056	1.3715	1.3458	1.3915	1.4078	1.3993
C	39 - C	42	1.3896	1.4130	1.4666	1.5271	1.4937	1.5850
C	39 - H	45	1.0908	1.0279	0.9232	0.9686	0.9748	0.8975
C	41 - C	43	2.7940	0.0516	0.0916	0.0949	0.0878	0.0972
C	41 - C	46	1.4099	1.3371	1.3405	1.3897	1.3777	1.4246
C	42 - H	47	1.0877	1.0174	0.9215	0.9639	0.9776	0.9030
C	43 - H	44	1.0916	1.0302	0.9268	0.9688	0.9791	0.9057
C	43 - C	48	1.4012	1.3641	1.4018	1.4586	1.4194	1.5185
C	46 - C	48	1.3911	1.4162	1.4680	1.5280	1.4866	1.5921
C	46 - H	49	1.0904	1.0256	0.9266	0.9634	0.9746	0.9098
C	48 - H	50	1.0902	1.0311	0.9282	0.9721	0.9856	0.9126
Sum :				73.0920	73.9395	78.3976	78.3976	78.3976

Atomic summation :

C	1	3.9621	3.9820	4.1562	4.1535	4.1884
H	2	1.0750	0.9780	1.0271	1.0416	0.9404
O	3	2.2940	2.5121	2.7408	2.7441	2.7870
C	4	3.9843	3.9576	4.1464	4.1100	4.1516
C	5	3.9287	3.9752	4.1489	4.1277	4.1965
Cl	6	1.1067	1.0056	1.2677	1.3564	1.4715
C	7	3.3918	3.6364	3.9417	3.8741	3.9062
N	8	3.1966	3.4871	3.6939	3.6981	3.7630
O	9	2.2775	2.5025	2.7335	2.7393	2.7819
C	10	3.9657	3.9864	4.1454	4.1393	4.1529
O	11	2.2933	2.5112	2.7404	2.7439	2.7870
H	12	1.0413	0.9801	1.0251	1.0360	0.9593
C	13	3.3668	3.6165	3.9114	3.8571	3.8612
C	14	4.1104	4.0033	4.1565	4.1498	4.1592
C	15	3.3958	3.6377	3.9448	3.8766	3.9090
Ru	16	4.3883	4.5880	5.1495	5.2200	4.9705
H	17	1.0764	0.9777	1.0270	1.0417	0.9400
Ru	18	4.3389	4.5733	5.1422	5.2123	4.9602
C	19	4.0365	4.0202	4.1434	4.1311	4.1866
C	20	3.3929	3.6238	3.9159	3.8555	3.8779
C	21	3.7915	3.9741	4.1400	4.0969	4.2196
C	22	3.9887	3.9567	4.1466	4.1091	4.1530
O	23	1.9896	1.9593	2.4427	2.6368	2.6008
H	24	1.0389	0.9868	1.0260	1.0346	0.9672
H	25	1.0463	0.9742	1.0251	1.0380	0.9539
C	26	3.9671	3.9921	4.1497	4.1429	4.1988
O	27	2.2740	2.4969	2.7276	2.7371	2.7855
N	28	3.1930	3.4801	3.6895	3.6965	3.7638
H	29	1.0713	0.9830	1.0254	1.0354	0.9616
C	30	3.9607	3.9815	4.1559	4.1527	4.1868
C	31	4.0117	3.9885	4.1286	4.1221	4.1917
H	32	1.0694	0.9841	1.0260	1.0352	0.9644
C	33	3.7869	3.9695	4.1387	4.0962	4.2217
C	34	3.9570	3.9857	4.1536	4.1459	4.2218
C	35	4.0143	3.9878	4.1284	4.1200	4.1870
C	36	3.9711	3.9853	4.1497	4.1351	4.2129
H	37	1.0446	0.9805	1.0267	1.0369	0.9632

C	38	4.1062	4.0035	4.1580	4.1488	4.1688
C	39	3.9318	3.9746	4.1490	4.1274	4.1963
H	40	1.0411	0.9797	1.0238	1.0350	0.9572
C	41	4.0324	4.0187	4.1436	4.1316	4.1944
C	42	3.9641	3.9860	4.1456	4.1403	4.1555
C	43	3.9742	3.9845	4.1490	4.1343	4.2091
H	44	1.0402	0.9793	1.0236	1.0352	0.9560
H	45	1.0379	0.9755	1.0235	1.0378	0.9469
C	46	3.9632	3.9920	4.1504	4.1440	4.2028
H	47	1.0432	0.9797	1.0251	1.0360	0.9591
C	48	3.9579	3.9853	4.1536	4.1456	4.2215
H	49	1.0398	0.9868	1.0262	1.0346	0.9677
H	50	1.0442	0.9802	1.0266	1.0370	0.9626
H	51	1.0368	0.9759	1.0236	1.0377	0.9476
H	52	1.0459	0.9746	1.0252	1.0378	0.9548
H	53	1.1261	0.8818	1.1103	1.0528	1.0910

(*) Values from:
- Mayer bond-order analysis
- Gophinatan-Jug bond order analysis
- Nalewajski-Mrozek bond order analysis
  a) N-M (1) - bond-orders calculated from two-electron valence indices based on partitioning of tr(Delta_P^2] (3-index set)
  b) N-M (2) - bond-orders calculated from two-electron valence indices based on partitioning of tr(Delta_P^2] (4-index set)
  c) N-M (3) - bond-orders calculated from valence indices based on partitioning of tr(P*Delta_P]

A. Michalak, R.L. DeKock, T. Ziegler, J. Comp. Chem., subm.
and original articles by Nalewajski et al.)

(2) NPA- NBO (gennbo extension for ADF)

```
********************************** NBO 5.0 ***********************************
          N A T U R A L   A T O M I C   O R B I T A L   A N D
        N A T U R A L   B O N D   O R B I T A L   A N A L Y S I S
******************************************************************************
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         Cite this program as:

         NBO 5.0.  E. D. Glendening, J. K. Badenhoop, A. E. Reed,
         J. E. Carpenter, J. A. Bohmann, C. M. Morales, and F. Weinhold
         (Theoretical Chemistry Institute, University of Wisconsin,
         Madison, WI, 2001); http://www.chem.wisc.edu/~nbo5

      /3CBOND / : Search for 3-center bonds
      /NLMO   / : Form Natural Localized Molecular Orbitals
      /NRT    / : Natural Resonance Theory Analysis
      /AONBO  / : Write the AO to NBO transformation to LFN 37
      /AONLMO / : Write the AO to NLMO transformation to LFN 39
      /NAOMO  / : Print core and valence MOs in the NAO basis
      /NBONLMO/ : Write the NBO to NLMO transformation to LFN 49
      /NLMOMO / : Write the NLMO to MO transformation to LFN 49
      /STERIC / : Print NBO/NLMO steric analysis
      /CMO    / : Print analysis of canonical MOs
      /FILE   / : Set to nbodata

Job title: ***axial-OH
```

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C 1	-0.25120	1.99935	4.23956	0.01230	6.25120
C 2	0.03320	1.99936	3.94726	0.02018	5.96680
C 3	-0.16496	1.99938	4.15427	0.01131	6.16496
C 4	0.59977	1.99945	3.35633	0.04445	5.40023
C 5	-0.22612	1.99929	4.21548	0.01135	6.22612
C 6	0.60719	1.99946	3.34582	0.04752	5.39281
C 7	0.20481	1.99926	3.77282	0.02311	5.79519
C 8	0.59860	1.99945	3.35766	0.04429	5.40140
C 9	-0.13788	1.99918	4.11823	0.02047	6.13788
C 10	0.58710	1.99946	3.36488	0.04855	5.41290
C 11	-0.02592	1.99908	3.98746	0.03938	6.02592
C 12	0.03265	1.99936	3.94735	0.02065	5.96735
C 13	-0.18368	1.99930	4.17247	0.01191	6.18368
C 14	-0.24986	1.99935	4.23820	0.01231	6.24986
C 15	-0.26811	1.99930	4.25308	0.01574	6.26811
C 16	-0.03141	1.99908	3.99306	0.03927	6.03141
C 17	-0.23275	1.99937	4.22049	0.01290	6.23275
C 18	-0.25893	1.99930	4.24397	0.01566	6.25893
C 19	-0.19217	1.99937	4.18049	0.01231	6.19217
C 20	0.19458	1.99926	3.78315	0.02301	5.80542
C 21	-0.16440	1.99938	4.15367	0.01135	6.16440
C 22	-0.14973	1.99919	4.13036	0.02018	6.14973
C 23	-0.22898	1.99929	4.21823	0.01147	6.22898
C 24	-0.18951	1.99937	4.17794	0.01220	6.18951
C 25	-0.18684	1.99930	4.17545	0.01209	6.18684
C 26	-0.23225	1.99937	4.21999	0.01289	6.23225
H 27	0.23467	0.00000	0.76240	0.00293	0.76533
H 28	0.22130	0.00000	0.77698	0.00172	0.77870
H 29	0.23671	0.00000	0.76032	0.00297	0.76329
H 30	0.20382	0.00000	0.79423	0.00195	0.79618
H 31	0.23351	0.00000	0.76500	0.00149	0.76649
H 32	0.21756	0.00000	0.77981	0.00263	0.78244
H 33	0.21556	0.00000	0.78174	0.00270	0.78444
H 34	0.21690	0.00000	0.78135	0.00174	0.78310
H 35	0.21692	0.00000	0.78156	0.00152	0.78308

```
   H 36    0.21787      0.00000     0.78065    0.00148     0.78213
   H 37    0.22629      0.00000     0.77231    0.00140     0.77371
   H 38    0.22251      0.00000     0.77577    0.00172     0.77749
   H 39    0.20415      0.00000     0.79388    0.00197     0.79585
   H 40    0.21749      0.00000     0.78078    0.00173     0.78251
   H 41    0.22513      0.00000     0.77346    0.00141     0.77487
   H 42    0.23236      0.00000     0.76613    0.00151     0.76764
   H 43    0.50339      0.00000     0.49164    0.00497     0.49661
   O 44   -0.43489      1.99980     6.40100    0.03409     8.43489
   O 45   -0.45091      1.99980     6.41665    0.03446     8.45091
   O 46   -0.43573      1.99980     6.40184    0.03409     8.43573
   O 47   -0.94819      1.99987     6.92089    0.02743     8.94819
   O 48   -0.45692      1.99980     6.42229    0.03484     8.45692
  Cl 49   -0.48298      9.99988     7.46932    0.01377    17.48298
   N 50   -0.38079      1.99948     5.34038    0.04094     7.38079
   N 51   -0.39102      1.99948     5.35090    0.04064     7.39102
  Ru 52    0.22620     35.96823     7.75737    0.04820    43.77380
  Ru 53    0.22590     35.96857     7.75674    0.04878    43.77410
=======================================================================
* Total *  0.00000    147.91700   183.12305    0.95995   332.00000

                            Natural Population
-----------------------------------------------------------
  Core                    147.91700 ( 99.9439% of 148)
  Valence                 183.12305 ( 99.5234% of 184)
  Natural Minimal Basis   331.04005 ( 99.7109% of 332)
  Natural Rydberg Basis     0.95995 (  0.2891% of 332)
-----------------------------------------------------------


NATURAL LOCALIZED MOLECULAR ORBITAL (NLMO) ANALYSIS:

Maximum off-diagonal element of DM in NLMO basis:  0.62882D-06

Hybridization/Polarization Analysis of NLMOs in NAO Basis:
NLMO/Occupancy/Percent from Parent NBO/ Atomic Hybrid Contributions
-------------------------------------------------------------------------------
  1. (2.00000)  99.1514%  BD ( 1) C  1- C  2
                        49.783%  C  1 s( 32.90%)p 2.04( 67.00%)d 0.00(  0.09%)
                        49.398%  C  2 s( 35.96%)p 1.78( 63.95%)d 0.00(  0.09%)
                         0.156%  C  3 s(  4.42%)p21.25( 93.88%)d 0.39(  1.70%)
                         0.023%  C  4 s( 23.81%)p 3.19( 76.05%)d 0.01(  0.14%)
                         0.011%  C  7 s( 65.20%)p 0.52( 33.99%)d 0.01(  0.81%)
                         0.077%  C 10 s( 81.74%)p 0.22( 18.18%)d 0.00(  0.08%)
                         0.018%  C 11 s( 21.45%)p 3.66( 78.43%)d 0.01(  0.12%)
                         0.011%  H 27 s( 78.80%)p 0.27( 21.20%)
                         0.163%  H 41 s( 99.48%)p 0.01(  0.52%)
                         0.015%  H 42 s( 89.58%)p 0.12( 10.42%)
                         0.151%  N 50 s(  3.78%)p25.20( 95.36%)d 0.23(  0.85%)
                         0.148% Ru 52 s( 13.12%)p 0.31(  4.07%)d 6.31( 82.82%)
  2. (2.00000)  80.5654%  BD ( 2) C  1- C  2
                        44.635%  C  1 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                        35.946%  C  2 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                         8.765%  C  3 s(  0.00%)p 1.00( 99.79%)d 0.00(  0.21%)
                         2.070%  C  5 s(  0.00%)p 1.00( 99.66%)d 0.00(  0.34%)
                         4.884%  C  7 s(  0.00%)p 1.00( 99.93%)d 0.00(  0.07%)
                         0.300%  C  9 s(  0.00%)p 1.00( 98.43%)d 0.02(  1.57%)
                         0.120%  C 11 s(  0.06%)p99.99( 99.73%)d 3.47(  0.21%)
                         0.105%  C 13 s(  0.01%)p 1.00( 99.61%)d 0.00(  0.38%)
                         0.012%  C 15 s(  0.03%)p99.99( 98.10%)d73.87(  1.87%)
                         0.097%  C 19 s(  0.00%)p 1.00( 99.93%)d 0.00(  0.07%)
                         0.015%  H 42 s(  0.40%)p99.99( 99.60%)
                         2.997%  N 50 s(  0.01%)p 1.00( 99.36%)d 0.01(  0.64%)
                         0.012% Ru 52 s(  0.67%)p43.39( 29.09%)d99.99( 70.24%)
  3. (2.00000)  99.2320%  BD ( 1) C  1- C  3
                        49.594%  C  1 s( 33.47%)p 1.98( 66.43%)d 0.00(  0.09%)
                         0.159%  C  2 s(  2.13%)p45.37( 96.51%)d 0.64(  1.37%)
                        49.675%  C  3 s( 33.31%)p 2.00( 66.60%)d 0.00(  0.09%)
                         0.164%  C  5 s(  2.75%)p34.86( 95.86%)d 0.50(  1.39%)
                         0.020%  C  7 s( 49.74%)p 1.00( 49.82%)d 0.01(  0.43%)
                         0.149%  H 27 s( 99.66%)p 0.00(  0.34%)
                         0.165%  H 28 s( 99.50%)p 0.01(  0.50%)
                         0.015%  H 41 s( 81.30%)p 0.23( 18.70%)
                         0.020%  H 42 s( 85.81%)p 0.17( 14.19%)
                         0.019%  N 50 s( 26.28%)p 2.80( 73.57%)d 0.01(  0.15%)
  4. (2.00000)  98.8123%  BD ( 1) C  1- H 42
                        60.928%  C  1 s( 28.77%)p 2.47( 71.16%)d 0.00(  0.07%)
                         0.362%  C  2 s(  7.77%)p11.76( 91.33%)d 0.12(  0.91%)
                         0.226%  C  3 s(  6.17%)p15.01( 92.56%)d 0.21(  1.28%)
                         0.171%  C  5 s( 33.93%)p 1.93( 65.42%)d 0.02(  0.64%)
                         0.038%  C  7 s( 26.53%)p 2.77( 73.37%)d 0.00(  0.10%)
                         0.050%  H 27 s( 99.32%)p 0.01(  0.68%)
                         0.012%  H 28 s( 99.16%)p 0.01(  0.84%)
                         0.060%  H 41 s( 99.47%)p 0.01(  0.53%)
                        37.896%  H 42 s( 99.95%)p 0.00(  0.05%)
                         0.217%  N 50 s( 32.97%)p 2.02( 66.58%)d 0.01(  0.45%)
                         0.011% Ru 52 s(  9.17%)p 0.33(  3.01%)d 9.57( 87.81%)
  5. (2.00000)  98.6915%  BD ( 1) C  2- H 27
                         0.220%  C  1 s(  8.67%)p10.36( 89.81%)d 0.18(  1.52%)
                        61.364%  C  2 s( 29.82%)p 2.35( 70.12%)d 0.00(  0.06%)
                         0.169%  C  3 s( 35.29%)p 1.82( 64.06%)d 0.02(  0.65%)
                         0.023%  C  5 s( 52.63%)p 0.89( 47.09%)d 0.01(  0.28%)
                         0.384%  C  7 s( 26.13%)p 2.82( 73.67%)d 0.01(  0.20%)
                         0.012%  C 10 s( 40.71%)p 1.44( 58.56%)d 0.02(  0.73%)
                        37.333%  H 27 s( 99.89%)p 0.00(  0.11%)
                         0.013%  H 41 s( 98.03%)p 0.02(  1.97%)
                         0.050%  H 42 s( 99.46%)p 0.01(  0.54%)
                         0.348%  N 50 s( 16.16%)p 5.11( 82.53%)d 0.08(  1.31%)
                         0.019% Ru 52 s(  5.62%)p 3.92( 22.02%)d12.87( 72.36%)
  6. (2.00000)  99.3136%  BD ( 1) C  2- N 50
                         0.080%  C  1 s(  6.09%)p15.11( 91.99%)d 0.32(  1.93%)
                        39.741%  C  2 s( 30.83%)p 2.24( 69.08%)d 0.00(  0.09%)
                         0.011%  C  4 s( 32.53%)p 2.06( 67.08%)d 0.01(  0.39%)
                         0.185%  C  7 s(  9.18%)p 9.67( 88.81%)d 0.22(  2.01%)
                         0.119%  C  9 s( 29.66%)p 2.35( 69.68%)d 0.02(  0.65%)
                         0.017%  C 10 s( 12.81%)p 6.75( 86.43%)d 0.06(  0.76%)
                         0.011%  C 11 s( 28.24%)p 2.50( 70.66%)d 0.04(  1.10%)
                         0.015%  H 27 s( 95.18%)p 0.05(  4.82%)
                         0.090%  H 42 s( 99.16%)p 0.01(  0.84%)
                        59.579%  N 50 s( 35.23%)p 1.83( 64.59%)d 0.00(  0.17%)
                         0.101% Ru 52 s(  7.09%)p 3.46( 24.51%)d 9.65( 68.40%)
  7. (2.00000)  99.1904%  BD ( 1) C  3- C  5
                         0.153%  C  1 s(  2.59%)p37.02( 95.91%)d 0.58(  1.50%)
                         0.015%  C  2 s( 51.84%)p 0.90( 46.80%)d 0.03(  1.36%)
                        49.323%  C  3 s( 33.65%)p 1.97( 66.26%)d 0.00(  0.09%)
                        49.909%  C  5 s( 33.96%)p 1.94( 65.95%)d 0.00(  0.09%)
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                    0.219%  C  7 s(  3.52%)p27.05( 95.18%)d 0.37(  1.30%)
                    0.141%  C  9 s( 30.89%)p 2.23( 68.72%)d 0.01(  0.39%)
                    0.019%  H 28 s( 88.98%)p 0.12( 11.02%)
                    0.017%  H 41 s( 83.19%)p 0.20( 16.81%)
                    0.154%  H 42 s( 99.57%)p 0.00(  0.43%)
                    0.021%  N 50 s( 25.17%)p 2.96( 74.52%)d 0.01(  0.31%)
 8. (2.00000)  80.9478%  BD ( 2) C  3- C  5
                    3.229%  C  1 s(  0.00%)p 1.00( 99.52%)d 0.00(  0.48%)
                    2.851%  C  2 s(  0.00%)p 1.00( 99.85%)d 0.00(  0.15%)
                   35.996%  C  3 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                   45.054%  C  5 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                    9.937%  C  7 s(  0.00%)p 1.00( 99.79%)d 0.00(  0.20%)
                    0.182%  C  9 s(  0.00%)p 1.00( 98.46%)d 0.02(  1.54%)
                    0.023%  C 10 s(  0.12%)p99.99( 99.40%)d 3.84(  0.47%)
                    0.115%  C 11 s(  0.34%)p99.99( 99.61%)d 0.15(  0.05%)
                    0.050%  C 13 s(  0.02%)p99.99( 98.89%)d60.18(  1.09%)
                    0.053%  C 19 s(  0.02%)p99.99( 99.93%)d 3.03(  0.06%)
                    0.012%  H 28 s(  0.20%)p99.99( 99.80%)
                    0.010%  H 41 s(  0.08%)p99.99( 99.92%)
                    2.431%  N 50 s(  0.01%)p99.99( 99.82%)d16.44(  0.17%)
 9. (2.00000)  98.9221%  BD ( 1) C  3- H 41
                    0.220%  C  1 s(  6.07%)p15.30( 92.81%)d 0.19(  1.13%)
                    0.180%  C  2 s( 39.86%)p 1.49( 59.49%)d 0.02(  0.65%)
                   60.722%  C  3 s( 28.37%)p 2.52( 71.56%)d 0.00(  0.08%)
                    0.251%  C  5 s(  6.09%)p15.23( 92.78%)d 0.19(  1.13%)
                    0.199%  C  7 s( 30.57%)p 2.25( 68.84%)d 0.02(  0.59%)
                    0.013%  C  9 s( 40.52%)p 1.46( 59.16%)d 0.01(  0.32%)
                    0.010%  H 27 s( 99.93%)p 0.00(  0.07%)
                    0.063%  H 28 s( 99.30%)p 0.01(  0.70%)
                   38.208%  H 41 s( 99.96%)p 0.00(  0.04%)
                    0.061%  H 42 s( 99.29%)p 0.01(  0.71%)
                    0.036%  N 50 s( 66.31%)p 0.50( 33.19%)d 0.01(  0.49%)
                    0.011% Ru 52 s( 37.34%)p 0.31( 11.66%)d 1.37( 51.00%)
10. (2.00000)  99.8741%  BD ( 1) C  4- O 44
                   25.075%  C  4 s(  0.01%)p99.99( 99.76%)d22.19(  0.23%)
                    0.013%  C 11 s( 22.06%)p 3.51( 77.52%)d 0.02(  0.42%)
                   74.800%  O 44 s(  0.01%)p 1.00( 99.60%)d 0.00(  0.39%)
                    0.078% Ru 52 s(  0.37%)p56.21( 21.08%)d99.99( 78.55%)
11. (2.00000)  99.8665%  BD ( 2) C  4- O 44
                   25.641%  C  4 s(  0.00%)p 1.00( 99.78%)d 0.00(  0.22%)
                    0.023%  C 10 s( 21.81%)p 3.55( 77.33%)d 0.04(  0.86%)
                   74.226%  O 44 s(  0.00%)p 1.00( 99.61%)d 0.00(  0.39%)
                    0.069% Ru 52 s(  0.02%)p99.99( 23.48%)d99.99( 76.50%)
12. (2.00000)  99.7651%  BD ( 3) C  4- O 44
                   31.712%  C  4 s( 39.96%)p 1.50( 59.98%)d 0.00(  0.06%)
                    0.020%  C 10 s( 56.26%)p 0.77( 43.31%)d 0.01(  0.43%)
                    0.014%  C 11 s( 14.81%)p 5.74( 85.03%)d 0.01(  0.17%)
                   68.059%  O 44 s( 43.21%)p 1.30( 56.01%)d 0.02(  0.78%)
                    0.166% Ru 52 s( 28.94%)p 1.22( 35.36%)d 1.23( 35.70%)
13. (2.00000)  96.2396%  BD ( 1) C  4-Ru 52
                    0.042%  C  2 s(  8.14%)p11.20( 91.26%)d 0.07(  0.60%)
                    0.011%  C  3 s(  3.71%)p25.95( 96.18%)d 0.03(  0.12%)
                   65.485%  C  4 s( 65.43%)p 0.53( 34.56%)d 0.00(  0.01%)
                    0.056%  C  7 s(  8.72%)p10.43( 90.89%)d 0.04(  0.39%)
                    0.040%  C  9 s(  7.20%)p12.82( 92.31%)d 0.07(  0.49%)
                    0.711%  C 10 s( 16.63%)p 4.99( 82.99%)d 0.02(  0.38%)
                    0.494%  C 11 s(  4.54%)p20.98( 95.21%)d 0.06(  0.26%)
                    0.047%  C 15 s(  4.07%)p23.48( 95.55%)d 0.09(  0.38%)
                    0.011%  C 17 s(  3.42%)p28.22( 96.48%)d 0.03(  0.11%)
                    0.022%  H 43 s( 99.64%)p 0.00(  0.36%)
                    0.070%  O 44 s( 66.04%)p 0.34( 22.40%)d 0.18( 11.56%)
                    0.039%  O 47 s( 45.38%)p 1.19( 53.97%)d 0.01(  0.64%)
                    0.134%  O 48 s(  1.82%)p52.98( 96.58%)d 0.88(  1.60%)
                    0.106% Cl 49 s( 14.85%)p 5.68( 84.30%)d 0.06(  0.85%)
                    0.265%  N 50 s(  8.05%)p11.31( 91.11%)d 0.10(  0.83%)
                   32.386% Ru 52 s( 15.25%)p 0.01(  0.08%)d 5.55( 84.67%)
                    0.033% Ru 53 s( 24.28%)p 0.48( 11.62%)d 2.64( 64.10%)
14. (2.00000)  98.9824%  BD ( 1) C  5- C  7
                    0.161%  C  3 s(  4.40%)p21.37( 94.06%)d 0.35(  1.54%)
                    0.025%  C  4 s( 21.40%)p 3.67( 78.45%)d 0.01(  0.14%)
                   49.262%  C  5 s( 32.45%)p 2.08( 67.46%)d 0.00(  0.09%)
                   49.763%  C  7 s( 33.71%)p 1.96( 66.22%)d 0.00(  0.07%)
                    0.139%  C  9 s( 11.52%)p 7.56( 87.12%)d 0.12(  1.36%)
                    0.068%  C 10 s( 83.82%)p 0.19( 16.09%)d 0.00(  0.08%)
                    0.116%  C 11 s( 42.91%)p 1.31( 56.38%)d 0.02(  0.71%)
                    0.013%  H 28 s( 93.08%)p 0.07(  6.92%)
                    0.155%  H 41 s( 99.39%)p 0.01(  0.61%)
                    0.116%  N 50 s(  5.35%)p17.45( 93.28%)d 0.26(  1.37%)
                    0.135% Ru 52 s( 23.77%)p 0.13(  3.04%)d 3.08( 73.19%)
15. (2.00000)  98.7123%  BD ( 1) C  5- H 28
                    0.176%  C  1 s( 37.21%)p 1.67( 62.18%)d 0.02(  0.61%)
                    0.028%  C  2 s( 64.76%)p 0.54( 35.02%)d 0.00(  0.22%)
                    0.236%  C  3 s(  5.22%)p17.89( 93.42%)d 0.26(  1.36%)
                   60.354%  C  5 s( 28.16%)p 2.55( 71.77%)d 0.00(  0.07%)
                    0.391%  C  7 s( 10.94%)p 8.04( 88.00%)d 0.10(  1.06%)
                    0.026%  C  9 s( 85.05%)p 0.17( 14.39%)d 0.01(  0.55%)
                    0.015%  C 11 s(  7.55%)p12.20( 92.05%)d 0.05(  0.40%)
                    0.025%  C 13 s( 43.90%)p 1.25( 54.80%)d 0.03(  1.30%)
                    0.012%  C 17 s( 35.40%)p 1.79( 63.52%)d 0.03(  1.08%)
                   38.373%  H 28 s( 99.94%)p 0.00(  0.06%)
                    0.016%  H 30 s( 87.75%)p 0.14( 12.25%)
                    0.064%  H 41 s( 99.45%)p 0.01(  0.55%)
                    0.011%  H 42 s( 98.90%)p 0.01(  1.10%)
                    0.234%  N 50 s( 30.90%)p 2.22( 68.61%)d 0.02(  0.49%)
                    0.011% Ru 52 s( 14.12%)p 0.11(  1.52%)d 5.97( 84.36%)
16. (2.00000)  99.8295%  BD ( 1) C  6- O 45
                   25.129%  C  6 s(  1.63%)p60.25( 98.14%)d 0.14(  0.23%)
                    0.011%  C 18 s( 22.66%)p 3.39( 76.79%)d 0.02(  0.55%)
                   74.717%  O 45 s(  1.27%)p77.51( 98.33%)d 0.32(  0.41%)
                    0.078% Ru 53 s(  1.77%)p11.04( 19.59%)d44.34( 78.64%)
17. (2.00000)  99.8049%  BD ( 2) C  6- O 45
                    0.015%  C  2 s( 10.73%)p 8.24( 88.45%)d 0.08(  0.82%)
                   25.338%  C  6 s(  1.20%)p82.34( 98.58%)d 0.19(  0.22%)
                    0.012%  C  8 s( 28.74%)p 2.43( 69.81%)d 0.05(  1.44%)
                   74.479%  O 45 s(  0.77%)p99.99( 98.82%)d 0.52(  0.40%)
                    0.015%  N 51 s(  3.72%)p25.86( 96.17%)d 0.03(  0.11%)
                    0.074% Ru 53 s(  0.88%)p23.56( 20.84%)d88.47( 78.27%)
18. (2.00000)  99.7257%  BD ( 3) C  6- O 45
                    0.010%  C  2 s( 11.28%)p 7.85( 88.48%)d 0.02(  0.24%)
                   31.066%  C  6 s( 38.03%)p 1.63( 61.90%)d 0.00(  0.07%)
                    0.023%  C  8 s( 56.97%)p 0.75( 42.84%)d 0.00(  0.19%)
                    0.013%  C 16 s( 15.29%)p 5.53( 84.60%)d 0.01(  0.11%)
                   68.689%  O 45 s( 41.23%)p 1.41( 58.01%)d 0.02(  0.75%)
                    0.158% Ru 53 s( 28.57%)p 1.17( 33.52%)d 1.33( 37.91%)
19. (2.00000)  96.2480%  BD ( 1) C  6-Ru 53
                    0.023%  C  2 s( 14.15%)p 6.04( 85.42%)d 0.03(  0.43%)
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                    65.355%  C  6 s( 65.98%)p 0.52( 34.01%)d 0.00(  0.01%)
                     0.712%  C  8 s( 28.38%)p 2.51( 71.35%)d 0.01(  0.27%)
                     0.011%  C 12 s( 54.25%)p 0.83( 44.96%)d 0.01(  0.79%)
                     0.469%  C 16 s(  4.83%)p19.70( 95.07%)d 0.02(  0.11%)
                     0.042%  C 18 s( 40.19%)p 1.48( 59.35%)d 0.01(  0.46%)
                     0.010%  C 20 s( 15.98%)p 5.23( 83.49%)d 0.03(  0.53%)
                     0.085%  C 22 s( 24.99%)p 3.00( 74.90%)d 0.00(  0.11%)
                     0.026%  C 24 s( 34.59%)p 1.89( 65.37%)d 0.00(  0.05%)
                     0.083%  O 45 s( 68.32%)p 0.31( 20.88%)d 0.16( 10.80%)
                     0.095%  O 46 s(  3.62%)p26.20( 94.83%)d 0.43(  1.55%)
                     0.165%  O 47 s( 14.71%)p 5.70( 83.82%)d 0.10(  1.46%)
                     0.154% Cl 49 s( 13.64%)p 6.27( 85.51%)d 0.06(  0.84%)
                     0.048%  N 51 s( 57.73%)p 0.72( 41.61%)d 0.01(  0.66%)
                     0.040% Ru 52 s( 44.48%)p 0.21(  9.42%)d 1.04( 46.10%)
                    32.615% Ru 53 s( 17.40%)p 0.00(  0.05%)d 4.74( 82.54%)
20. (2.00000)  98.6202%  BD ( 1) C  7- C  9
                     0.015%  C  1 s( 73.79%)p 0.35( 25.94%)d 0.00(  0.27%)
                     0.218%  C  2 s( 33.36%)p 1.99( 66.29%)d 0.01(  0.35%)
                     0.092%  C  3 s( 34.72%)p 1.85( 64.25%)d 0.03(  1.03%)
                     0.148%  C  5 s(  4.60%)p20.32( 93.49%)d 0.41(  1.91%)
                    50.088%  C  7 s( 32.68%)p 2.06( 67.28%)d 0.00(  0.05%)
                    48.568%  C  9 s( 28.83%)p 2.47( 71.10%)d 0.00(  0.07%)
                     0.155%  C 11 s(  6.38%)p14.43( 92.02%)d 0.25(  1.60%)
                     0.147%  C 13 s(  2.90%)p32.95( 95.46%)d 0.57(  1.64%)
                     0.101%  C 15 s( 35.46%)p 1.80( 63.86%)d 0.02(  0.68%)
                     0.091%  C 17 s( 35.86%)p 1.76( 63.23%)d 0.03(  0.91%)
                     0.016%  C 19 s( 69.11%)p 0.44( 30.57%)d 0.00(  0.32%)
                     0.044%  H 28 s( 99.43%)p 0.01(  0.57%)
                     0.045%  H 30 s( 99.71%)p 0.00(  0.29%)
                     0.197%  N 50 s( 15.46%)p 5.36( 82.80%)d 0.11(  1.74%)
                     0.023% Ru 52 s( 45.29%)p 0.38( 17.41%)d 0.82( 37.30%)
21. (2.00000)  99.0942%  BD ( 1) C  7- N 50
                     0.160%  C  2 s(  6.83%)p13.37( 91.29%)d 0.27(  1.88%)
                     0.086%  C  5 s(  7.71%)p11.66( 89.85%)d 0.32(  2.45%)
                    40.468%  C  7 s( 28.76%)p 2.47( 71.17%)d 0.00(  0.07%)
                     0.103%  C  9 s(  8.60%)p10.43( 89.73%)d 0.19(  1.66%)
                     0.023%  C 10 s(  5.46%)p17.18( 93.72%)d 0.15(  0.82%)
                     0.035%  C 11 s( 64.39%)p 0.54( 34.85%)d 0.01(  0.76%)
                     0.057%  C 13 s( 22.41%)p 3.45( 77.21%)d 0.02(  0.38%)
                     0.150%  H 27 s( 99.93%)p 0.00(  0.07%)
                     0.106%  H 28 s( 99.18%)p 0.01(  0.82%)
                    58.637%  N 50 s( 33.93%)p 1.94( 65.89%)d 0.01(  0.18%)
                     0.115% Ru 52 s( 25.94%)p 0.78( 20.27%)d 2.07( 53.78%)
22. (2.00000)  85.5208%  BD ( 2) C  7- N 50
                     2.062%  C  1 s(  0.01%)p 1.00( 99.82%)d 0.00(  0.18%)
                     6.392%  C  2 s(  0.01%)p 1.00( 99.46%)d 0.01(  0.53%)
                     2.162%  C  3 s(  0.00%)p 1.00( 99.86%)d 0.00(  0.14%)
                     0.023%  C  4 s( 19.94%)p 3.92( 78.09%)d 0.10(  1.97%)
                     2.257%  C  5 s(  0.00%)p 1.00( 99.53%)d 0.00(  0.47%)
                     0.018%  C  6 s( 10.21%)p 8.78( 89.62%)d 0.02(  0.18%)
                    27.686%  C  7 s(  0.00%)p 1.00( 99.91%)d 0.00(  0.09%)
                     0.615%  C  9 s(  0.02%)p99.99( 98.66%)d61.68(  1.32%)
                     0.118%  C 10 s(  0.17%)p99.99( 99.39%)d 2.60(  0.44%)
                     0.175%  C 11 s(  0.52%)p99.99( 98.62%)d 1.67(  0.86%)
                     0.231%  C 13 s(  0.03%)p99.99( 99.84%)d 4.41(  0.13%)
                     0.034%  C 15 s(  0.20%)p99.99( 97.84%)d 9.96(  1.97%)
                     0.121%  C 19 s(  0.04%)p99.99( 99.88%)d 1.97(  0.08%)
                     0.041%  O 48 s(  0.03%)p99.99( 99.92%)d 1.84(  0.05%)
                    57.879%  N 50 s(  0.00%)p 1.00( 99.91%)d 0.00(  0.09%)
                     0.133% Ru 52 s(  0.97%)p22.46( 21.86%)d79.29( 77.17%)
                     0.017% Ru 53 s( 28.71%)p 0.46( 13.25%)d 2.02( 58.04%)
23. (2.00000)  99.8714%  BD ( 1) C  8- O 46
                    25.170%  C  8 s(  0.05%)p99.99( 99.72%)d 4.71(  0.23%)
                     0.011%  C 16 s( 18.47%)p 4.40( 81.21%)d 0.02(  0.32%)
                    74.704%  O 46 s(  0.03%)p99.99( 99.58%)d14.79(  0.39%)
                     0.076% Ru 53 s(  0.33%)p68.98( 22.53%)d99.99( 77.14%)
24. (2.00000)  99.8725%  BD ( 2) C  8- O 46
                     0.015%  C  6 s( 24.25%)p 3.08( 74.70%)d 0.04(  1.06%)
                    25.543%  C  8 s(  0.00%)p 1.00( 99.77%)d 0.00(  0.22%)
                    74.330%  O 46 s(  0.01%)p 1.00( 99.60%)d 0.00(  0.39%)
                     0.070% Ru 53 s(  0.08%)p99.99( 22.88%)d99.99( 77.04%)
25. (2.00000)  99.7643%  BD ( 3) C  8- O 46
                     0.021%  C  6 s( 57.72%)p 0.73( 41.89%)d 0.01(  0.39%)
                    31.722%  C  8 s( 39.96%)p 1.50( 59.98%)d 0.00(  0.06%)
                     0.014%  C 16 s( 14.85%)p 5.72( 84.99%)d 0.01(  0.16%)
                    68.049%  O 46 s( 43.13%)p 1.30( 56.09%)d 0.02(  0.78%)
                     0.166% Ru 53 s( 29.31%)p 1.21( 35.38%)d 1.20( 35.31%)
26. (2.00000)  96.2625%  BD ( 1) C  8-Ru 53
                     0.678%  C  6 s( 19.31%)p 4.16( 80.32%)d 0.02(  0.37%)
                    65.534%  C  8 s( 65.46%)p 0.53( 34.53%)d 0.00(  0.01%)
                     0.048%  C 12 s(  7.49%)p12.28( 91.95%)d 0.08(  0.57%)
                     0.483%  C 16 s(  4.48%)p21.29( 95.28%)d 0.06(  0.25%)
                     0.047%  C 18 s(  4.62%)p20.59( 95.04%)d 0.07(  0.34%)
                     0.058%  C 20 s(  8.29%)p11.01( 91.31%)d 0.05(  0.40%)
                     0.014%  C 21 s(  2.87%)p33.78( 97.02%)d 0.04(  0.10%)
                     0.038%  C 22 s(  7.03%)p13.15( 92.45%)d 0.07(  0.52%)
                     0.010%  C 26 s(  3.79%)p25.37( 96.10%)d 0.03(  0.11%)
                     0.018%  H 43 s( 99.47%)p 0.01(  0.53%)
                     0.117%  O 45 s(  2.01%)p47.81( 96.21%)d 0.88(  1.78%)
                     0.070%  O 46 s( 65.69%)p 0.35( 22.72%)d 0.18( 11.58%)
                     0.040%  O 47 s( 48.80%)p 1.04( 50.76%)d 0.01(  0.44%)
                     0.107% Cl 49 s( 14.04%)p 6.06( 85.15%)d 0.06(  0.81%)
                     0.265%  N 51 s(  8.22%)p11.04( 90.80%)d 0.12(  0.97%)
                     0.031% Ru 52 s( 23.63%)p 0.54( 12.85%)d 2.69( 63.52%)
                    32.390% Ru 53 s( 15.39%)p 0.01(  0.08%)d 5.49( 84.53%)
27. (2.00000)  98.5820%  BD ( 1) C  9- C 11
                     0.019%  C  2 s( 30.76%)p 2.24( 68.84%)d 0.01(  0.40%)
                     0.011%  C  4 s( 34.28%)p 1.90( 65.09%)d 0.02(  0.63%)
                     0.113%  C  5 s( 26.14%)p 2.80( 73.10%)d 0.03(  0.76%)
                     0.196%  C  7 s(  4.11%)p22.79( 93.74%)d 0.52(  2.15%)
                    52.679%  C  9 s( 32.03%)p 2.12( 67.91%)d 0.00(  0.06%)
                     0.062%  C 10 s( 23.59%)p 3.23( 76.25%)d 0.01(  0.16%)
                    45.951%  C 11 s( 35.10%)p 1.85( 64.80%)d 0.00(  0.10%)
                     0.170%  C 13 s(  1.40%)p69.10( 96.77%)d 1.31(  1.83%)
                     0.173%  C 15 s(  7.98%)p11.37( 90.74%)d 0.16(  1.28%)
                     0.015%  H 28 s( 99.52%)p 0.00(  0.48%)
                     0.172%  H 30 s( 98.97%)p 0.01(  1.03%)
                     0.190%  H 33 s( 99.76%)p 0.00(  0.24%)
                     0.013%  O 48 s(  1.09%)p90.32( 98.71%)d 0.18(  0.19%)
                     0.057%  N 50 s( 83.18%)p 0.18( 14.94%)d 0.02(  1.88%)
                     0.136% Ru 52 s( 25.19%)p 0.84( 21.08%)d 2.13( 53.73%)
28. (2.00000)  98.6941%  BD ( 1) C  9- C 13
                     0.018%  C  4 s( 57.27%)p 0.74( 42.65%)d 0.00(  0.07%)
                     0.200%  C  7 s(  9.07%)p 9.83( 89.18%)d 0.19(  1.75%)
                    50.283%  C  9 s( 31.83%)p 2.14( 68.11%)d 0.00(  0.07%)
                     0.014%  C 10 s( 61.89%)p 0.61( 37.97%)d 0.00(  0.13%)
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                    0.264%  C 11 s(  3.69%)p25.78( 95.24%)d 0.29(  1.06%)
                   48.484%  C 13 s( 33.13%)p 2.02( 66.79%)d 0.00(  0.08%)
                    0.162%  C 17 s(  4.44%)p21.18( 94.02%)d 0.35(  1.54%)
                    0.015%  C 19 s( 63.12%)p 0.56( 35.23%)d 0.03(  1.64%)
                    0.011%  H 30 s( 87.01%)p 0.15( 12.99%)
                    0.150%  H 34 s( 99.36%)p 0.01(  0.64%)
                    0.038% Cl 49 s( 14.69%)p 5.76( 84.68%)d 0.04(  0.63%)
                    0.116%  N 50 s( 58.26%)p 0.69( 40.37%)d 0.02(  1.37%)
                    0.206% Ru 52 s( 16.11%)p 0.08(  1.34%)d 5.12( 82.55%)
29. (2.00000)  81.1519%  BD ( 2) C  9- C 13
                    0.616%  C  1 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                    0.204%  C  3 s(  0.00%)p 1.00( 99.04%)d 0.01(  0.96%)
                    0.015%  C  4 s(  1.76%)p55.22( 97.24%)d 0.57(  1.00%)
                    0.551%  C  5 s(  0.01%)p 1.00( 99.49%)d 0.01(  0.50%)
                    2.305%  C  7 s(  0.00%)p 1.00( 99.04%)d 0.01(  0.96%)
                   43.006%  C  9 s(  0.00%)p 1.00( 99.99%)d 0.00(  0.01%)
                    5.973%  C 11 s(  0.00%)p 1.00( 99.71%)d 0.00(  0.29%)
                   38.149%  C 13 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                    1.149%  C 15 s(  0.00%)p 1.00( 99.56%)d 0.00(  0.44%)
                    5.303%  C 17 s(  0.00%)p 1.00( 99.71%)d 0.00(  0.29%)
                    1.727%  C 19 s(  0.00%)p 1.00( 99.73%)d 0.00(  0.27%)
                    0.014%  H 30 s(  0.06%)p99.99( 99.94%)
                    0.921%  N 50 s(  0.00%)p 1.00( 99.60%)d 0.00(  0.39%)
                    0.022% Ru 52 s(  0.56%)p29.43( 16.50%)d99.99( 82.94%)
30. (2.00000)  99.8088%  BD ( 1) C 10- O 48
                    0.012%  C  4 s(  9.62%)p 9.26( 89.16%)d 0.13(  1.22%)
                   25.351%  C 10 s(  2.32%)p42.03( 97.46%)d 0.10(  0.22%)
                   74.480%  O 48 s(  1.85%)p52.86( 97.74%)d 0.22(  0.41%)
                    0.010%  N 50 s(  6.50%)p14.30( 93.00%)d 0.08(  0.50%)
                    0.083% Ru 52 s(  1.86%)p11.12( 20.64%)d41.74( 77.50%)
31. (2.00000)  99.7877%  BD ( 2) C 10- O 48
                    0.011%  C  4 s( 29.62%)p 2.34( 69.25%)d 0.04(  1.13%)
                   25.144%  C 10 s(  0.93%)p99.99( 98.84%)d 0.24(  0.23%)
                    0.023%  C 12 s( 11.72%)p 7.44( 87.19%)d 0.09(  1.09%)
                   74.655%  O 48 s(  0.60%)p99.99( 99.00%)d 0.66(  0.40%)
                    0.013%  N 50 s(  5.08%)p18.65( 94.73%)d 0.04(  0.19%)
                    0.012%  N 51 s(  4.67%)p20.28( 94.78%)d 0.12(  0.55%)
                    0.070% Ru 52 s(  0.74%)p28.32( 21.01%)d99.99( 78.25%)
32. (2.00000)  99.7178%  BD ( 3) C 10- O 48
                    0.022%  C  4 s( 53.78%)p 0.86( 46.04%)d 0.00(  0.18%)
                   30.976%  C 10 s( 37.61%)p 1.66( 62.32%)d 0.00(  0.07%)
                    0.014%  C 11 s( 14.49%)p 5.89( 85.39%)d 0.01(  0.12%)
                    0.013%  C 12 s( 13.49%)p 6.39( 86.24%)d 0.02(  0.27%)
                   68.773%  O 48 s( 40.90%)p 1.43( 58.35%)d 0.02(  0.75%)
                    0.156% Ru 52 s( 28.37%)p 1.18( 33.49%)d 1.34( 38.15%)
33. (2.00000)  96.2795%  BD ( 1) C 10-Ru 52
                    0.011%  C  2 s( 57.02%)p 0.74( 42.24%)d 0.01(  0.74%)
                    0.686%  C  4 s( 27.23%)p 2.66( 72.49%)d 0.01(  0.27%)
                    0.011%  C  7 s( 15.60%)p 5.38( 83.91%)d 0.03(  0.49%)
                    0.087%  C  9 s( 23.72%)p 3.21( 76.19%)d 0.00(  0.09%)
                   65.533%  C 10 s( 66.10%)p 0.51( 33.90%)d 0.00(  0.01%)
                    0.508%  C 11 s(  5.30%)p17.84( 94.60%)d 0.02(  0.10%)
                    0.027%  C 12 s( 14.34%)p 5.93( 85.07%)d 0.04(  0.59%)
                    0.043%  C 15 s( 38.94%)p 1.56( 60.58%)d 0.01(  0.48%)
                    0.027%  C 19 s( 33.77%)p 1.96( 66.19%)d 0.00(  0.04%)
                    0.011%  H 43 s( 99.54%)p 0.00(  0.46%)
                    0.093%  O 44 s(  3.77%)p25.09( 94.63%)d 0.42(  1.60%)
                    0.162%  O 47 s( 27.37%)p 2.58( 70.64%)d 0.07(  2.00%)
                    0.084%  O 48 s( 68.27%)p 0.30( 20.77%)d 0.16( 10.96%)
                    0.138% Cl 49 s( 12.93%)p 6.65( 86.08%)d 0.08(  0.99%)
                    0.050%  N 50 s( 56.70%)p 0.75( 42.61%)d 0.01(  0.69%)
                   32.437% Ru 52 s( 17.77%)p 0.00(  0.05%)d 4.63( 82.18%)
                    0.033% Ru 53 s( 43.85%)p 0.26( 11.62%)d 1.02( 44.54%)
34. (2.00000)  98.9969%  BD ( 1) C 11- C 15
                    0.020%  C  4 s( 58.23%)p 0.71( 41.61%)d 0.00(  0.16%)
                    0.157%  C  7 s( 33.39%)p 1.98( 66.18%)d 0.01(  0.43%)
                    0.222%  C  9 s( 10.47%)p 8.43( 88.31%)d 0.12(  1.22%)
                    0.047%  C 10 s( 41.94%)p 1.38( 57.83%)d 0.01(  0.23%)
                   47.632%  C 11 s( 37.19%)p 1.69( 62.71%)d 0.00(  0.09%)
                   51.394%  C 15 s( 34.49%)p 1.90( 65.42%)d 0.00(  0.09%)
                    0.144%  C 19 s(  2.13%)p45.23( 96.37%)d 0.70(  1.50%)
                    0.027%  H 33 s( 93.39%)p 0.07(  6.61%)
                    0.146%  H 35 s( 99.09%)p 0.01(  0.91%)
                    0.012%  N 50 s( 19.42%)p 4.08( 79.19%)d 0.07(  1.38%)
                    0.135% Ru 52 s( 24.88%)p 1.30( 32.46%)d 1.71( 42.66%)
35. (2.00000)  78.0796%  BD ( 2) C 11- C 15
                    0.044%  C  1 s(  0.05%)p99.99( 99.92%)d 0.79(  0.04%)
                    0.013%  C  2 s(  0.92%)p99.99( 96.46%)d 2.87(  2.63%)
                    0.062%  C  4 s( 11.02%)p 7.99( 87.97%)d 0.09(  1.02%)
                    0.096%  C  5 s(  0.09%)p99.99( 99.91%)d 0.02(  0.00%)
                    0.176%  C  7 s(  0.09%)p99.99( 98.62%)d13.67(  1.29%)
                    4.514%  C  9 s(  0.00%)p 1.00( 99.61%)d 0.00(  0.39%)
                    0.036%  C 10 s( 11.31%)p 7.75( 87.63%)d 0.09(  1.06%)
                   35.499%  C 11 s(  0.01%)p 1.00( 99.94%)d 0.00(  0.05%)
                    5.766%  C 13 s(  0.00%)p 1.00( 99.91%)d 0.00(  0.09%)
                   42.585%  C 15 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.02%)
                    5.086%  C 17 s(  0.00%)p 1.00( 99.88%)d 0.00(  0.11%)
                    5.860%  C 19 s(  0.00%)p 1.00( 99.66%)d 0.00(  0.34%)
                    0.012%  H 30 s(  0.28%)p99.99( 99.72%)
                    0.012%  H 33 s(  0.90%)p99.99( 99.10%)
                    0.013%  H 34 s(  0.03%)p99.99( 99.97%)
                    0.014%  O 44 s(  4.68%)p20.10( 94.05%)d 0.27(  1.27%)
                    0.010%  O 48 s(  0.47%)p99.99( 96.14%)d 7.19(  3.39%)
                    0.039%  N 50 s(  3.51%)p26.44( 92.77%)d 1.06(  3.73%)
                    0.092% Ru 52 s(  1.13%)p16.87( 19.10%)d70.47( 79.77%)
                    0.024% Ru 53 s(  8.03%)p 0.39(  3.16%)d11.06( 88.81%)
36. (2.00000)  93.0234%  BD ( 1) C 11-Ru 52
                    0.059%  C  2 s( 41.26%)p 1.42( 58.41%)d 0.01(  0.33%)
                    0.842%  C  4 s( 33.41%)p 1.98( 66.27%)d 0.01(  0.32%)
                    0.042%  C  5 s( 29.10%)p 2.43( 70.77%)d 0.00(  0.13%)
                    0.117%  C  7 s( 74.29%)p 0.34( 25.49%)d 0.00(  0.22%)
                    0.415%  C  9 s( 18.51%)p 4.31( 79.77%)d 0.09(  1.72%)
                    0.950%  C 10 s( 36.74%)p 1.72( 63.03%)d 0.01(  0.23%)
                   54.567%  C 11 s( 28.68%)p 2.49( 71.31%)d 0.00(  0.01%)
                    0.342%  C 13 s( 38.16%)p 1.61( 61.31%)d 0.01(  0.52%)
                    0.408%  C 15 s( 11.33%)p 7.68( 87.03%)d 0.14(  1.64%)
                    0.046%  C 17 s( 59.20%)p 0.68( 40.28%)d 0.01(  0.52%)
                    0.304%  C 19 s( 43.16%)p 1.30( 56.29%)d 0.01(  0.55%)
                    0.029%  H 30 s( 98.21%)p 0.02(  1.79%)
                    0.127%  H 33 s( 99.57%)p 0.00(  0.43%)
                    0.021%  H 35 s( 98.01%)p 0.02(  1.99%)
                    0.133%  O 44 s(  0.68%)p99.99( 98.39%)d 1.37(  0.93%)
                    0.242%  O 47 s( 21.62%)p 3.59( 77.67%)d 0.03(  0.70%)
                    0.137%  O 48 s(  1.19%)p82.54( 98.00%)d 0.69(  0.82%)
                    0.043% Cl 49 s( 18.67%)p 2.22( 41.53%)d 2.13( 39.80%)
                    0.310%  N 50 s( 14.87%)p 5.68( 84.55%)d 0.04(  0.58%)
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                      40.771% Ru 52 s( 10.69%)p 0.00(  0.03%)d 8.35( 89.28%)
                       0.051% Ru 53 s(  1.17%)p 5.50(  6.44%)d78.86( 92.39%)
37. (2.00000)  99.1632%  BD ( 1) C 12- C 14
                       0.076%  C  6 s( 81.72%)p 0.22( 18.20%)d 0.00(  0.08%)
                       0.022%  C  8 s( 21.34%)p 3.68( 78.52%)d 0.01(  0.14%)
                      49.390%  C 12 s( 35.99%)p 1.78( 63.92%)d 0.00(  0.09%)
                      49.802%  C 14 s( 32.93%)p 2.03( 66.98%)d 0.00(  0.09%)
                       0.018%  C 16 s( 21.01%)p 3.75( 78.88%)d 0.01(  0.11%)
                       0.011%  C 20 s( 66.18%)p 0.50( 33.01%)d 0.01(  0.81%)
                       0.155%  C 21 s(  4.42%)p21.26( 93.87%)d 0.39(  1.71%)
                       0.011%  H 29 s( 78.77%)p 0.27( 21.23%)
                       0.015%  H 31 s( 89.99%)p 0.11( 10.01%)
                       0.162%  H 37 s( 99.50%)p 0.01(  0.50%)
                       0.146%  N 51 s(  3.81%)p24.98( 95.31%)d 0.23(  0.87%)
                       0.147% Ru 53 s( 14.44%)p 0.29(  4.15%)d 5.64( 81.41%)
38. (2.00000)  80.4566%  BD ( 2) C 12- C 14
                      35.969%  C 12 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.04%)
                      44.503%  C 14 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                       0.115%  C 16 s(  0.00%)p 1.00( 99.78%)d 0.00(  0.22%)
                       0.010%  C 18 s(  0.02%)p99.99( 97.91%)d97.19(  2.07%)
                       4.928%  C 20 s(  0.00%)p 1.00( 99.93%)d 0.00(  0.07%)
                       8.817%  C 21 s(  0.00%)p 1.00( 99.79%)d 0.00(  0.21%)
                       0.296%  C 22 s(  0.01%)p99.99( 98.39%)d99.99(  1.60%)
                       2.049%  C 23 s(  0.00%)p 1.00( 99.65%)d 0.00(  0.35%)
                       0.098%  C 24 s(  0.00%)p 1.00( 99.93%)d 0.00(  0.07%)
                       0.107%  C 25 s(  0.04%)p99.99( 99.60%)d10.23(  0.37%)
                       0.014%  H 31 s(  0.34%)p99.99( 99.66%)
                       3.036%  N 51 s(  0.00%)p 1.00( 99.36%)d 0.01(  0.64%)
                       0.015% Ru 53 s(  1.49%)p17.66( 26.35%)d48.37( 72.16%)
39. (2.00000)  98.6865%  BD ( 1) C 12- H 29
                       0.011%  C  6 s( 41.34%)p 1.40( 57.93%)d 0.02(  0.73%)
                       0.012%  C 10 s(  1.71%)p56.87( 97.33%)d 0.56(  0.96%)
                      61.474%  C 12 s( 29.87%)p 2.35( 70.07%)d 0.00(  0.06%)
                       0.220%  C 14 s(  8.61%)p10.43( 89.86%)d 0.18(  1.52%)
                       0.385%  C 20 s( 26.09%)p 2.83( 73.71%)d 0.01(  0.20%)
                       0.169%  C 21 s( 35.33%)p 1.81( 64.02%)d 0.02(  0.65%)
                       0.023%  C 23 s( 53.00%)p 0.88( 46.73%)d 0.01(  0.27%)
                      37.218%  H 29 s( 99.89%)p 0.00(  0.11%)
                       0.050%  H 31 s( 99.44%)p 0.01(  0.56%)
                       0.013%  H 37 s( 98.06%)p 0.02(  1.94%)
                       0.347%  N 51 s( 16.54%)p 4.97( 82.14%)d 0.08(  1.32%)
                       0.019% Ru 53 s(  7.14%)p 3.21( 22.90%)d 9.80( 69.96%)
40. (2.00000)  99.3178%  BD ( 1) C 12- N 51
                       0.017%  C  6 s( 11.96%)p 7.30( 87.31%)d 0.06(  0.74%)
                       0.010%  C  8 s( 28.65%)p 2.48( 70.95%)d 0.01(  0.40%)
                      39.687%  C 12 s( 30.77%)p 2.25( 69.14%)d 0.00(  0.09%)
                       0.080%  C 14 s(  6.31%)p14.56( 91.80%)d 0.30(  1.90%)
                       0.011%  C 16 s( 27.77%)p 2.56( 71.17%)d 0.04(  1.06%)
                       0.183%  C 20 s(  9.34%)p 9.49( 88.63%)d 0.22(  2.03%)
                       0.119%  C 22 s( 30.46%)p 2.26( 68.88%)d 0.02(  0.65%)
                       0.016%  H 29 s( 95.59%)p 0.05(  4.41%)
                       0.090%  H 31 s( 99.19%)p 0.01(  0.81%)
                      59.637%  N 51 s( 35.27%)p 1.83( 64.56%)d 0.00(  0.17%)
                       0.099% Ru 53 s(  6.92%)p 3.65( 25.21%)d 9.82( 67.88%)
41. (2.00000)  99.1624%  BD ( 1) C 13- C 17
                       0.150%  C  7 s( 39.97%)p 1.49( 59.55%)d 0.01(  0.48%)
                       0.233%  C  9 s(  4.41%)p21.38( 94.37%)d 0.27(  1.21%)
                       0.018%  C 11 s( 30.98%)p 2.22( 68.68%)d 0.01(  0.34%)
                      49.976%  C 13 s( 34.04%)p 1.94( 65.88%)d 0.00(  0.09%)
                       0.011%  C 15 s( 61.98%)p 0.58( 36.06%)d 0.03(  1.96%)
                      49.234%  C 17 s( 33.57%)p 1.98( 66.34%)d 0.00(  0.09%)
                       0.153%  C 19 s(  2.87%)p33.29( 95.57%)d 0.54(  1.56%)
                       0.018%  H 30 s( 87.76%)p 0.14( 12.24%)
                       0.017%  H 34 s( 82.56%)p 0.21( 17.44%)
                       0.151%  H 35 s( 99.50%)p 0.01(  0.50%)
42. (2.00000)  98.7323%  BD ( 1) C 13- H 30
                       0.012%  C  3 s( 35.11%)p 1.81( 63.55%)d 0.04(  1.34%)
                       0.033%  C  5 s( 31.09%)p 2.18( 67.76%)d 0.04(  1.15%)
                       0.048%  C  7 s( 87.20%)p 0.14( 12.62%)d 0.00(  0.18%)
                       0.303%  C  9 s(  9.71%)p 9.19( 89.21%)d 0.11(  1.09%)
                       0.269%  C 11 s( 40.82%)p 1.44( 58.81%)d 0.01(  0.37%)
                      59.542%  C 13 s( 27.52%)p 2.63( 72.41%)d 0.00(  0.07%)
                       0.025%  C 15 s( 57.20%)p 0.74( 42.25%)d 0.01(  0.55%)
                       0.233%  C 17 s(  5.91%)p15.73( 92.88%)d 0.21(  1.22%)
                       0.176%  C 19 s( 39.81%)p 1.50( 59.58%)d 0.02(  0.62%)
                       0.022%  H 28 s( 87.07%)p 0.15( 12.93%)
                      39.199%  H 30 s( 99.94%)p 0.00(  0.06%)
                       0.059%  H 34 s( 99.47%)p 0.01(  0.53%)
                       0.012%  H 35 s( 98.18%)p 0.02(  1.82%)
                       0.016%  N 50 s(  6.87%)p13.46( 92.51%)d 0.09(  0.61%)
                       0.023% Ru 52 s(  5.97%)p 0.28(  1.65%)d15.49( 92.38%)
43. (2.00000)  99.2317%  BD ( 1) C 14- C 21
                       0.160%  C 12 s(  2.12%)p45.51( 96.52%)d 0.64(  1.36%)
                      49.581%  C 14 s( 33.43%)p 1.99( 66.47%)d 0.00(  0.09%)
                       0.020%  C 20 s( 47.16%)p 1.11( 52.38%)d 0.01(  0.45%)
                      49.687%  C 21 s( 33.31%)p 2.00( 66.60%)d 0.00(  0.09%)
                       0.164%  C 23 s(  2.81%)p34.04( 95.78%)d 0.50(  1.40%)
                       0.149%  H 29 s( 99.68%)p 0.00(  0.32%)
                       0.020%  H 31 s( 85.89%)p 0.16( 14.11%)
                       0.015%  H 37 s( 81.68%)p 0.22( 18.32%)
                       0.165%  H 38 s( 99.50%)p 0.01(  0.50%)
                       0.018%  N 51 s( 24.37%)p 3.10( 75.48%)d 0.01(  0.16%)
44. (2.00000)  98.8067%  BD ( 1) C 14- H 31
                       0.366%  C 12 s(  7.75%)p11.79( 91.35%)d 0.12(  0.90%)
                      60.980%  C 14 s( 28.75%)p 2.48( 71.18%)d 0.00(  0.07%)
                       0.038%  C 20 s( 26.66%)p 2.75( 73.24%)d 0.00(  0.10%)
                       0.226%  C 21 s(  6.15%)p15.06( 92.58%)d 0.21(  1.27%)
                       0.172%  C 23 s( 33.82%)p 1.94( 65.54%)d 0.02(  0.64%)
                       0.050%  H 29 s( 99.31%)p 0.01(  0.69%)
                      37.839%  H 31 s( 99.95%)p 0.00(  0.05%)
                       0.060%  H 37 s( 99.46%)p 0.01(  0.54%)
                       0.012%  H 38 s( 99.19%)p 0.01(  0.81%)
                       0.219%  N 51 s( 32.89%)p 2.03( 66.66%)d 0.01(  0.45%)
45. (2.00000)  98.8865%  BD ( 1) C 15- C 19
                       0.028%  C  4 s( 60.35%)p 0.66( 39.54%)d 0.00(  0.11%)
                       0.014%  C  9 s( 37.27%)p 1.65( 61.41%)d 0.04(  1.32%)
                       0.023%  C 10 s( 67.03%)p 0.48( 32.26%)d 0.01(  0.70%)
                       0.319%  C 11 s(  6.09%)p15.29( 93.07%)d 0.14(  0.84%)
                       0.010%  C 13 s( 49.24%)p 0.99( 48.55%)d 0.04(  2.21%)
                      49.413%  C 15 s( 32.99%)p 2.03( 66.92%)d 0.00(  0.10%)
                       0.156%  C 17 s(  4.51%)p20.82( 93.84%)d 0.37(  1.65%)
                      49.519%  C 19 s( 34.11%)p 1.93( 65.81%)d 0.00(  0.08%)
                       0.015%  H 33 s( 81.27%)p 0.23( 18.73%)
                       0.158%  H 34 s( 99.35%)p 0.01(  0.65%)
                       0.015%  H 35 s( 81.52%)p 0.23( 18.48%)
                       0.045% Cl 49 s( 13.84%)p 6.16( 85.22%)d 0.07(  0.93%)
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                     0.010%  N 50 s( 30.84%)p 2.24( 68.97%)d 0.01(  0.18%)
                     0.248% Ru 52 s(  8.92%)p 0.28(  2.47%)d 9.94( 88.61%)
46. (2.00000)  98.7405%  BD ( 1) C 15- H 33
                     0.013%  C  7 s( 30.05%)p 2.30( 68.97%)d 0.03(  0.98%)
                     0.199%  C  9 s( 30.07%)p 2.31( 69.35%)d 0.02(  0.58%)
                     0.042%  C 10 s(  4.75%)p19.76( 93.81%)d 0.30(  1.44%)
                     0.338%  C 11 s(  8.19%)p11.06( 90.64%)d 0.14(  1.17%)
                     0.030%  C 13 s( 58.28%)p 0.71( 41.42%)d 0.01(  0.31%)
                    60.226%  C 15 s( 27.03%)p 2.70( 72.91%)d 0.00(  0.07%)
                     0.192%  C 17 s( 39.12%)p 1.54( 60.35%)d 0.01(  0.53%)
                     0.253%  C 19 s(  6.86%)p13.39( 91.80%)d 0.20(  1.34%)
                    38.526%  H 33 s( 99.92%)p 0.00(  0.08%)
                     0.011%  H 34 s( 97.47%)p 0.03(  2.53%)
                     0.064%  H 35 s( 99.56%)p 0.00(  0.44%)
                     0.013%  O 48 s(  4.83%)p18.57( 89.64%)d 1.15(  5.54%)
                     0.010% Cl 49 s( 12.71%)p 6.71( 85.28%)d 0.16(  2.00%)
                     0.046% Ru 52 s(  6.34%)p 0.41(  2.58%)d14.36( 91.08%)
47. (2.00000)  98.9969%  BD ( 1) C 16- C 18
                     0.047%  C  6 s( 38.31%)p 1.61( 61.50%)d 0.01(  0.20%)
                     0.018%  C  8 s( 57.00%)p 0.75( 42.83%)d 0.00(  0.17%)
                    47.679%  C 16 s( 37.07%)p 1.70( 62.84%)d 0.00(  0.09%)
                    51.346%  C 18 s( 34.49%)p 1.90( 65.42%)d 0.00(  0.09%)
                     0.161%  C 20 s( 33.13%)p 2.01( 66.45%)d 0.01(  0.42%)
                     0.224%  C 22 s( 10.80%)p 8.15( 87.94%)d 0.12(  1.26%)
                     0.143%  C 24 s(  2.17%)p44.43( 96.29%)d 0.71(  1.54%)
                     0.027%  H 32 s( 93.36%)p 0.07(  6.64%)
                     0.147%  H 36 s( 99.08%)p 0.01(  0.92%)
                     0.011%  N 51 s( 21.17%)p 3.66( 77.41%)d 0.07(  1.42%)
                     0.134% Ru 53 s( 24.62%)p 1.33( 32.81%)d 1.73( 42.57%)
48. (2.00000)  98.5648%  BD ( 1) C 16- C 22
                     0.061%  C  6 s( 23.10%)p 3.32( 76.75%)d 0.01(  0.15%)
                     0.011%  C  8 s( 35.27%)p 1.82( 64.16%)d 0.02(  0.57%)
                     0.019%  C 12 s( 30.54%)p 2.26( 69.06%)d 0.01(  0.40%)
                    45.846%  C 16 s( 34.99%)p 1.86( 64.91%)d 0.00(  0.10%)
                     0.171%  C 18 s(  7.74%)p11.75( 90.98%)d 0.16(  1.28%)
                     0.200%  C 20 s(  4.22%)p22.19( 93.66%)d 0.50(  2.11%)
                    52.767%  C 22 s( 32.06%)p 2.12( 67.88%)d 0.00(  0.06%)
                     0.116%  C 23 s( 26.09%)p 2.80( 73.16%)d 0.03(  0.75%)
                     0.172%  C 25 s(  1.47%)p65.77( 96.73%)d 1.22(  1.80%)
                     0.190%  H 32 s( 99.78%)p 0.00(  0.22%)
                     0.016%  H 38 s( 99.54%)p 0.00(  0.46%)
                     0.172%  H 39 s( 99.00%)p 0.01(  1.00%)
                     0.013%  O 45 s(  0.74%)p99.99( 99.07%)d 0.25(  0.19%)
                     0.060%  N 51 s( 83.07%)p 0.18( 15.13%)d 0.02(  1.80%)
                     0.136% Ru 53 s( 25.95%)p 0.81( 21.09%)d 2.04( 52.96%)
49. (2.00000)  93.1540%  BD ( 1) C 16-Ru 53
                     0.921%  C  6 s( 37.95%)p 1.63( 61.82%)d 0.01(  0.23%)
                     0.837%  C  8 s( 33.57%)p 1.97( 66.12%)d 0.01(  0.31%)
                     0.062%  C 12 s( 41.33%)p 1.41( 58.29%)d 0.01(  0.38%)
                    54.834%  C 16 s( 28.89%)p 2.46( 71.10%)d 0.00(  0.01%)
                     0.405%  C 18 s( 11.10%)p 7.85( 87.20%)d 0.15(  1.70%)
                     0.120%  C 20 s( 73.57%)p 0.36( 26.23%)d 0.00(  0.20%)
                     0.422%  C 22 s( 18.53%)p 4.31( 79.78%)d 0.09(  1.69%)
                     0.043%  C 23 s( 28.82%)p 2.46( 71.04%)d 0.01(  0.14%)
                     0.303%  C 24 s( 43.28%)p 1.30( 56.17%)d 0.01(  0.55%)
                     0.348%  C 25 s( 38.07%)p 1.61( 61.40%)d 0.01(  0.53%)
                     0.046%  C 26 s( 59.66%)p 0.67( 39.82%)d 0.01(  0.52%)
                     0.126%  H 32 s( 99.49%)p 0.01(  0.51%)
                     0.021%  H 36 s( 98.04%)p 0.02(  1.96%)
                     0.029%  H 39 s( 98.20%)p 0.02(  1.80%)
                     0.126%  O 45 s(  1.30%)p75.15( 97.86%)d 0.64(  0.83%)
                     0.134%  O 46 s(  0.68%)p99.99( 98.40%)d 1.35(  0.92%)
                     0.242%  O 47 s( 24.15%)p 3.11( 75.10%)d 0.03(  0.76%)
                     0.055% Cl 49 s( 20.51%)p 2.32( 47.55%)d 1.56( 31.93%)
                     0.288%  N 51 s( 13.85%)p 6.17( 85.48%)d 0.05(  0.67%)
                     0.049% Ru 52 s(  0.25%)p26.13(  6.56%)d99.99( 93.19%)
                    40.543% Ru 53 s( 10.83%)p 0.00(  0.02%)d 8.23( 89.15%)
50. (2.00000)  99.2274%  BD ( 1) C 17- C 19
                     0.018%  C  9 s( 65.12%)p 0.53( 34.28%)d 0.01(  0.61%)
                     0.015%  C 11 s( 38.41%)p 1.60( 61.48%)d 0.00(  0.11%)
                     0.170%  C 13 s(  2.86%)p33.51( 95.70%)d 0.51(  1.45%)
                     0.157%  C 15 s(  5.24%)p17.87( 93.69%)d 0.20(  1.07%)
                    49.810%  C 17 s( 33.34%)p 2.00( 66.57%)d 0.00(  0.09%)
                    49.459%  C 19 s( 33.57%)p 1.98( 66.34%)d 0.00(  0.09%)
                     0.167%  H 30 s( 99.34%)p 0.01(  0.66%)
                     0.145%  H 33 s( 99.68%)p 0.00(  0.32%)
                     0.017%  H 34 s( 81.85%)p 0.22( 18.15%)
                     0.015%  H 35 s( 77.26%)p 0.29( 22.74%)
51. (2.00000)  81.4793%  BD ( 2) C 17- C 19
                     0.235%  C  1 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                     0.055%  C  3 s(  0.03%)p99.99( 99.05%)d33.57(  0.92%)
                     0.200%  C  5 s(  0.01%)p 1.00( 99.79%)d 0.00(  0.20%)
                     0.749%  C  7 s(  0.01%)p 1.00( 99.28%)d 0.01(  0.72%)
                     3.579%  C  9 s(  0.00%)p 1.00( 99.82%)d 0.00(  0.18%)
                     1.642%  C 11 s(  0.02%)p99.99( 99.70%)d12.48(  0.28%)
                     5.323%  C 13 s(  0.00%)p 1.00( 99.67%)d 0.00(  0.33%)
                     6.391%  C 15 s(  0.00%)p 1.00( 99.78%)d 0.00(  0.22%)
                    40.470%  C 17 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                    41.044%  C 19 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                     0.016%  H 34 s(  0.01%)p 1.00( 99.99%)
                     0.016%  H 35 s(  0.01%)p99.99( 99.99%)
                     0.231%  N 50 s(  0.16%)p99.99( 99.17%)d 4.28(  0.68%)
                     0.011% Ru 52 s(  0.74%)p12.50(  9.30%)d99.99( 89.96%)
52. (2.00000)  98.8650%  BD ( 1) C 17- H 34
                     0.013%  C  7 s( 43.93%)p 1.26( 55.47%)d 0.01(  0.60%)
                     0.195%  C  9 s( 28.45%)p 2.49( 70.94%)d 0.02(  0.61%)
                     0.055%  C 11 s( 43.52%)p 1.30( 56.38%)d 0.00(  0.10%)
                     0.268%  C 13 s(  7.00%)p13.15( 91.97%)d 0.15(  1.03%)
                     0.181%  C 15 s( 34.54%)p 1.88( 64.85%)d 0.02(  0.61%)
                    60.251%  C 17 s( 27.98%)p 2.57( 71.94%)d 0.00(  0.08%)
                     0.241%  C 19 s(  6.93%)p13.29( 92.12%)d 0.14(  0.95%)
                     0.061%  H 30 s( 99.44%)p 0.01(  0.56%)
                    38.623%  H 34 s( 99.96%)p 0.00(  0.04%)
                     0.059%  H 35 s( 99.32%)p 0.01(  0.68%)
                     0.025% Ru 52 s( 30.49%)p 0.17(  5.32%)d 2.11( 64.19%)
53. (2.00000)  98.9017%  BD ( 1) C 18- C 24
                     0.022%  C  6 s( 65.94%)p 0.51( 33.33%)d 0.01(  0.73%)
                     0.029%  C  8 s( 62.73%)p 0.59( 37.17%)d 0.00(  0.10%)
                     0.311%  C 16 s(  6.22%)p14.93( 92.92%)d 0.14(  0.86%)
                    49.378%  C 18 s( 32.98%)p 2.03( 66.93%)d 0.00(  0.10%)
                     0.014%  C 22 s( 38.58%)p 1.56( 60.08%)d 0.03(  1.34%)
                    49.569%  C 24 s( 34.16%)p 1.93( 65.76%)d 0.00(  0.08%)
                     0.010%  C 25 s( 48.68%)p 1.01( 49.13%)d 0.04(  2.19%)
                     0.155%  C 26 s(  4.66%)p20.12( 93.69%)d 0.36(  1.66%)
                     0.015%  H 32 s( 80.59%)p 0.24( 19.41%)
                     0.015%  H 36 s( 81.95%)p 0.22( 18.05%)
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                    0.158%  H 40 s( 99.33%)p 0.01(  0.67%)
                    0.046% Cl 49 s( 13.88%)p 6.14( 85.23%)d 0.06(  0.89%)
                    0.010%  N 51 s( 31.09%)p 2.21( 68.68%)d 0.01(  0.23%)
                    0.249% Ru 53 s(  8.37%)p 0.30(  2.48%)d10.65( 89.15%)
54. (2.00000)  80.9416%  BD ( 2) C 18- C 24
                    0.012%  C  6 s(  4.87%)p19.16( 93.29%)d 0.38(  1.84%)
                    0.176%  C 14 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                    6.237%  C 16 s(  0.00%)p 1.00( 99.72%)d 0.00(  0.28%)
                   41.307%  C 18 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                    0.629%  C 20 s(  0.00%)p 1.00( 99.21%)d 0.01(  0.79%)
                    0.089%  C 21 s(  0.03%)p99.99( 99.38%)d21.88(  0.59%)
                    3.413%  C 22 s(  0.00%)p 1.00( 99.75%)d 0.00(  0.24%)
                    0.101%  C 23 s(  0.11%)p99.99( 99.01%)d 8.06(  0.88%)
                   39.636%  C 24 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                    4.084%  C 25 s(  0.00%)p 1.00( 99.88%)d 0.00(  0.12%)
                    3.991%  C 26 s(  0.00%)p 1.00( 99.59%)d 0.00(  0.41%)
                    0.010%  H 32 s(  0.12%)p99.99( 99.88%)
                    0.016%  H 36 s(  0.01%)p99.99( 99.99%)
                    0.239%  N 51 s(  0.17%)p99.99( 99.66%)d 0.97(  0.16%)
                    0.021% Ru 53 s(  0.44%)p70.65( 31.14%)d99.99( 68.42%)
55. (2.00000)  98.7365%  BD ( 1) C 18- H 32
                    0.041%  C  6 s(  5.05%)p18.52( 93.52%)d 0.28(  1.43%)
                    0.340%  C 16 s(  8.11%)p11.19( 90.70%)d 0.15(  1.20%)
                   60.315%  C 18 s( 27.08%)p 2.69( 72.85%)d 0.00(  0.07%)
                    0.014%  C 20 s( 30.06%)p 2.29( 68.95%)d 0.03(  0.99%)
                    0.197%  C 22 s( 30.06%)p 2.31( 69.33%)d 0.02(  0.61%)
                    0.256%  C 24 s(  6.82%)p13.46( 91.82%)d 0.20(  1.36%)
                    0.030%  C 25 s( 58.68%)p 0.70( 41.01%)d 0.01(  0.31%)
                    0.194%  C 26 s( 39.15%)p 1.54( 60.32%)d 0.01(  0.53%)
                   38.434%  H 32 s( 99.92%)p 0.00(  0.08%)
                    0.065%  H 36 s( 99.56%)p 0.00(  0.44%)
                    0.011%  H 40 s( 97.50%)p 0.03(  2.50%)
                    0.013%  O 45 s(  3.76%)p24.16( 90.94%)d 1.41(  5.30%)
                    0.011% Cl 49 s( 13.70%)p 6.16( 84.38%)d 0.14(  1.92%)
                    0.047% Ru 53 s(  6.50%)p 0.41(  2.68%)d13.96( 90.82%)
56. (2.00000)  98.8262%  BD ( 1) C 19- H 35
                    0.037%  C  9 s( 26.04%)p 2.83( 73.61%)d 0.01(  0.36%)
                    0.251%  C 11 s( 42.19%)p 1.36( 57.46%)d 0.01(  0.35%)
                    0.184%  C 13 s( 38.31%)p 1.59( 61.09%)d 0.02(  0.60%)
                    0.276%  C 15 s(  6.43%)p14.41( 92.69%)d 0.14(  0.88%)
                    0.237%  C 17 s(  7.03%)p13.09( 91.97%)d 0.14(  1.00%)
                   60.211%  C 19 s( 27.77%)p 2.60( 72.15%)d 0.00(  0.08%)
                    0.012%  H 30 s( 98.43%)p 0.02(  1.57%)
                    0.066%  H 33 s( 99.56%)p 0.00(  0.44%)
                    0.061%  H 34 s( 99.52%)p 0.00(  0.48%)
                   38.620%  H 35 s( 99.96%)p 0.00(  0.04%)
                    0.019% Ru 52 s(  4.18%)p 0.89(  3.73%)d22.02( 92.09%)
57. (2.00000)  98.6211%  BD ( 1) C 20- C 22
                    0.219%  C 12 s( 33.17%)p 2.00( 66.48%)d 0.01(  0.35%)
                    0.015%  C 14 s( 74.11%)p 0.35( 25.62%)d 0.00(  0.26%)
                    0.153%  C 16 s(  6.71%)p13.67( 91.75%)d 0.23(  1.54%)
                    0.100%  C 18 s( 35.23%)p 1.82( 64.12%)d 0.02(  0.65%)
                   50.142%  C 20 s( 32.69%)p 2.06( 67.26%)d 0.00(  0.05%)
                    0.092%  C 21 s( 34.66%)p 1.86( 64.32%)d 0.03(  1.02%)
                   48.514%  C 22 s( 28.77%)p 2.47( 71.16%)d 0.00(  0.07%)
                    0.148%  C 23 s(  4.62%)p20.25( 93.49%)d 0.41(  1.89%)
                    0.016%  C 24 s( 69.09%)p 0.44( 30.61%)d 0.00(  0.30%)
                    0.145%  C 25 s(  2.89%)p33.04( 95.49%)d 0.56(  1.61%)
                    0.090%  C 26 s( 35.73%)p 1.77( 63.36%)d 0.03(  0.91%)
                    0.044%  H 38 s( 99.43%)p 0.01(  0.57%)
                    0.045%  H 39 s( 99.71%)p 0.00(  0.29%)
                    0.198%  N 51 s( 15.63%)p 5.29( 82.65%)d 0.11(  1.72%)
                    0.021% Ru 53 s( 49.88%)p 0.36( 17.75%)d 0.65( 32.37%)
58. (2.00000)  98.9889%  BD ( 1) C 20- C 23
                    0.068%  C  6 s( 83.63%)p 0.19( 16.29%)d 0.00(  0.08%)
                    0.024%  C  8 s( 19.01%)p 4.25( 80.86%)d 0.01(  0.14%)
                    0.116%  C 16 s( 42.53%)p 1.33( 56.77%)d 0.02(  0.70%)
                   49.801%  C 20 s( 33.74%)p 1.96( 66.19%)d 0.00(  0.07%)
                    0.160%  C 21 s(  4.26%)p22.11( 94.21%)d 0.36(  1.53%)
                    0.139%  C 22 s( 11.42%)p 7.64( 87.22%)d 0.12(  1.35%)
                   49.230%  C 23 s( 32.43%)p 2.08( 67.48%)d 0.00(  0.09%)
                    0.154%  H 37 s( 99.41%)p 0.01(  0.59%)
                    0.013%  H 38 s( 93.23%)p 0.07(  6.77%)
                    0.115%  N 51 s(  5.39%)p17.31( 93.25%)d 0.25(  1.36%)
                    0.134% Ru 53 s( 24.84%)p 0.13(  3.20%)d 2.90( 71.97%)
59. (2.00000)  99.0904%  BD ( 1) C 20- N 51
                    0.022%  C  6 s(  5.39%)p17.39( 93.78%)d 0.15(  0.82%)
                    0.160%  C 12 s(  6.75%)p13.54( 91.42%)d 0.27(  1.83%)
                    0.036%  C 16 s( 63.27%)p 0.57( 36.00%)d 0.01(  0.73%)
                   40.478%  C 20 s( 28.71%)p 2.48( 71.22%)d 0.00(  0.07%)
                    0.103%  C 22 s(  8.77%)p10.21( 89.60%)d 0.19(  1.63%)
                    0.086%  C 23 s(  7.71%)p11.66( 89.87%)d 0.31(  2.42%)
                    0.057%  C 25 s( 22.46%)p 3.44( 77.17%)d 0.02(  0.38%)
                    0.148%  H 29 s( 99.95%)p 0.00(  0.05%)
                    0.106%  H 38 s( 99.21%)p 0.01(  0.79%)
                   58.624%  N 51 s( 33.85%)p 1.95( 65.97%)d 0.01(  0.18%)
                    0.115% Ru 53 s( 24.97%)p 0.83( 20.64%)d 2.18( 54.39%)
60. (2.00000)  85.7160%  BD ( 2) C 20- N 51
                    0.117%  C  6 s(  1.60%)p61.19( 97.96%)d 0.27(  0.44%)
                    0.025%  C  8 s( 20.29%)p 3.83( 77.74%)d 0.10(  1.97%)
                    0.023%  C 10 s( 11.00%)p 8.06( 88.67%)d 0.03(  0.33%)
                    6.286%  C 12 s(  0.01%)p99.99( 99.46%)d40.81(  0.52%)
                    2.032%  C 14 s(  0.01%)p 1.00( 99.82%)d 0.00(  0.17%)
                    0.167%  C 16 s(  0.32%)p99.99( 98.80%)d 2.77(  0.88%)
                    0.031%  C 18 s(  0.45%)p99.99( 97.48%)d 4.66(  2.08%)
                   27.838%  C 20 s(  0.00%)p 1.00( 99.91%)d 0.00(  0.09%)
                    2.142%  C 21 s(  0.00%)p 1.00( 99.86%)d 0.00(  0.14%)
                    0.599%  C 22 s(  0.05%)p99.99( 98.60%)d25.95(  1.35%)
                    2.242%  C 23 s(  0.00%)p 1.00( 99.54%)d 0.00(  0.46%)
                    0.122%  C 24 s(  0.03%)p99.99( 99.89%)d 2.25(  0.07%)
                    0.240%  C 25 s(  0.03%)p99.99( 99.85%)d 4.21(  0.12%)
                    0.040%  O 45 s(  0.04%)p99.99( 99.90%)d 1.78(  0.07%)
                   57.918%  N 51 s(  0.00%)p 1.00( 99.91%)d 0.00(  0.09%)
                    0.016% Ru 52 s( 32.27%)p 0.46( 14.98%)d 1.63( 52.75%)
                    0.127% Ru 53 s(  0.59%)p37.81( 22.39%)d99.99( 77.02%)
61. (2.00000)  99.1915%  BD ( 1) C 21- C 23
                    0.015%  C 12 s( 52.35%)p 0.88( 46.29%)d 0.03(  1.36%)
                    0.152%  C 14 s(  2.60%)p36.87( 95.90%)d 0.58(  1.50%)
                    0.219%  C 20 s(  3.55%)p26.80( 95.14%)d 0.37(  1.31%)
                   49.297%  C 21 s( 33.62%)p 1.97( 66.28%)d 0.00(  0.09%)
                    0.143%  C 22 s( 30.87%)p 2.23( 68.74%)d 0.01(  0.39%)
                   49.936%  C 23 s( 33.94%)p 1.94( 65.97%)d 0.00(  0.09%)
                    0.153%  H 31 s( 99.58%)p 0.00(  0.42%)
                    0.016%  H 37 s( 83.29%)p 0.20( 16.71%)
                    0.020%  H 38 s( 89.23%)p 0.12( 10.77%)
                    0.020%  N 51 s( 25.35%)p 2.93( 74.34%)d 0.01(  0.31%)
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62. (2.00000)  80.8607%  BD ( 2) C 21- C 23
                          0.023%  C  6 s(  1.68%)p58.35( 97.85%)d 0.28(  0.48%)
                          0.012%  C 10 s(  6.56%)p14.16( 92.83%)d 0.09(  0.62%)
                          2.820%  C 12 s(  0.00%)p 1.00( 99.85%)d 0.00(  0.15%)
                          3.232%  C 14 s(  0.00%)p 1.00( 99.53%)d 0.00(  0.47%)
                          0.109%  C 16 s(  0.07%)p99.99( 99.88%)d 0.66(  0.05%)
                          9.983%  C 20 s(  0.00%)p 1.00( 99.80%)d 0.00(  0.20%)
                         35.844%  C 21 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                          0.179%  C 22 s(  0.01%)p99.99( 98.46%)d99.99(  1.53%)
                         45.120%  C 23 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                          0.051%  C 24 s(  0.02%)p99.99( 99.92%)d 2.58(  0.05%)
                          0.051%  C 25 s(  0.08%)p99.99( 98.88%)d12.70(  1.04%)
                          0.012%  H 38 s(  0.49%)p99.99( 99.51%)
                          2.501%  N 51 s(  0.01%)p99.99( 99.83%)d12.71(  0.16%)
                          0.011% Ru 53 s(  1.25%)p 3.04(  3.79%)d76.24( 94.97%)
63. (2.00000)  98.9191%  BD ( 1) C 21- H 37
                          0.180%  C 12 s( 39.82%)p 1.50( 59.53%)d 0.02(  0.65%)
                          0.220%  C 14 s(  5.96%)p15.59( 92.92%)d 0.19(  1.12%)
                          0.200%  C 20 s( 30.63%)p 2.25( 68.78%)d 0.02(  0.59%)
                         60.775%  C 21 s( 28.39%)p 2.52( 71.54%)d 0.00(  0.08%)
                          0.013%  C 22 s( 41.08%)p 1.43( 58.59%)d 0.01(  0.33%)
                          0.252%  C 23 s(  6.09%)p15.25( 92.78%)d 0.19(  1.13%)
                          0.010%  H 29 s( 99.95%)p 0.00(  0.05%)
                          0.062%  H 31 s( 99.28%)p 0.01(  0.72%)
                         38.151%  H 37 s( 99.96%)p 0.00(  0.04%)
                          0.063%  H 38 s( 99.31%)p 0.01(  0.69%)
                          0.036%  N 51 s( 66.93%)p 0.49( 32.57%)d 0.01(  0.50%)
                          0.011% Ru 53 s( 38.44%)p 0.30( 11.55%)d 1.30( 50.01%)
64. (2.00000)  98.6995%  BD ( 1) C 22- C 25
                          0.013%  C  6 s( 60.25%)p 0.66( 39.60%)d 0.00(  0.15%)
                          0.020%  C  8 s( 58.51%)p 0.71( 41.42%)d 0.00(  0.07%)
                          0.260%  C 16 s(  3.51%)p27.17( 95.43%)d 0.30(  1.06%)
                          0.202%  C 20 s(  9.26%)p 9.61( 88.98%)d 0.19(  1.75%)
                         50.323%  C 22 s( 31.86%)p 2.14( 68.08%)d 0.00(  0.07%)
                          0.015%  C 24 s( 63.68%)p 0.54( 34.65%)d 0.03(  1.67%)
                         48.451%  C 25 s( 33.07%)p 2.02( 66.84%)d 0.00(  0.08%)
                          0.162%  C 26 s(  4.21%)p22.38( 94.27%)d 0.36(  1.52%)
                          0.011%  H 39 s( 87.06%)p 0.15( 12.94%)
                          0.150%  H 40 s( 99.39%)p 0.01(  0.61%)
                          0.038% Cl 49 s( 14.28%)p 5.96( 85.10%)d 0.04(  0.62%)
                          0.117%  N 51 s( 57.47%)p 0.72( 41.17%)d 0.02(  1.36%)
                          0.204% Ru 53 s( 15.34%)p 0.09(  1.36%)d 5.43( 83.30%)
65. (2.00000)  98.7096%  BD ( 1) C 23- H 38
                          0.029%  C 12 s( 64.68%)p 0.54( 35.11%)d 0.00(  0.21%)
                          0.176%  C 14 s( 36.97%)p 1.69( 62.43%)d 0.02(  0.60%)
                          0.016%  C 16 s(  7.52%)p12.25( 92.12%)d 0.05(  0.36%)
                          0.394%  C 20 s( 11.06%)p 7.94( 87.88%)d 0.10(  1.06%)
                          0.235%  C 21 s(  5.16%)p18.12( 93.49%)d 0.26(  1.35%)
                          0.026%  C 22 s( 84.93%)p 0.17( 14.51%)d 0.01(  0.56%)
                         60.411%  C 23 s( 28.16%)p 2.55( 71.77%)d 0.00(  0.07%)
                          0.024%  C 25 s( 43.26%)p 1.28( 55.42%)d 0.03(  1.32%)
                          0.012%  C 26 s( 35.02%)p 1.82( 63.89%)d 0.03(  1.08%)
                          0.011%  H 31 s( 98.93%)p 0.01(  1.07%)
                          0.064%  H 37 s( 99.44%)p 0.01(  0.56%)
                         38.313%  H 38 s( 99.94%)p 0.00(  0.06%)
                          0.015%  H 39 s( 87.29%)p 0.15( 12.71%)
                          0.236%  N 51 s( 30.58%)p 2.25( 68.92%)d 0.02(  0.49%)
                          0.011% Ru 53 s( 13.54%)p 0.13(  1.80%)d 6.25( 84.66%)
66. (2.00000)  99.2273%  BD ( 1) C 24- C 26
                          0.015%  C 16 s( 38.91%)p 1.57( 61.00%)d 0.00(  0.10%)
                          0.157%  C 18 s(  5.19%)p18.05( 93.75%)d 0.20(  1.06%)
                          0.018%  C 22 s( 67.08%)p 0.48( 32.30%)d 0.01(  0.62%)
                         49.427%  C 24 s( 33.54%)p 1.98( 66.37%)d 0.00(  0.09%)
                          0.171%  C 25 s(  2.88%)p33.17( 95.65%)d 0.51(  1.46%)
                         49.841%  C 26 s( 33.32%)p 2.00( 66.59%)d 0.00(  0.09%)
                          0.144%  H 32 s( 99.69%)p 0.00(  0.31%)
                          0.014%  H 36 s( 76.88%)p 0.30( 23.12%)
                          0.169%  H 39 s( 99.33%)p 0.01(  0.67%)
                          0.016%  H 40 s( 82.09%)p 0.22( 17.91%)
67. (2.00000)  98.8252%  BD ( 1) C 24- H 36
                          0.249%  C 16 s( 41.95%)p 1.38( 57.71%)d 0.01(  0.35%)
                          0.277%  C 18 s(  6.34%)p14.63( 92.79%)d 0.14(  0.87%)
                          0.037%  C 22 s( 26.07%)p 2.82( 73.57%)d 0.01(  0.36%)
                         60.256%  C 24 s( 27.79%)p 2.60( 72.14%)d 0.00(  0.08%)
                          0.184%  C 25 s( 37.98%)p 1.62( 61.41%)d 0.02(  0.61%)
                          0.237%  C 26 s(  7.02%)p13.09( 91.97%)d 0.14(  1.01%)
                          0.066%  H 32 s( 99.54%)p 0.00(  0.46%)
                         38.575%  H 36 s( 99.96%)p 0.00(  0.04%)
                          0.012%  H 39 s( 98.49%)p 0.02(  1.51%)
                          0.062%  H 40 s( 99.53%)p 0.00(  0.47%)
                          0.019% Ru 53 s(  4.20%)p 0.85(  3.55%)d21.98( 92.25%)
68. (2.00000)  99.1668%  BD ( 1) C 25- C 26
                          0.017%  C 16 s( 34.81%)p 1.86( 64.87%)d 0.01(  0.33%)
                          0.012%  C 18 s( 63.80%)p 0.54( 34.38%)d 0.03(  1.82%)
                          0.150%  C 20 s( 40.06%)p 1.48( 59.44%)d 0.01(  0.49%)
                          0.232%  C 22 s(  4.39%)p21.48( 94.38%)d 0.28(  1.23%)
                          0.151%  C 24 s(  2.83%)p33.83( 95.63%)d 0.55(  1.55%)
                         50.015%  C 25 s( 34.05%)p 1.93( 65.87%)d 0.00(  0.09%)
                         49.200%  C 26 s( 33.57%)p 1.98( 66.33%)d 0.00(  0.09%)
                          0.149%  H 36 s( 99.50%)p 0.00(  0.50%)
                          0.018%  H 39 s( 87.97%)p 0.14( 12.03%)
                          0.017%  H 40 s( 82.58%)p 0.21( 17.42%)
69. (2.00000)  83.7465%  BD ( 2) C 25- C 26
                          0.016%  C  6 s(  7.01%)p13.21( 92.60%)d 0.06(  0.40%)
                          0.010%  C  8 s( 29.45%)p 2.35( 69.21%)d 0.05(  1.34%)
                          0.012%  C 12 s(  0.33%)p99.99( 99.67%)d 0.02(  0.01%)
                          3.610%  C 16 s(  0.02%)p99.99( 99.94%)d 1.49(  0.03%)
                          2.303%  C 18 s(  0.00%)p 1.00( 99.81%)d 0.00(  0.19%)
                          0.021%  C 20 s(  0.55%)p99.99( 94.09%)d 9.75(  5.36%)
                          2.863%  C 22 s(  0.00%)p 1.00( 99.43%)d 0.01(  0.57%)
                          7.232%  C 24 s(  0.00%)p 1.00( 99.75%)d 0.00(  0.25%)
                         39.036%  C 25 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                         44.760%  C 26 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                          0.017%  H 39 s(  0.03%)p99.99( 99.97%)
                          0.020%  H 40 s(  0.03%)p99.99( 99.97%)
                          0.022%  N 51 s(  2.49%)p38.82( 96.69%)d 0.33(  0.82%)
                          0.019% Ru 53 s(  1.88%)p 3.24(  6.08%)d49.04( 92.04%)
70. (2.00000)  98.7355%  BD ( 1) C 25- H 39
                          0.269%  C 16 s( 40.66%)p 1.45( 58.97%)d 0.01(  0.37%)
                          0.025%  C 18 s( 57.17%)p 0.74( 42.30%)d 0.01(  0.54%)
                          0.049%  C 20 s( 86.98%)p 0.15( 12.83%)d 0.00(  0.19%)
                          0.012%  C 21 s( 35.35%)p 1.79( 63.31%)d 0.04(  1.34%)
                          0.302%  C 22 s(  9.94%)p 8.95( 88.97%)d 0.11(  1.09%)
                          0.033%  C 23 s( 30.76%)p 2.21( 68.10%)d 0.04(  1.14%)
                          0.176%  C 24 s( 39.95%)p 1.49( 59.44%)d 0.02(  0.61%)
                         59.564%  C 25 s( 27.53%)p 2.63( 72.40%)d 0.00(  0.07%)
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                      0.233%  C 26 s(  5.93%)p15.67( 92.87%)d 0.20(  1.21%)
                      0.012%  H 36 s( 98.16%)p 0.02(  1.84%)
                      0.021%  H 38 s( 86.85%)p 0.15( 13.15%)
                     39.180%  H 39 s( 99.94%)p 0.00(  0.06%)
                      0.059%  H 40 s( 99.45%)p 0.01(  0.55%)
                      0.016%  N 51 s(  7.12%)p12.96( 92.27%)d 0.09(  0.62%)
                      0.023% Ru 53 s(  6.10%)p 0.29(  1.75%)d15.10( 92.15%)
 71. (2.00000)  98.8650%  BD ( 1) C 26- H 40
                      0.055%  C 16 s( 44.37%)p 1.25( 55.54%)d 0.00(  0.09%)
                      0.180%  C 18 s( 34.46%)p 1.88( 64.93%)d 0.02(  0.61%)
                      0.013%  C 20 s( 43.73%)p 1.27( 55.65%)d 0.01(  0.62%)
                      0.198%  C 22 s( 28.51%)p 2.49( 70.87%)d 0.02(  0.61%)
                      0.239%  C 24 s(  6.91%)p13.33( 92.13%)d 0.14(  0.96%)
                      0.269%  C 25 s(  6.93%)p13.29( 92.04%)d 0.15(  1.03%)
                     60.280%  C 26 s( 28.00%)p 2.57( 71.92%)d 0.00(  0.08%)
                      0.059%  H 36 s( 99.30%)p 0.01(  0.70%)
                      0.061%  H 39 s( 99.45%)p 0.01(  0.55%)
                     38.595%  H 40 s( 99.96%)p 0.00(  0.04%)
                      0.025% Ru 53 s( 30.48%)p 0.18(  5.44%)d 2.10( 64.07%)
 72. (2.00000)  99.3945%  BD ( 1) H 43- O 47
                      0.069%  C  4 s( 14.41%)p 5.92( 85.22%)d 0.03(  0.37%)
                      0.013%  C  6 s( 54.90%)p 0.81( 44.52%)d 0.01(  0.59%)
                      0.073%  C  8 s( 11.65%)p 7.56( 88.01%)d 0.03(  0.34%)
                      0.017%  C 10 s( 27.63%)p 2.58( 71.41%)d 0.03(  0.96%)
                      0.012%  C 11 s( 23.50%)p 3.23( 75.84%)d 0.03(  0.66%)
                      0.014%  C 16 s( 14.44%)p 5.85( 84.48%)d 0.07(  1.08%)
                     24.295%  H 43 s( 99.97%)p 0.00(  0.03%)
                      0.019%  O 44 s(  2.42%)p40.21( 97.36%)d 0.09(  0.22%)
                      0.021%  O 46 s(  2.26%)p43.09( 97.52%)d 0.09(  0.21%)
                     75.100%  O 47 s( 23.13%)p 3.31( 76.65%)d 0.01(  0.23%)
                      0.012%  N 50 s( 35.84%)p 1.71( 61.12%)d 0.09(  3.05%)
                      0.015%  N 51 s( 39.66%)p 1.48( 58.81%)d 0.04(  1.53%)
                      0.135% Ru 52 s( 17.06%)p 1.39( 23.64%)d 3.48( 59.30%)
                      0.150% Ru 53 s( 21.10%)p 0.94( 19.90%)d 2.80( 59.01%)


CMO: NBO Analysis of Canonical Molecular Orbitals


SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

    Threshold for printing:   0.50 kcal/mol
   (Intermolecular threshold: 0.05 kcal/mol)
                                                            E(2)  E(j)-E(i) F(i,j)
     Donor NBO (i)              Acceptor NBO (j)       kcal/mol   a.u.    a.u.
================================================================================

within unit  1
  1. BD ( 1) C 1- C 2      199. RY*( 2) C 3             0.94    2.37    0.042
  1. BD ( 1) C 1- C 2      737. RY*( 1) N50             1.70    2.49    0.058
  1. BD ( 1) C 1- C 2      869. BD*( 1) C 3- H41        2.46    1.03    0.045
  1. BD ( 1) C 1- C 2      876. BD*( 1) C10-Ru52        0.50    0.77    0.019
  1. BD ( 1) C 1- C 2      880. BD*( 1) C 1- C 3        0.71    1.11    0.025
  1. BD ( 1) C 1- C 2      884. BD*( 1) C 2- N50        0.52    1.10    0.021
  2. BD ( 2) C 1- C 2      200. RY*( 3) C 3             0.94    0.77    0.027
  2. BD ( 2) C 1- C 2      738. RY*( 2) N50             0.80    1.13    0.030
  2. BD ( 2) C 1- C 2      868. BD*( 2) C 3- C 5       16.54    0.23    0.056
  2. BD ( 2) C 1- C 2      882. BD*( 2) C 1- C 2        0.61    0.23    0.011
  2. BD ( 2) C 1- C 2      887. BD*( 2) C 7- N50       10.73    0.21    0.044
  3. BD ( 1) C 1- C 3      230. RY*( 3) C 5             0.93    2.30    0.041
  3. BD ( 1) C 1- C 3      867. BD*( 1) C 3- C 5        0.82    1.12    0.027
  3. BD ( 1) C 1- C 3      871. BD*( 1) C 5- H28        2.50    1.03    0.045
  3. BD ( 1) C 1- C 3      881. BD*( 1) C 1- C 2        0.75    1.12    0.026
  3. BD ( 1) C 1- C 3      885. BD*( 1) C 2- H27        2.38    1.03    0.044
  4. BD ( 1) C 1- H42      183. RY*( 1) C 2             0.63    2.03    0.032
  4. BD ( 1) C 1- H42      198. RY*( 1) C 3             0.84    2.23    0.039
  4. BD ( 1) C 1- H42      867. BD*( 1) C 3- C 5        3.38    0.95    0.051
  4. BD ( 1) C 1- H42      884. BD*( 1) C 2- N50        5.29    0.92    0.062
  5. BD ( 1) C 2- H27      168. RY*( 1) C 1             0.88    2.14    0.039
  5. BD ( 1) C 2- H27      737. RY*( 1) N50             1.76    2.31    0.057
  5. BD ( 1) C 2- H27      778. RY*(12)Ru52             0.57    6.38    0.054
  5. BD ( 1) C 2- H27      880. BD*( 1) C 1- C 3        3.32    0.93    0.050
  5. BD ( 1) C 2- H27      886. BD*( 1) C 7- N50        6.74    0.90    0.070
  6. BD ( 1) C 2- N50      170. RY*( 3) C 1             0.82    2.64    0.042
  6. BD ( 1) C 2- N50      188. RY*( 6) C 2             0.64    3.82    0.044
  6. BD ( 1) C 2- N50      196. RY*(14) C 2             0.63   40.84    0.143
  6. BD ( 1) C 2- N50      197. RY*(15) C 2             0.93   26.69    0.141
  6. BD ( 1) C 2- N50      258. RY*( 1) C 7             0.82    2.30    0.039
  6. BD ( 1) C 2- N50      260. RY*( 3) C 7             1.73    2.71    0.061
  6. BD ( 1) C 2- N50      740. RY*( 4) N50             1.33    5.86    0.079
  6. BD ( 1) C 2- N50      744. RY*( 8) N50             0.51   14.46    0.077
  6. BD ( 1) C 2- N50      767. RY*( 1)Ru52             1.08    7.57    0.081
  6. BD ( 1) C 2- N50      768. RY*( 2)Ru52             1.45    4.31    0.071
  6. BD ( 1) C 2- N50      773. RY*( 7)Ru52             1.97    9.01    0.119
  6. BD ( 1) C 2- N50      775. RY*( 9)Ru52             1.43   10.79    0.111
  6. BD ( 1) C 2- N50      776. RY*(10)Ru52             0.93    9.12    0.083
  6. BD ( 1) C 2- N50      778. RY*(12)Ru52             2.03    6.67    0.104
  6. BD ( 1) C 2- N50      779. RY*(13)Ru52             2.53   15.51    0.177
  6. BD ( 1) C 2- N50      783. RY*(17)Ru52             1.12   13.24    0.109
  6. BD ( 1) C 2- N50      789. RY*(23)Ru52             1.15   11.21    0.102
  6. BD ( 1) C 2- N50      790. RY*(24)Ru52             1.19 3605.71    3.603
  6. BD ( 1) C 2- N50      791. RY*(25)Ru52             0.61 3395.14    4.053
  6. BD ( 1) C 2- N50      792. RY*(26)Ru52             1.39 1160.17    1.138
  6. BD ( 1) C 2- N50      795. RY*(29)Ru52             1.27   53.71    0.234
  6. BD ( 1) C 2- N50      796. RY*(30)Ru52             0.87   19.37    0.116
  6. BD ( 1) C 2- N50      804. RY*(38)Ru52             1.55  259.07    0.568
  6. BD ( 1) C 2- N50      876. BD*( 1) C10-Ru52        4.24    0.88    0.059
  6. BD ( 1) C 2- N50      881. BD*( 1) C 1- C 2        0.78    1.23    0.028
  6. BD ( 1) C 2- N50      883. BD*( 1) C 1- H42        1.59    1.15    0.038
  6. BD ( 1) C 2- N50      886. BD*( 1) C 7- N50        0.62    1.19    0.024
  6. BD ( 1) C 2- N50      888. BD*( 1) C 7- C 9        2.74    1.19    0.051
  7. BD ( 1) C 3- C 5      170. RY*( 3) C 1             0.88    2.53    0.042
  7. BD ( 1) C 3- C 5      258. RY*( 1) C 7             0.69    2.19    0.035
  7. BD ( 1) C 3- C 5      870. BD*( 1) C 5- C 7        1.08    1.13    0.031
  7. BD ( 1) C 3- C 5      880. BD*( 1) C 1- C 3        0.78    1.11    0.026
  7. BD ( 1) C 3- C 5      883. BD*( 1) C 1- H42        2.47    1.04    0.045
  7. BD ( 1) C 3- C 5      888. BD*( 1) C 7- C 9        3.53    1.08    0.055
  8. BD ( 2) C 3- C 5      169. RY*( 2) C 1             1.08    0.81    0.029
  8. BD ( 2) C 3- C 5      264. RY*( 7) C 7             0.62    2.10    0.035
  8. BD ( 2) C 3- C 5      882. BD*( 2) C 1- C 2       12.44    0.23    0.048
  8. BD ( 2) C 3- C 5      887. BD*( 2) C 7- N50       22.33    0.21    0.064
  9. BD ( 1) C 3- H41      168. RY*( 1) C 1             0.88    2.15    0.039
  9. BD ( 1) C 3- H41      228. RY*( 1) C 5             0.90    2.03    0.038
  9. BD ( 1) C 3- H41      870. BD*( 1) C 5- C 7        3.86    0.96    0.054
  9. BD ( 1) C 3- H41      881. BD*( 1) C 1- C 2        3.36    0.95    0.051
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12. BD (3) C 4- O44	188. RY*(6) C 2	1.15	4.14	0.062
12. BD (3) C 4- O44	213. RY*(1) C 4	8.16	2.90	0.138
12. BD (3) C 4- O44	216. RY*(4) C 4	1.20	3.27	0.056
12. BD (3) C 4- O44	219. RY*(7) C 4	4.67	7.74	0.170
12. BD (3) C 4- O44	221. RY*(9) C 4	0.83	5.39	0.060
12. BD (3) C 4- O44	227. RY*(15) C 4	0.75	27.99	0.130
12. BD (3) C 4- O44	263. RY*(6) C 7	0.77	5.31	0.057
12. BD (3) C 4- O44	292. RY*(5) C 9	0.76	4.29	0.051
12. BD (3) C 4- O44	303. RY*(1) C10	1.01	3.02	0.049
12. BD (3) C 4- O44	310. RY*(8) C10	0.54	4.40	0.044
12. BD (3) C 4- O44	321. RY*(4) C11	0.80	3.36	0.046
12. BD (3) C 4- O44	383. RY*(6) C15	1.75	4.34	0.078
12. BD (3) C 4- O44	645. RY*(3) O44	0.91	2.84	0.045
12. BD (3) C 4- O44	646. RY*(4) O44	1.28	1.84	0.043
12. BD (3) C 4- O44	706. RY*(4) O48	0.68	1.74	0.031
12. BD (3) C 4- O44	767. RY*(1)Ru52	12.29	7.89	0.278
12. BD (3) C 4- O44	768. RY*(2)Ru52	7.90	4.62	0.171
12. BD (3) C 4- O44	769. RY*(3)Ru52	2.69	2.69	0.076
12. BD (3) C 4- O44	770. RY*(4)Ru52	5.13	3.39	0.118
12. BD (3) C 4- O44	771. RY*(5)Ru52	7.93	7.97	0.224
12. BD (3) C 4- O44	772. RY*(6)Ru52	1.33	5.48	0.076
12. BD (3) C 4- O44	773. RY*(7)Ru52	5.03	9.32	0.193
12. BD (3) C 4- O44	774. RY*(8)Ru52	1.28	4.72	0.070
12. BD (3) C 4- O44	775. RY*(9)Ru52	9.98	11.10	0.297
12. BD (3) C 4- O44	776. RY*(10)Ru52	2.44	9.44	0.135
12. BD (3) C 4- O44	777. RY*(11)Ru52	0.58	6.06	0.053
12. BD (3) C 4- O44	778. RY*(12)Ru52	3.07	6.99	0.131
12. BD (3) C 4- O44	779. RY*(13)Ru52	3.97	15.82	0.224
12. BD (3) C 4- O44	780. RY*(14)Ru52	2.07	9.88	0.128
12. BD (3) C 4- O44	781. RY*(15)Ru52	2.42	8.63	0.129
12. BD (3) C 4- O44	783. RY*(17)Ru52	5.73	13.56	0.249
12. BD (3) C 4- O44	785. RY*(19)Ru52	3.62	8.20	0.154
12. BD (3) C 4- O44	787. RY*(21)Ru52	0.85	13.57	0.096
12. BD (3) C 4- O44	788. RY*(22)Ru52	0.57	10.82	0.070
12. BD (3) C 4- O44	789. RY*(23)Ru52	6.74	11.52	0.249
12. BD (3) C 4- O44	790. RY*(24)Ru52	6.96	13606.02	8.698
12. BD (3) C 4- O44	791. RY*(25)Ru52	3.60	33395.46	9.795
12. BD (3) C 4- O44	792. RY*(26)Ru52	8.23	1160.48	2.762
12. BD (3) C 4- O44	793. RY*(27)Ru52	0.70	51.36	0.169
12. BD (3) C 4- O44	795. RY*(29)Ru52	8.11	54.02	0.591
12. BD (3) C 4- O44	796. RY*(30)Ru52	5.66	19.68	0.298
12. BD (3) C 4- O44	799. RY*(33)Ru52	1.62	89.29	0.340
12. BD (3) C 4- O44	804. RY*(38)Ru52	9.17	259.39	1.378
12. BD (3) C 4- O44	807. RY*(41)Ru52	0.64	82.08	0.205
12. BD (3) C 4- O44	811. RY*(45)Ru52	0.99	51.78	0.203
12. BD (3) C 4- O44	812. RY*(46)Ru52	0.69	187.20	0.321
13. BD (1) C 4-Ru52	213. RY*(1) C 4	0.52	2.34	0.031
13. BD (1) C 4-Ru52	303. RY*(1) C10	0.51	2.46	0.032
13. BD (1) C 4-Ru52	304. RY*(2) C10	2.33	1.49	0.054
13. BD (1) C 4-Ru52	305. RY*(3) C10	4.10	3.20	0.104
13. BD (1) C 4-Ru52	307. RY*(5) C10	0.53	2.49	0.033
13. BD (1) C 4-Ru52	309. RY*(7) C10	1.03	6.97	0.077
13. BD (1) C 4-Ru52	310. RY*(8) C10	0.82	3.84	0.051
13. BD (1) C 4-Ru52	317. RY*(15) C10	0.71	25.64	0.123
13. BD (1) C 4-Ru52	319. RY*(2) C11	0.53	1.18	0.023
13. BD (1) C 4-Ru52	645. RY*(3) O44	1.17	2.27	0.047
13. BD (1) C 4-Ru52	737. RY*(1) N50	4.47	2.36	0.093
13. BD (1) C 4-Ru52	767. RY*(1)Ru52	0.51	7.33	0.056
13. BD (1) C 4-Ru52	768. RY*(2)Ru52	1.02	4.06	0.058
13. BD (1) C 4-Ru52	771. RY*(5)Ru52	1.10	7.41	0.082
13. BD (1) C 4-Ru52	775. RY*(9)Ru52	0.62	10.54	0.073
13. BD (1) C 4-Ru52	776. RY*(10)Ru52	0.53	8.88	0.062
13. BD (1) C 4-Ru52	785. RY*(19)Ru52	0.54	7.64	0.058
13. BD (1) C 4-Ru52	792. RY*(26)Ru52	0.63	1159.92	0.776
13. BD (1) C 4-Ru52	795. RY*(29)Ru52	0.88	53.46	0.197
13. BD (1) C 4-Ru52	804. RY*(38)Ru52	0.62	258.82	0.364
13. BD (1) C 4-Ru52	874. BD*(3) C 4- O44	0.56	1.13	0.023
13. BD (1) C 4-Ru52	875. BD*(1) C 4-Ru52	1.15	0.63	0.026
13. BD (1) C 4-Ru52	876. BD*(1) C10-Ru52	11.72	0.64	0.083
13. BD (1) C 4-Ru52	877. BD*(1) C10- O48	2.10	0.54	0.031
13. BD (1) C 4-Ru52	878. BD*(2) C10- O48	2.03	0.52	0.030
13. BD (1) C 4-Ru52	879. BD*(3) C10- O48	1.79	1.10	0.040
13. BD (1) C 4-Ru52	884. BD*(1) C 2- N50	0.62	0.96	0.022
13. BD (1) C 4-Ru52	886. BD*(1) C 7- N50	0.78	0.94	0.024
13. BD (1) C 4-Ru52	891. BD*(1) C 9- C11	0.59	1.02	0.022
13. BD (1) C 4-Ru52	894. BD*(1) C11-Ru52	12.49	0.53	0.077
13. BD (1) C 4-Ru52	895. BD*(1) C11- C15	0.65	1.03	0.023
13. BD (1) C 4-Ru52	896. BD*(2) C11- C15	0.61	0.54	0.017
14. BD (1) C 5- C 7	199. RY*(2) C 3	1.56	2.36	0.054
14. BD (1) C 5- C 7	290. RY*(3) C 9	0.84	2.45	0.041
14. BD (1) C 5- C 7	737. RY*(1) N50	0.55	2.49	0.033
14. BD (1) C 5- C 7	739. RY*(3) N50	0.54	2.77	0.035
14. BD (1) C 5- C 7	867. BD*(1) C 3- C 5	0.92	1.11	0.029
14. BD (1) C 5- C 7	869. BD*(1) C 3- H41	2.34	1.02	0.044
14. BD (1) C 5- C 7	886. BD*(1) C 7- N50	0.52	1.07	0.021
14. BD (1) C 5- C 7	888. BD*(1) C 7- C 9	1.09	1.07	0.030
14. BD (1) C 5- C 7	891. BD*(1) C 9- C11	2.18	1.14	0.045
15. BD (1) C 5- H28	198. RY*(1) C 3	0.90	2.23	0.040
15. BD (1) C 5- H28	258. RY*(1) C 7	1.00	2.02	0.040
15. BD (1) C 5- H28	880. BD*(1) C 1- C 3	3.49	0.93	0.051
15. BD (1) C 5- H28	886. BD*(1) C 7- N50	5.67	0.91	0.064
20. BD (1) C 7- C 9	228. RY*(1) C 5	0.79	2.14	0.037
20. BD (1) C 7- C 9	318. RY*(1) C11	1.04	1.67	0.037
20. BD (1) C 7- C 9	348. RY*(1) C13	0.89	2.15	0.039
20. BD (1) C 7- C 9	354. RY*(7) C13	0.57	8.15	0.061
20. BD (1) C 7- C 9	737. RY*(1) N50	0.79	2.43	0.039
20. BD (1) C 7- C 9	867. BD*(1) C 3- C 5	2.02	1.06	0.042
20. BD (1) C 7- C 9	870. BD*(1) C 5- C 7	0.96	1.06	0.029
20. BD (1) C 7- C 9	884. BD*(1) C 2- N50	4.63	1.04	0.062
20. BD (1) C 7- C 9	889. BD*(1) C 9- C13	0.88	1.08	0.028
20. BD (1) C 7- C 9	891. BD*(1) C 9- C11	1.03	1.09	0.030
20. BD (1) C 7- C 9	892. BD*(1) C13- C17	2.11	1.08	0.043
20. BD (1) C 7- C 9	895. BD*(1) C11- C15	2.59	1.10	0.048
21. BD (1) C 7- N50	185. RY*(3) C 2	2.49	2.59	0.072
21. BD (1) C 7- N50	233. RY*(6) C 5	0.56	7.08	0.056
21. BD (1) C 7- N50	235. RY*(8) C 5	0.58	3.89	0.043
21. BD (1) C 7- N50	266. RY*(9) C 7	0.68	12.25	0.082
21. BD (1) C 7- N50	268. RY*(11) C 7	0.54	6.06	0.051
21. BD (1) C 7- N50	271. RY*(14) C 7	0.75	42.76	0.160
21. BD (1) C 7- N50	272. RY*(15) C 7	0.99	24.44	0.139
21. BD (1) C 7- N50	739. RY*(3) N50	0.96	2.87	0.047
21. BD (1) C 7- N50	767. RY*(1)Ru52	0.53	7.56	0.056
21. BD (1) C 7- N50	773. RY*(7)Ru52	0.75	8.99	0.074
21. BD (1) C 7- N50	774. RY*(8)Ru52	0.68	4.39	0.049
21. BD (1) C 7- N50	778. RY*(12)Ru52	0.97	6.66	0.072
21. BD (1) C 7- N50	779. RY*(13)Ru52	0.87	15.49	0.104

21. BD (1) C 7- N50	783. RY*(17)Ru52	0.51	13.23	0.074
21. BD (1) C 7- N50	870. BD*(1) C 5- C 7	1.02	1.22	0.032
21. BD (1) C 7- N50	871. BD*(1) C 5- H28	1.64	1.13	0.038
21. BD (1) C 7- N50	876. BD*(1) C10-Ru52	5.03	0.87	0.064
21. BD (1) C 7- N50	885. BD*(1) C 2- H27	1.92	1.13	0.042
21. BD (1) C 7- N50	888. BD*(1) C 7- C 9	0.63	1.17	0.024
21. BD (1) C 7- N50	889. BD*(1) C 9- C13	2.30	1.24	0.048
22. BD (2) C 7- N50	184. RY*(2) C 2	2.74	0.92	0.048
22. BD (2) C 7- N50	229. RY*(2) C 5	0.93	0.76	0.026
22. BD (2) C 7- N50	289. RY*(2) C 9	0.72	0.83	0.024
22. BD (2) C 7- N50	769. RY*(3)Ru52	0.51	1.90	0.030
22. BD (2) C 7- N50	868. BD*(2) C 3- C 5	7.62	0.27	0.041
22. BD (2) C 7- N50	882. BD*(2) C 1- C 2	20.36	0.27	0.067
22. BD (2) C 7- N50	890. BD*(2) C 9- C13	7.56	0.30	0.044
27. BD (1) C 9- C11	258. RY*(1) C 7	0.87	2.14	0.039
27. BD (1) C 9- C11	290. RY*(3) C 9	0.61	2.41	0.034
27. BD (1) C 9- C11	292. RY*(5) C 9	0.53	3.81	0.040
27. BD (1) C 9- C11	296. RY*(9) C 9	0.83	15.13	0.101
27. BD (1) C 9- C11	301. RY*(14) C 9	0.81	42.44	0.166
27. BD (1) C 9- C11	302. RY*(15) C 9	0.94	25.97	0.140
27. BD (1) C 9- C11	318. RY*(1) C11	0.66	1.68	0.030
27. BD (1) C 9- C11	350. RY*(3) C13	0.76	2.37	0.038
27. BD (1) C 9- C11	351. RY*(4) C13	0.97	2.13	0.041
27. BD (1) C 9- C11	355. RY*(8) C13	0.51	3.39	0.037
27. BD (1) C 9- C11	380. RY*(3) C15	1.51	2.34	0.053
27. BD (1) C 9- C11	767. RY*(1)Ru52	0.98	7.41	0.076
27. BD (1) C 9- C11	770. RY*(4)Ru52	0.69	2.91	0.040
27. BD (1) C 9- C11	773. RY*(7)Ru52	1.40	8.84	0.100
27. BD (1) C 9- C11	774. RY*(8)Ru52	0.72	4.24	0.050
27. BD (1) C 9- C11	775. RY*(9)Ru52	0.52	10.62	0.067
27. BD (1) C 9- C11	778. RY*(12)Ru52	0.95	6.51	0.071
27. BD (1) C 9- C11	779. RY*(13)Ru52	1.06	15.34	0.115
27. BD (1) C 9- C11	780. RY*(14)Ru52	0.54	9.40	0.064
27. BD (1) C 9- C11	781. RY*(15)Ru52	0.62	8.15	0.064
27. BD (1) C 9- C11	783. RY*(17)Ru52	0.50	13.08	0.073
27. BD (1) C 9- C11	788. RY*(22)Ru52	0.63	10.34	0.073
27. BD (1) C 9- C11	790. RY*(24)Ru52	0.57	13605.54	2.502
27. BD (1) C 9- C11	792. RY*(26)Ru52	0.66	1160.00	0.787
27. BD (1) C 9- C11	795. RY*(29)Ru52	0.54	53.54	0.152
27. BD (1) C 9- C11	796. RY*(30)Ru52	0.51	19.20	0.089
27. BD (1) C 9- C11	800. RY*(34)Ru52	0.62	50.17	0.159
27. BD (1) C 9- C11	804. RY*(38)Ru52	0.74	258.91	0.394
27. BD (1) C 9- C11	870. BD*(1) C 5- C 7	3.41	1.07	0.054
27. BD (1) C 9- C11	888. BD*(1) C 7- C 9	1.02	1.02	0.029
27. BD (1) C 9- C11	889. BD*(1) C 9- C13	2.08	1.09	0.042
27. BD (1) C 9- C11	893. BD*(1) C13- H30	2.31	1.00	0.043
27. BD (1) C 9- C11	895. BD*(1) C11- C15	0.55	1.11	0.022
27. BD (1) C 9- C11	902. BD*(1) C15- H33	2.88	1.01	0.048
28. BD (1) C 9- C13	260. RY*(3) C 7	1.19	2.56	0.049
28. BD (1) C 9- C13	320. RY*(3) C11	0.65	1.66	0.029
28. BD (1) C 9- C13	410. RY*(3) C17	1.74	2.54	0.060
28. BD (1) C 9- C13	886. BD*(1) C 7- N50	2.78	1.04	0.048
28. BD (1) C 9- C13	888. BD*(1) C 7- C 9	0.98	1.04	0.028
28. BD (1) C 9- C13	891. BD*(1) C 9- C11	2.13	1.12	0.044
28. BD (1) C 9- C13	892. BD*(1) C13- C17	1.01	1.11	0.030
28. BD (1) C 9- C13	894. BD*(1) C11-Ru52	3.42	0.63	0.045
28. BD (1) C 9- C13	899. BD*(1) C17- H34	2.30	1.02	0.043
29. BD (2) C 9- C13	289. RY*(2) C 9	0.81	0.76	0.024
29. BD (2) C 9- C13	319. RY*(2) C11	0.98	0.87	0.029
29. BD (2) C 9- C13	409. RY*(2) C17	1.02	0.73	0.027
29. BD (2) C 9- C13	887. BD*(2) C 7- N50	23.39	0.18	0.060
29. BD (2) C 9- C13	890. BD*(2) C 9- C13	0.52	0.23	0.010
29. BD (2) C 9- C13	896. BD*(2) C11- C15	15.44	0.24	0.055
29. BD (2) C 9- C13	898. BD*(2) C17- C19	14.39	0.22	0.051
30. BD (1) C10- O48	769. RY*(3)Ru52	0.86	2.02	0.037
30. BD (1) C10- O48	877. BD*(1) C10- O48	0.51	0.43	0.014
32. BD (3) C10- O48	188. RY*(6) C 2	1.00	4.10	0.057
32. BD (3) C10- O48	213. RY*(1) C 4	0.99	2.86	0.048
32. BD (3) C10- O48	219. RY*(7) C 4	1.20	7.70	0.086
32. BD (3) C10- O48	263. RY*(6) C 7	0.53	5.27	0.047
32. BD (3) C10- O48	303. RY*(1) C10	8.89	2.98	0.146
32. BD (3) C10- O48	305. RY*(3) C10	2.22	3.72	0.081
32. BD (3) C10- O48	309. RY*(7) C10	3.96	7.49	0.154
32. BD (3) C10- O48	310. RY*(8) C10	0.92	4.36	0.057
32. BD (3) C10- O48	311. RY*(9) C10	0.80	5.61	0.060
32. BD (3) C10- O48	316. RY*(14) C10	0.71	46.70	0.163
32. BD (3) C10- O48	317. RY*(15) C10	0.95	26.16	0.141
32. BD (3) C10- O48	321. RY*(4) C11	0.64	3.32	0.041
32. BD (3) C10- O48	383. RY*(6) C15	2.11	4.30	0.085
32. BD (3) C10- O48	646. RY*(4) O44	0.80	1.80	0.034
32. BD (3) C10- O48	648. RY*(6) O44	0.54	3.55	0.039
32. BD (3) C10- O48	705. RY*(3) O48	1.27	3.05	0.056
32. BD (3) C10- O48	706. RY*(4) O48	0.95	1.70	0.036
32. BD (3) C10- O48	767. RY*(1)Ru52	9.90	7.85	0.249
32. BD (3) C10- O48	768. RY*(2)Ru52	10.66	4.58	0.197
32. BD (3) C10- O48	769. RY*(3)Ru52	4.43	2.65	0.097
32. BD (3) C10- O48	770. RY*(4)Ru52	1.28	3.35	0.059
32. BD (3) C10- O48	771. RY*(5)Ru52	13.67	7.93	0.294
32. BD (3) C10- O48	772. RY*(6)Ru52	2.44	5.44	0.103
32. BD (3) C10- O48	773. RY*(7)Ru52	7.76	9.28	0.240
32. BD (3) C10- O48	774. RY*(8)Ru52	1.25	4.68	0.068
32. BD (3) C10- O48	775. RY*(9)Ru52	9.01	11.06	0.282
32. BD (3) C10- O48	776. RY*(10)Ru52	5.09	9.40	0.195
32. BD (3) C10- O48	778. RY*(12)Ru52	1.81	6.95	0.100
32. BD (3) C10- O48	779. RY*(13)Ru52	3.12	15.78	0.198
32. BD (3) C10- O48	780. RY*(14)Ru52	0.59	9.84	0.068
32. BD (3) C10- O48	781. RY*(15)Ru52	1.70	8.59	0.108
32. BD (3) C10- O48	783. RY*(17)Ru52	7.74	13.52	0.289
32. BD (3) C10- O48	784. RY*(18)Ru52	2.15	7.00	0.110
32. BD (3) C10- O48	785. RY*(19)Ru52	3.33	8.16	0.147
32. BD (3) C10- O48	789. RY*(23)Ru52	9.90	11.48	0.301
32. BD (3) C10- O48	790. RY*(24)Ru52	7.90	13605.98	9.269
32. BD (3) C10- O48	791. RY*(25)Ru52	4.05	33395.42	10.401
32. BD (3) C10- O48	792. RY*(26)Ru52	9.34	1160.44	2.943
32. BD (3) C10- O48	795. RY*(29)Ru52	9.76	53.98	0.649
32. BD (3) C10- O48	796. RY*(30)Ru52	6.69	19.64	0.324
32. BD (3) C10- O48	799. RY*(33)Ru52	1.86	89.25	0.364
32. BD (3) C10- O48	800. RY*(34)Ru52	0.76	50.61	0.176
32. BD (3) C10- O48	804. RY*(38)Ru52	10.37	259.34	1.466
32. BD (3) C10- O48	807. RY*(41)Ru52	0.72	82.04	0.217
33. BD (1) C10-Ru52	216. RY*(4) C 4	2.72	2.71	0.078
33. BD (1) C10-Ru52	218. RY*(6) C 4	0.79	2.64	0.042
33. BD (1) C10-Ru52	219. RY*(7) C 4	0.90	7.19	0.073
33. BD (1) C10-Ru52	303. RY*(1) C10	0.96	2.47	0.044
33. BD (1) C10-Ru52	317. RY*(15) C10	0.51	25.65	0.104
33. BD (1) C10-Ru52	318. RY*(1) C11	0.97	1.60	0.036

33. BD (1) C10-Ru52	705. RY*(3) O48	1.92	2.53	0.063
33. BD (1) C10-Ru52	706. RY*(4) O48	0.60	1.18	0.024
33. BD (1) C10-Ru52	740. RY*(4) N50	0.50	5.62	0.048
33. BD (1) C10-Ru52	767. RY*(1)Ru52	0.58	7.33	0.059
33. BD (1) C10-Ru52	795. RY*(29)Ru52	0.63	53.47	0.167
33. BD (1) C10-Ru52	873. BD*(2) C 4- O44	1.75	0.52	0.028
33. BD (1) C10-Ru52	874. BD*(3) C 4- O44	2.07	1.14	0.044
33. BD (1) C10-Ru52	875. BD*(1) C 4-Ru52	12.29	0.64	0.084
33. BD (1) C10-Ru52	876. BD*(1) C10-Ru52	1.06	0.64	0.025
33. BD (1) C10-Ru52	879. BD*(3) C10- O48	0.67	1.10	0.024
33. BD (1) C10-Ru52	891. BD*(1) C 9- C11	2.06	1.03	0.041
33. BD (1) C10-Ru52	894. BD*(1) C11-Ru52	13.24	0.54	0.080
34. BD (1) C11- C15	219. RY*(7) C 4	0.60	7.28	0.059
34. BD (1) C11- C15	288. RY*(1) C 9	1.47	2.00	0.048
34. BD (1) C11- C15	290. RY*(3) C 9	1.09	2.41	0.046
34. BD (1) C11- C15	303. RY*(1) C10	0.53	2.55	0.033
34. BD (1) C11- C15	318. RY*(1) C11	0.52	1.69	0.027
34. BD (1) C11- C15	320. RY*(3) C11	0.69	1.65	0.030
34. BD (1) C11- C15	321. RY*(4) C11	2.38	2.89	0.074
34. BD (1) C11- C15	326. RY*(9) C11	0.66	13.42	0.085
34. BD (1) C11- C15	380. RY*(3) C15	0.61	2.35	0.034
34. BD (1) C11- C15	383. RY*(6) C15	1.62	3.87	0.071
34. BD (1) C11- C15	384. RY*(7) C15	0.56	8.60	0.062
34. BD (1) C11- C15	390. RY*(13) C15	0.59	40.95	0.139
34. BD (1) C11- C15	392. RY*(15) C15	0.74	27.28	0.128
34. BD (1) C11- C15	440. RY*(3) C19	1.41	2.50	0.053
34. BD (1) C11- C15	589. RY*(2) H33	0.54	2.52	0.033
34. BD (1) C11- C15	767. RY*(1)Ru52	2.41	7.42	0.120
34. BD (1) C11- C15	768. RY*(2)Ru52	2.67	4.15	0.094
34. BD (1) C11- C15	769. RY*(3)Ru52	1.75	2.22	0.056
34. BD (1) C11- C15	770. RY*(4)Ru52	3.64	2.92	0.092
34. BD (1) C11- C15	771. RY*(5)Ru52	2.76	7.50	0.129
34. BD (1) C11- C15	772. RY*(6)Ru52	0.80	5.01	0.057
34. BD (1) C11- C15	773. RY*(7)Ru52	3.03	8.85	0.147
34. BD (1) C11- C15	774. RY*(8)Ru52	1.70	4.25	0.076
34. BD (1) C11- C15	775. RY*(9)Ru52	1.37	10.63	0.108
34. BD (1) C11- C15	777. RY*(11)Ru52	0.81	5.60	0.061
34. BD (1) C11- C15	778. RY*(12)Ru52	1.90	6.52	0.100
34. BD (1) C11- C15	779. RY*(13)Ru52	1.67	15.35	0.143
34. BD (1) C11- C15	780. RY*(14)Ru52	1.05	9.41	0.089
34. BD (1) C11- C15	781. RY*(15)Ru52	1.87	8.16	0.111
34. BD (1) C11- C15	783. RY*(17)Ru52	2.44	13.09	0.160
34. BD (1) C11- C15	784. RY*(18)Ru52	0.51	6.57	0.052
34. BD (1) C11- C15	785. RY*(19)Ru52	1.51	7.74	0.097
34. BD (1) C11- C15	788. RY*(22)Ru52	0.51	10.35	0.065
34. BD (1) C11- C15	789. RY*(23)Ru52	2.19	11.05	0.140
34. BD (1) C11- C15	790. RY*(24)Ru52	2.17	13605.55	4.873
34. BD (1) C11- C15	791. RY*(25)Ru52	1.17	33394.99	5.605
34. BD (1) C11- C15	792. RY*(26)Ru52	2.57	1160.01	1.550
34. BD (1) C11- C15	793. RY*(27)Ru52	0.77	50.89	0.178
34. BD (1) C11- C15	794. RY*(28)Ru52	0.52	186.75	0.280
34. BD (1) C11- C15	795. RY*(29)Ru52	2.46	53.55	0.326
34. BD (1) C11- C15	796. RY*(30)Ru52	2.11	19.21	0.180
34. BD (1) C11- C15	804. RY*(38)Ru52	2.87	258.92	0.773
34. BD (1) C11- C15	888. BD*(1) C 7- C 9	3.60	1.03	0.055
34. BD (1) C11- C15	891. BD*(1) C 9- C11	0.69	1.11	0.025
34. BD (1) C11- C15	900. BD*(1) C19- H35	2.21	1.01	0.042
34. BD (1) C11- C15	901. BD*(1) C15- C19	1.15	1.09	0.032
34. BD (1) C11- C15	902. BD*(1) C15- H33	0.67	1.02	0.023
35. BD (2) C11- C15	289. RY*(2) C 9	1.81	0.75	0.037
35. BD (2) C11- C15	319. RY*(2) C11	0.68	0.86	0.024
35. BD (2) C11- C15	439. RY*(2) C19	1.43	0.72	0.032
35. BD (2) C11- C15	875. BD*(1) C 4-Ru52	0.83	0.32	0.015
35. BD (2) C11- C15	890. BD*(2) C 9- C13	14.60	0.22	0.050
35. BD (2) C11- C15	898. BD*(2) C17- C19	17.96	0.21	0.056
36. BD (1) C11-Ru52	216. RY*(4) C 4	0.72	2.54	0.040
36. BD (1) C11-Ru52	288. RY*(1) C 9	0.79	1.74	0.034
36. BD (1) C11-Ru52	304. RY*(2) C10	0.71	1.33	0.028
36. BD (1) C11-Ru52	305. RY*(3) C10	1.89	3.04	0.070
36. BD (1) C11-Ru52	321. RY*(4) C11	0.55	2.64	0.035
36. BD (1) C11-Ru52	378. RY*(1) C15	0.84	2.00	0.038
36. BD (1) C11-Ru52	737. RY*(1) N50	3.13	2.20	0.076
36. BD (1) C11-Ru52	778. RY*(12)Ru52	0.71	6.26	0.062
36. BD (1) C11-Ru52	870. BD*(1) C 5- C 7	0.64	0.83	0.021
36. BD (1) C11-Ru52	872. BD*(1) C 4- O44	1.29	0.35	0.020
36. BD (1) C11-Ru52	874. BD*(3) C 4- O44	0.88	0.97	0.027
36. BD (1) C11-Ru52	875. BD*(1) C 4-Ru52	17.37	0.47	0.084
36. BD (1) C11-Ru52	876. BD*(1) C10-Ru52	18.65	0.48	0.088
36. BD (1) C11-Ru52	878. BD*(2) C10- O48	0.91	0.35	0.016
36. BD (1) C11-Ru52	879. BD*(3) C10- O48	1.67	0.93	0.036
36. BD (1) C11-Ru52	884. BD*(1) C 2- N50	1.71	0.80	0.034
36. BD (1) C11-Ru52	888. BD*(1) C 7- C 9	0.57	0.78	0.019
36. BD (1) C11-Ru52	889. BD*(1) C 9- C13	6.38	0.84	0.067
36. BD (1) C11-Ru52	894. BD*(1) C11-Ru52	3.33	0.37	0.033
36. BD (1) C11-Ru52	901. BD*(1) C15- C19	5.63	0.84	0.063
36. BD (1) C11-Ru52	902. BD*(1) C15- H33	0.86	0.76	0.024
41. BD (1) C13- C17	288. RY*(1) C 9	0.71	2.01	0.034
41. BD (1) C13- C17	440. RY*(3) C19	1.01	2.51	0.045
41. BD (1) C13- C17	888. BD*(1) C 7- C 9	3.42	1.05	0.054
41. BD (1) C13- C17	889. BD*(1) C 9- C13	1.25	1.11	0.033
41. BD (1) C13- C17	897. BD*(1) C17- C19	0.87	1.10	0.028
41. BD (1) C13- C17	900. BD*(1) C19- H35	2.34	1.03	0.044
42. BD (1) C13- H30	288. RY*(1) C 9	1.15	1.85	0.041
42. BD (1) C13- H30	408. RY*(1) C17	0.96	2.16	0.041
42. BD (1) C13- H30	891. BD*(1) C 9- C11	4.92	0.96	0.062
42. BD (1) C13- H30	897. BD*(1) C17- C19	3.57	0.94	0.052
45. BD (1) C15- C19	318. RY*(1) C11	1.05	1.69	0.038
45. BD (1) C15- C19	410. RY*(3) C17	0.96	2.54	0.044
45. BD (1) C15- C19	894. BD*(1) C11-Ru52	3.73	0.63	0.047
45. BD (1) C15- C19	895. BD*(1) C11- C15	1.44	1.13	0.036
45. BD (1) C15- C19	897. BD*(1) C17- C19	0.77	1.09	0.026
45. BD (1) C15- C19	899. BD*(1) C17- H34	2.36	1.02	0.044
46. BD (1) C15- H33	318. RY*(1) C11	1.53	1.52	0.043
46. BD (1) C15- H33	438. RY*(1) C19	0.96	2.04	0.040
46. BD (1) C15- H33	444. RY*(7) C19	0.53	6.60	0.053
46. BD (1) C15- H33	891. BD*(1) C 9- C11	3.77	0.95	0.053
46. BD (1) C15- H33	897. BD*(1) C17- C19	3.71	0.92	0.052
50. BD (1) C17- C19	350. RY*(3) C13	0.98	2.38	0.043
50. BD (1) C17- C19	381. RY*(4) C15	0.63	1.64	0.029
50. BD (1) C17- C19	892. BD*(1) C13- C17	0.95	1.11	0.029
50. BD (1) C17- C19	893. BD*(1) C13- H30	2.51	1.01	0.045
50. BD (1) C17- C19	901. BD*(1) C15- C19	0.81	1.10	0.027
50. BD (1) C17- C19	902. BD*(1) C15- H33	2.18	1.02	0.042
51. BD (2) C17- C19	349. RY*(2) C13	0.58	0.75	0.021
51. BD (2) C17- C19	379. RY*(2) C15	0.71	0.71	0.022
51. BD (2) C17- C19	890. BD*(2) C 9- C13	16.14	0.23	0.055

51. BD (2) C17- C19	896. BD*(2) C11- C15	12.40	0.24	0.049
52. BD (1) C17- H34	348. RY*(1) C13	0.97	2.01	0.040
52. BD (1) C17- H34	438. RY*(1) C19	0.97	2.05	0.040
52. BD (1) C17- H34	889. BD*(1) C 9- C13	4.03	0.95	0.055
52. BD (1) C17- H34	901. BD*(1) C15- C19	3.74	0.94	0.053
56. BD (1) C19- H35	378. RY*(1) C15	0.92	2.09	0.039
56. BD (1) C19- H35	408. RY*(1) C17	0.93	2.15	0.040
56. BD (1) C19- H35	892. BD*(1) C13- C17	3.65	0.94	0.053
56. BD (1) C19- H35	895. BD*(1) C11- C15	4.78	0.96	0.061
73. CR (1) C 1	185. RY*(3) C 2	0.67	11.63	0.079
73. CR (1) C 1	186. RY*(4) C 2	0.80	11.04	0.084
73. CR (1) C 1	199. RY*(2) C 3	1.02	11.50	0.097
73. CR (1) C 1	884. BD*(1) C 2- N50	0.69	10.23	0.075
74. CR (1) C 2	168. RY*(1) C 1	0.71	11.48	0.080
74. CR (1) C 2	170. RY*(3) C 1	0.65	11.69	0.078
74. CR (1) C 2	886. BD*(1) C 7- N50	1.04	10.25	0.093
75. CR (1) C 3	170. RY*(3) C 1	1.36	11.67	0.112
75. CR (1) C 3	230. RY*(3) C 5	1.34	11.45	0.111
76. CR (1) C 4	646. RY*(4) O44	0.89	10.64	0.087
77. CR (1) C 5	199. RY*(2) C 3	1.18	11.51	0.104
77. CR (1) C 5	260. RY*(3) C 7	1.15	11.73	0.104
77. CR (1) C 5	886. BD*(1) C 7- N50	0.68	10.21	0.075
77. CR (1) C 5	888. BD*(1) C 7- C 9	0.90	10.21	0.086
79. CR (1) C 7	228. RY*(1) C 5	0.62	11.37	0.075
79. CR (1) C 7	288. RY*(1) C 9	0.54	11.21	0.069
79. CR (1) C 7	739. RY*(3) N50	0.51	11.95	0.070
79. CR (1) C 7	884. BD*(1) C 2- N50	0.91	10.27	0.087
79. CR (1) C 7	889. BD*(1) C 9- C13	0.61	10.32	0.072
79. CR (1) C 7	891. BD*(1) C 9- C11	0.60	10.33	0.071
81. CR (1) C 9	258. RY*(1) C 7	0.56	11.30	0.071
81. CR (1) C 9	318. RY*(1) C11	0.51	10.84	0.067
81. CR (1) C 9	320. RY*(3) C11	0.73	10.81	0.079
81. CR (1) C 9	348. RY*(1) C13	0.53	11.32	0.069
81. CR (1) C 9	350. RY*(3) C13	0.59	11.54	0.074
81. CR (1) C 9	870. BD*(1) C 5- C 7	0.77	10.24	0.080
81. CR (1) C 9	886. BD*(1) C 7- N50	0.51	10.20	0.065
81. CR (1) C 9	894. BD*(1) C11-Ru52	0.63	9.78	0.076
82. CR (1) C10	706. RY*(4) O48	0.93	10.54	0.088
83. CR (1) C11	288. RY*(1) C 9	0.55	11.16	0.070
83. CR (1) C11	290. RY*(3) C 9	0.87	11.58	0.090
83. CR (1) C11	378. RY*(1) C15	0.52	11.42	0.069
83. CR (1) C11	380. RY*(3) C15	0.98	11.52	0.095
83. CR (1) C11	888. BD*(1) C 7- C 9	0.66	10.20	0.074
83. CR (1) C11	889. BD*(1) C 9- C13	0.72	10.26	0.077
83. CR (1) C11	894. BD*(1) C11-Ru52	0.55	9.79	0.071
83. CR (1) C11	901. BD*(1) C15- C19	0.58	10.26	0.070
85. CR (1) C13	290. RY*(3) C 9	0.93	11.57	0.093
85. CR (1) C13	410. RY*(3) C17	1.26	11.69	0.108
85. CR (1) C13	888. BD*(1) C 7- C 9	0.77	10.19	0.080
85. CR (1) C13	891. BD*(1) C 9- C11	0.88	10.27	0.086
87. CR (1) C15	320. RY*(3) C11	1.00	10.80	0.093
87. CR (1) C15	440. RY*(3) C19	0.94	11.64	0.094
87. CR (1) C15	894. BD*(1) C11-Ru52	0.83	9.77	0.087
89. CR (1) C17	350. RY*(3) C13	1.30	11.53	0.109
89. CR (1) C17	440. RY*(3) C19	1.25	11.65	0.108
89. CR (1) C17	889. BD*(1) C 9- C13	0.57	10.25	0.069
91. CR (1) C19	380. RY*(3) C15	0.87	11.51	0.089
91. CR (1) C19	381. RY*(4) C15	0.59	10.79	0.071
91. CR (1) C19	410. RY*(3) C17	0.85	11.69	0.089
91. CR (1) C19	895. BD*(1) C11- C15	0.84	10.27	0.083
99. CR (1) O44	213. RY*(1) C 4	4.86	20.39	0.282
99. CR (1) O44	875. BD*(1) C 4-Ru52	0.65	18.68	0.107
103. CR (1) O48	303. RY*(1) C10	4.91	20.52	0.284
103. CR (1) O48	876. BD*(1) C10-Ru52	0.62	18.70	0.105
109. CR (1) N50	183. RY*(1) C 2	0.95	15.43	0.108
109. CR (1) N50	185. RY*(3) C 2	0.95	15.72	0.109
109. CR (1) N50	258. RY*(1) C 7	0.96	15.41	0.109
109. CR (1) N50	260. RY*(3) C 7	0.95	15.82	0.109
109. CR (1) N50	876. BD*(1) C10-Ru52	4.41	14.00	0.242
112. CR (2)Ru52	792. RY*(26)Ru52	3.58	1285.58	1.915
112. CR (2)Ru52	795. RY*(29)Ru52	0.89	179.12	0.356
112. CR (2)Ru52	804. RY*(38)Ru52	2.16	384.48	0.814
112. CR (2)Ru52	807. RY*(41)Ru52	2.07	207.18	0.585
112. CR (2)Ru52	874. BD*(3) C 4- O44	1.03	126.79	0.323
112. CR (2)Ru52	879. BD*(3) C10- O48	1.11	126.76	0.337
113. CR (3)Ru52	767. RY*(1)Ru52	1.03	28.70	0.154
113. CR (3)Ru52	771. RY*(5)Ru52	0.57	28.78	0.114
113. CR (3)Ru52	773. RY*(7)Ru52	1.00	30.13	0.155
113. CR (3)Ru52	775. RY*(9)Ru52	1.15	31.91	0.171
113. CR (3)Ru52	776. RY*(10)Ru52	0.51	30.25	0.111
113. CR (3)Ru52	779. RY*(13)Ru52	1.01	36.63	0.171
113. CR (3)Ru52	783. RY*(17)Ru52	0.90	34.37	0.157
113. CR (3)Ru52	789. RY*(23)Ru52	0.84	32.33	0.147
113. CR (3)Ru52	792. RY*(26)Ru52	7.55	1181.29	2.667
113. CR (3)Ru52	795. RY*(29)Ru52	2.97	74.83	0.421
113. CR (3)Ru52	796. RY*(30)Ru52	1.01	40.49	0.181
113. CR (3)Ru52	799. RY*(33)Ru52	5.08	110.10	0.668
113. CR (3)Ru52	804. RY*(38)Ru52	4.78	280.19	1.033
113. CR (3)Ru52	807. RY*(41)Ru52	18.55	102.89	1.233
113. CR (3)Ru52	874. BD*(3) C 4- O44	3.61	22.50	0.255
113. CR (3)Ru52	879. BD*(3) C10- O48	3.94	22.47	0.267
113. CR (3)Ru52	884. BD*(1) C 2- N50	0.82	22.33	0.122
113. CR (3)Ru52	886. BD*(1) C 7- N50	0.62	22.32	0.106
113. CR (3)Ru52	891. BD*(1) C 9- C11	0.63	22.39	0.107
113. CR (3)Ru52	894. BD*(1) C11-Ru52	0.86	21.90	0.133
113. CR (3)Ru52	895. BD*(1) C11- C15	1.47	22.40	0.163
114. CR (4)Ru52	213. RY*(1) C 4	3.11	6.42	0.126
114. CR (4)Ru52	303. RY*(1) C10	3.62	6.54	0.137
114. CR (4)Ru52	318. RY*(1) C11	0.69	5.68	0.056
114. CR (4)Ru52	767. RY*(1)Ru52	0.73	11.41	0.082
114. CR (4)Ru52	771. RY*(5)Ru52	0.63	11.49	0.076
114. CR (4)Ru52	773. RY*(7)Ru52	0.81	12.84	0.091
114. CR (4)Ru52	775. RY*(9)Ru52	0.84	14.62	0.099
114. CR (4)Ru52	779. RY*(13)Ru52	0.85	19.34	0.115
114. CR (4)Ru52	783. RY*(17)Ru52	0.83	17.08	0.106
114. CR (4)Ru52	789. RY*(23)Ru52	0.90	15.05	0.104
114. CR (4)Ru52	792. RY*(26)Ru52	1.87	1164.00	1.322
114. CR (4)Ru52	795. RY*(29)Ru52	1.33	57.54	0.247
114. CR (4)Ru52	796. RY*(30)Ru52	0.67	23.20	0.112
114. CR (4)Ru52	799. RY*(33)Ru52	0.65	92.81	0.220
114. CR (4)Ru52	804. RY*(38)Ru52	1.51	262.91	0.564
114. CR (4)Ru52	807. RY*(41)Ru52	1.74	85.60	0.345
114. CR (4)Ru52	874. BD*(3) C 4- O44	10.37	5.21	0.208
114. CR (4)Ru52	877. BD*(1) C10- O48	0.55	4.62	0.047
114. CR (4)Ru52	879. BD*(3) C10- O48	11.06	5.18	0.214
114. CR (4)Ru52	884. BD*(1) C 2- N50	2.45	5.05	0.100

114. CR (4)Ru52	886. BD*(1) C 7- N50	1.89	5.03	0.088
114. CR (4)Ru52	891. BD*(1) C 9- C11	1.54	5.10	0.080
114. CR (4)Ru52	894. BD*(1) C11-Ru52	2.65	4.62	0.106
114. CR (4)Ru52	895. BD*(1) C11- C15	4.00	5.11	0.128
117. CR (7)Ru52	876. BD*(1) C10-Ru52	3.18	1.95	0.077
117. CR (7)Ru52	877. BD*(1) C10- O48	0.55	1.85	0.030
117. CR (7)Ru52	879. BD*(3) C10- O48	1.45	2.41	0.053
117. CR (7)Ru52	884. BD*(1) C 2- N50	0.51	2.27	0.030
117. CR (7)Ru52	894. BD*(1) C11-Ru52	2.98	1.84	0.072
117. CR (7)Ru52	895. BD*(1) C11- C15	0.56	2.34	0.032
120. CR (10)Ru52	874. BD*(3) C 4- O44	1.37	2.45	0.052
120. CR (10)Ru52	875. BD*(1) C 4-Ru52	4.25	1.95	0.088
120. CR (10)Ru52	876. BD*(1) C10-Ru52	1.37	1.95	0.050
120. CR (10)Ru52	878. BD*(2) C10- O48	1.04	1.83	0.041
120. CR (10)Ru52	894. BD*(1) C11-Ru52	2.27	1.85	0.063
123. CR (13)Ru52	874. BD*(3) C 4- O44	1.25	2.44	0.049
123. CR (13)Ru52	875. BD*(1) C 4-Ru52	2.23	1.94	0.064
123. CR (13)Ru52	876. BD*(1) C10-Ru52	1.62	1.95	0.055
123. CR (13)Ru52	879. BD*(3) C10- O48	0.91	2.41	0.042
123. CR (13)Ru52	894. BD*(1) C11-Ru52	2.44	1.84	0.065
148. LP (1) O44	213. RY*(1) C 4	8.64	2.49	0.131
148. LP (1) O44	220. RY*(8) C 4	1.14	3.29	0.055
148. LP (1) O44	875. BD*(1) C 4-Ru52	3.28	0.78	0.049
154. LP (1) O48	303. RY*(1) C10	8.70	2.61	0.135
154. LP (1) O48	310. RY*(8) C10	2.14	4.00	0.083
154. LP (1) O48	876. BD*(1) C10-Ru52	3.17	0.79	0.049
159. LP (1) N50	183. RY*(1) C 2	2.16	1.92	0.063
159. LP (1) N50	185. RY*(3) C 2	0.65	2.20	0.037
159. LP (1) N50	258. RY*(1) C 7	1.99	1.90	0.060
159. LP (1) N50	260. RY*(3) C 7	1.07	2.31	0.049
159. LP (1) N50	773. RY*(7)Ru52	0.52	8.60	0.065
159. LP (1) N50	775. RY*(9)Ru52	0.58	10.39	0.076
159. LP (1) N50	870. BD*(1) C 5- C 7	7.40	0.83	0.076
159. LP (1) N50	873. BD*(2) C 4- O44	1.10	0.36	0.018
159. LP (1) N50	874. BD*(3) C 4- O44	0.87	0.97	0.028
159. LP (1) N50	876. BD*(1) C10-Ru52	72.05	0.48	0.167
159. LP (1) N50	881. BD*(1) C 1- C 2	7.06	0.83	0.074
159. LP (1) N50	885. BD*(1) C 2- H27	2.61	0.74	0.043
159. LP (1) N50	888. BD*(1) C 7- C 9	1.67	0.79	0.035
159. LP (1) N50	889. BD*(1) C 9- C13	0.53	0.85	0.021
159. LP (1) N50	894. BD*(1) C11-Ru52	1.61	0.38	0.022
159. LP (1) N50	895. BD*(1) C11- C15	1.45	0.87	0.035
161. LP (1)Ru52	306. RY*(4) C10	1.95	1.66	0.054
161. LP (1)Ru52	320. RY*(3) C11	0.58	1.24	0.025
161. LP (1)Ru52	739. RY*(3) N50	1.71	2.32	0.060
161. LP (1)Ru52	872. BD*(1) C 4- O44	4.76	0.19	0.027
161. LP (1)Ru52	877. BD*(1) C10- O48	11.98	0.22	0.046
161. LP (1)Ru52	878. BD*(2) C10- O48	9.56	0.20	0.039
161. LP (1)Ru52	884. BD*(1) C 2- N50	0.56	0.64	0.018
161. LP (1)Ru52	886. BD*(1) C 7- N50	0.51	0.62	0.017
161. LP (1)Ru52	895. BD*(1) C11- C15	0.73	0.71	0.021
161. LP (1)Ru52	896. BD*(2) C11- C15	1.71	0.22	0.018
162. LP (2)Ru52	215. RY*(3) C 4	2.02	2.03	0.062
162. LP (2)Ru52	306. RY*(4) C10	0.66	1.66	0.032
162. LP (2)Ru52	319. RY*(2) C11	1.74	0.85	0.037
162. LP (2)Ru52	872. BD*(1) C 4- O44	23.11	0.19	0.061
162. LP (2)Ru52	877. BD*(1) C10- O48	1.86	0.22	0.018
162. LP (2)Ru52	878. BD*(2) C10- O48	3.28	0.20	0.023
162. LP (2)Ru52	894. BD*(1) C11-Ru52	0.86	0.21	0.012
162. LP (2)Ru52	896. BD*(2) C11- C15	5.37	0.22	0.031
163. LP (3)Ru52	214. RY*(2) C 4	3.00	1.31	0.061
163. LP (3)Ru52	304. RY*(2) C10	2.44	1.18	0.053
163. LP (3)Ru52	738. RY*(2) N50	2.31	1.09	0.049
163. LP (3)Ru52	779. RY*(13)Ru52	0.59	14.95	0.093
163. LP (3)Ru52	873. BD*(2) C 4- O44	23.33	0.20	0.063
163. LP (3)Ru52	877. BD*(1) C10- O48	9.25	0.22	0.042
163. LP (3)Ru52	878. BD*(2) C10- O48	12.78	0.20	0.047
163. LP (3)Ru52	887. BD*(2) C 7- N50	3.53	0.17	0.023

from unit 1 to unit 2

6. BD (1) C 2- N50	570. RY*(3) H29	0.07	1.91	0.010
6. BD (1) C 2- N50	824. RY*(10)Ru53	0.08	7.81	0.022
6. BD (1) C 2- N50	826. RY*(12)Ru53	0.05	3.66	0.013
6. BD (1) C 2- N50	832. RY*(18)Ru53	0.09	5.99	0.021
10. BD (1) C 4- O44	821. RY*(7)Ru53	0.09	3.40	0.015
10. BD (1) C 4- O44	824. RY*(10)Ru53	0.09	7.42	0.023
10. BD (1) C 4- O44	834. RY*(20)Ru53	0.07	11.77	0.025
10. BD (1) C 4- O44	859. RY*(45)Ru53	0.06	50.96	0.049
12. BD (3) C 4- O44	253. RY*(11) C 6	0.05	2.97	0.011
12. BD (3) C 4- O44	338. RY*(6) C12	0.08	3.95	0.016
12. BD (3) C 4- O44	453. RY*(1) C20	0.07	2.63	0.012
12. BD (3) C 4- O44	457. RY*(5) C20	0.07	2.84	0.012
12. BD (3) C 4- O44	460. RY*(8) C20	0.08	6.33	0.020
12. BD (3) C 4- O44	570. RY*(3) H29	0.30	2.23	0.023
12. BD (3) C 4- O44	752. RY*(1) N51	0.05	2.88	0.011
12. BD (3) C 4- O44	753. RY*(2) N51	0.08	1.94	0.011
12. BD (3) C 4- O44	765. RY*(14) N51	0.06	5.56	0.017
12. BD (3) C 4- O44	824. RY*(10)Ru53	0.23	8.13	0.039
12. BD (3) C 4- O44	826. RY*(12)Ru53	0.05	3.98	0.013
12. BD (3) C 4- O44	832. RY*(18)Ru53	0.10	6.30	0.022
13. BD (1) C 4-Ru52	820. RY*(6)Ru53	0.17	4.04	0.024
13. BD (1) C 4-Ru52	906. BD*(1) C 6-Ru53	0.06	0.64	0.006
22. BD (2) C 7- N50	815. RY*(1)Ru53	0.09	7.26	0.024
22. BD (2) C 7- N50	822. RY*(8)Ru53	0.06	4.91	0.016
22. BD (2) C 7- N50	836. RY*(22)Ru53	0.06	10.86	0.025
22. BD (2) C 7- N50	840. RY*(26)Ru53	0.07	5743.78	0.626
22. BD (2) C 7- N50	847. RY*(33)Ru53	0.07	277.81	0.130
22. BD (2) C 7- N50	852. RY*(38)Ru53	0.07	355.97	0.153
22. BD (2) C 7- N50	856. RY*(42)Ru53	0.06	3162.73	0.416
31. BD (2) C10- O48	334. RY*(2) C12	0.16	1.04	0.011
31. BD (2) C10- O48	336. RY*(4) C12	0.07	1.68	0.010
31. BD (2) C10- O48	347. RY*(15) C12	0.05	26.43	0.033
31. BD (2) C10- O48	754. RY*(3) N51	0.05	2.54	0.010
31. BD (2) C10- O48	912. BD*(2) C12- C14	0.06	0.37	0.005
32. BD (3) C10- O48	285. RY*(13) C 8	0.06	3.37	0.012
32. BD (3) C10- O48	334. RY*(2) C12	0.15	1.69	0.014
32. BD (3) C10- O48	336. RY*(4) C12	0.12	2.33	0.015
32. BD (3) C10- O48	338. RY*(6) C12	0.07	3.91	0.015
32. BD (3) C10- O48	403. RY*(11) C16	0.05	4.11	0.013
32. BD (3) C10- O48	457. RY*(5) C20	0.07	2.79	0.012
32. BD (3) C10- O48	460. RY*(8) C20	0.08	6.29	0.021
32. BD (3) C10- O48	490. RY*(8) C22	0.06	5.04	0.016
32. BD (3) C10- O48	570. RY*(3) H29	0.58	2.19	0.032
32. BD (3) C10- O48	752. RY*(1) N51	0.06	2.84	0.011
32. BD (3) C10- O48	753. RY*(2) N51	0.07	1.90	0.010
32. BD (3) C10- O48	765. RY*(14) N51	0.06	5.51	0.016

32. BD (3) C10- O48	818. RY*(4)Ru53	0.06	3.26	0.012
32. BD (3) C10- O48	821. RY*(7)Ru53	0.06	4.06	0.013
32. BD (3) C10- O48	824. RY*(10)Ru53	0.25	8.09	0.040
32. BD (3) C10- O48	829. RY*(15)Ru53	0.05	8.17	0.019
32. BD (3) C10- O48	832. RY*(18)Ru53	0.15	6.26	0.028
32. BD (3) C10- O48	833. RY*(19)Ru53	0.11	8.03	0.026
33. BD (1) C10-Ru52	273. RY*(1) C 8	0.08	2.26	0.012
33. BD (1) C10-Ru52	276. RY*(4) C 8	0.09	2.75	0.015
33. BD (1) C10-Ru52	278. RY*(6) C 8	0.06	2.58	0.011
33. BD (1) C10-Ru52	279. RY*(7) C 8	0.14	7.12	0.029
33. BD (1) C10-Ru52	334. RY*(2) C12	0.23	1.18	0.015
33. BD (1) C10-Ru52	428. RY*(6) C18	0.09	3.53	0.016
33. BD (1) C10-Ru52	453. RY*(1) C20	0.10	2.07	0.013
33. BD (1) C10-Ru52	661. RY*(4) O45	0.06	1.14	0.007
33. BD (1) C10-Ru52	815. RY*(1)Ru53	0.26	7.49	0.040
33. BD (1) C10-Ru52	816. RY*(2)Ru53	0.24	2.37	0.021
33. BD (1) C10-Ru52	817. RY*(3)Ru53	0.14	1.65	0.014
33. BD (1) C10-Ru52	818. RY*(4)Ru53	0.07	2.74	0.012
33. BD (1) C10-Ru52	819. RY*(5)Ru53	0.18	6.96	0.032
33. BD (1) C10-Ru52	820. RY*(6)Ru53	0.09	4.05	0.017
33. BD (1) C10-Ru52	821. RY*(7)Ru53	0.42	3.55	0.035
33. BD (1) C10-Ru52	822. RY*(8)Ru53	0.14	5.15	0.024
33. BD (1) C10-Ru52	823. RY*(9)Ru53	0.36	9.61	0.053
33. BD (1) C10-Ru52	824. RY*(10)Ru53	0.28	7.57	0.042
33. BD (1) C10-Ru52	825. RY*(11)Ru53	0.23	6.52	0.035
33. BD (1) C10-Ru52	827. RY*(13)Ru53	0.13	14.28	0.040
33. BD (1) C10-Ru52	828. RY*(14)Ru53	0.05	9.17	0.020
33. BD (1) C10-Ru52	831. RY*(17)Ru53	0.16	12.95	0.041
33. BD (1) C10-Ru52	834. RY*(20)Ru53	0.12	11.93	0.034
33. BD (1) C10-Ru52	836. RY*(22)Ru53	0.24	11.10	0.047
33. BD (1) C10-Ru52	838. RY*(24)Ru53	0.13	35647.34	1.924
33. BD (1) C10-Ru52	839. RY*(25)Ru53	0.15	5348.39	0.820
33. BD (1) C10-Ru52	840. RY*(26)Ru53	0.25	5744.01	1.098
33. BD (1) C10-Ru52	843. RY*(29)Ru53	0.11	10.66	0.031
33. BD (1) C10-Ru52	844. RY*(30)Ru53	0.22	32.95	0.078
33. BD (1) C10-Ru52	847. RY*(33)Ru53	0.26	278.04	0.243
33. BD (1) C10-Ru52	852. RY*(38)Ru53	0.26	356.21	0.276
33. BD (1) C10-Ru52	855. RY*(41)Ru53	0.09	141.16	0.105
33. BD (1) C10-Ru52	856. RY*(42)Ru53	0.20	3162.97	0.727
33. BD (1) C10-Ru52	859. RY*(45)Ru53	0.07	51.11	0.056
33. BD (1) C10-Ru52	906. BD*(1) C 6-Ru53	0.08	0.64	0.007
33. BD (1) C10-Ru52	907. BD*(1) C 8-Ru53	0.50	0.64	0.017
33. BD (1) C10-Ru52	926. BD*(1) C16-Ru53	0.07	0.53	0.006
34. BD (1) C11- C15	338. RY*(6) C12	0.06	3.48	0.013
34. BD (1) C11- C15	570. RY*(3) H29	0.17	1.76	0.015
34. BD (1) C11- C15	824. RY*(10)Ru53	0.05	7.66	0.018
36. BD (1) C11-Ru52	393. RY*(1) C16	0.05	1.41	0.008
36. BD (1) C11-Ru52	815. RY*(1)Ru53	0.05	7.32	0.018
36. BD (1) C11-Ru52	817. RY*(3)Ru53	0.13	1.48	0.013
36. BD (1) C11-Ru52	818. RY*(4)Ru53	0.13	2.57	0.017
36. BD (1) C11-Ru52	820. RY*(6)Ru53	0.08	3.88	0.016
36. BD (1) C11-Ru52	822. RY*(8)Ru53	0.06	4.98	0.016
36. BD (1) C11-Ru52	825. RY*(11)Ru53	0.07	6.35	0.019
36. BD (1) C11-Ru52	907. BD*(1) C 8-Ru53	0.37	0.47	0.012
36. BD (1) C11-Ru52	926. BD*(1) C16-Ru53	0.16	0.36	0.007
113. CR (3)Ru52	906. BD*(1) C 6-Ru53	0.05	22.01	0.033
113. CR (3)Ru52	907. BD*(1) C 8-Ru53	0.07	22.00	0.037
114. CR (4)Ru52	906. BD*(1) C 6-Ru53	0.14	4.72	0.025
114. CR (4)Ru52	907. BD*(1) C 8-Ru53	0.27	4.72	0.035
120. CR (10)Ru52	907. BD*(1) C 8-Ru53	0.07	1.95	0.011
159. LP (1) N50	906. BD*(1) C 6-Ru53	0.10	0.48	0.006
161. LP (1)Ru52	816. RY*(2)Ru53	0.10	2.04	0.014
161. LP (1)Ru52	817. RY*(3)Ru53	0.08	1.32	0.010
161. LP (1)Ru52	821. RY*(7)Ru53	0.20	3.22	0.024
161. LP (1)Ru52	822. RY*(8)Ru53	0.13	4.82	0.024
161. LP (1)Ru52	823. RY*(9)Ru53	0.13	9.28	0.033
161. LP (1)Ru52	824. RY*(10)Ru53	0.15	7.25	0.031
161. LP (1)Ru52	827. RY*(13)Ru53	0.08	13.95	0.031
161. LP (1)Ru52	834. RY*(20)Ru53	0.17	11.60	0.042
161. LP (1)Ru52	836. RY*(22)Ru53	0.09	10.77	0.029
161. LP (1)Ru52	838. RY*(24)Ru53	0.08	35647.02	1.608
161. LP (1)Ru52	839. RY*(25)Ru53	0.09	5348.06	0.654
161. LP (1)Ru52	840. RY*(26)Ru53	0.16	5743.68	0.901
161. LP (1)Ru52	843. RY*(29)Ru53	0.07	10.33	0.026
161. LP (1)Ru52	844. RY*(30)Ru53	0.12	32.62	0.060
161. LP (1)Ru52	847. RY*(33)Ru53	0.14	277.72	0.189
161. LP (1)Ru52	852. RY*(38)Ru53	0.15	355.88	0.221
161. LP (1)Ru52	855. RY*(41)Ru53	0.06	140.83	0.088
161. LP (1)Ru52	856. RY*(42)Ru53	0.13	3162.64	0.600
161. LP (1)Ru52	859. RY*(45)Ru53	0.13	50.78	0.078
161. LP (1)Ru52	860. RY*(46)Ru53	0.08	186.34	0.118
162. LP (2)Ru52	245. RY*(3) C 6	0.11	2.81	0.017
162. LP (2)Ru52	249. RY*(7) C 6	0.08	7.13	0.022
162. LP (2)Ru52	815. RY*(1)Ru53	0.12	7.17	0.029
162. LP (2)Ru52	816. RY*(2)Ru53	0.09	2.04	0.013
162. LP (2)Ru52	817. RY*(3)Ru53	0.12	1.32	0.012
162. LP (2)Ru52	818. RY*(4)Ru53	0.06	2.41	0.011
162. LP (2)Ru52	820. RY*(6)Ru53	0.14	3.72	0.022
162. LP (2)Ru52	821. RY*(7)Ru53	0.70	3.22	0.046
162. LP (2)Ru52	822. RY*(8)Ru53	0.24	4.82	0.033
162. LP (2)Ru52	823. RY*(9)Ru53	0.39	9.28	0.058
162. LP (2)Ru52	824. RY*(10)Ru53	0.43	7.25	0.054
162. LP (2)Ru52	825. RY*(11)Ru53	0.24	6.19	0.037
162. LP (2)Ru52	826. RY*(12)Ru53	0.06	3.10	0.013
162. LP (2)Ru52	827. RY*(13)Ru53	0.18	13.95	0.049
162. LP (2)Ru52	830. RY*(16)Ru53	0.06	6.63	0.020
162. LP (2)Ru52	831. RY*(17)Ru53	0.28	12.62	0.057
162. LP (2)Ru52	834. RY*(20)Ru53	0.72	11.60	0.088
162. LP (2)Ru52	835. RY*(21)Ru53	0.11	12.52	0.036
162. LP (2)Ru52	836. RY*(22)Ru53	0.34	10.77	0.058
162. LP (2)Ru52	838. RY*(24)Ru53	0.27	35647.02	2.968
162. LP (2)Ru52	839. RY*(25)Ru53	0.29	5348.06	1.190
162. LP (2)Ru52	840. RY*(26)Ru53	0.52	5743.68	1.656
162. LP (2)Ru52	843. RY*(29)Ru53	0.21	10.33	0.045
162. LP (2)Ru52	844. RY*(30)Ru53	0.35	32.62	0.103
162. LP (2)Ru52	847. RY*(33)Ru53	0.46	277.72	0.344
162. LP (2)Ru52	852. RY*(38)Ru53	0.50	355.88	0.406
162. LP (2)Ru52	855. RY*(41)Ru53	0.20	140.83	0.163
162. LP (2)Ru52	856. RY*(42)Ru53	0.42	3162.64	1.103
162. LP (2)Ru52	859. RY*(45)Ru53	0.56	50.78	0.163
162. LP (2)Ru52	860. RY*(46)Ru53	0.35	186.34	0.245
162. LP (2)Ru52	906. BD*(1) C 6-Ru53	0.24	0.32	0.008
162. LP (2)Ru52	907. BD*(1) C 8-Ru53	0.07	0.31	0.004
163. LP (3)Ru52	816. RY*(2)Ru53	0.06	2.04	0.011
163. LP (3)Ru52	817. RY*(3)Ru53	0.09	1.33	0.011

from unit 1 to unit 3				
1. BD (1) C 1- C 2	638. RY*(1) H43	0.08	1.90	0.011
5. BD (1) C 2- H27	638. RY*(1) H43	0.09	1.73	0.011
5. BD (1) C 2- H27	688. RY*(1) O47	0.09	2.18	0.013
6. BD (1) C 2- N50	638. RY*(1) H43	0.16	2.02	0.016
6. BD (1) C 2- N50	639. RY*(2) H43	0.06	2.61	0.011
6. BD (1) C 2- N50	688. RY*(1) O47	0.23	2.47	0.021
6. BD (1) C 2- N50	693. RY*(6) O47	0.06	2.89	0.011
10. BD (1) C 4- O44	641. RY*(4) H43	0.05	2.52	0.010
12. BD (3) C 4- O44	638. RY*(1) H43	0.81	2.33	0.039
12. BD (3) C 4- O44	639. RY*(2) H43	0.14	2.92	0.018
12. BD (3) C 4- O44	640. RY*(3) H43	0.10	3.06	0.015
12. BD (3) C 4- O44	641. RY*(4) H43	0.32	3.22	0.029
12. BD (3) C 4- O44	688. RY*(1) O47	0.20	2.79	0.021
12. BD (3) C 4- O44	690. RY*(3) O47	0.07	3.64	0.015
12. BD (3) C 4- O44	692. RY*(5) O47	0.34	3.52	0.031
12. BD (3) C 4- O44	697. RY*(10) O47	0.10	5.90	0.022
12. BD (3) C 4- O44	698. RY*(11) O47	0.13	5.67	0.025
12. BD (3) C 4- O44	700. RY*(13) O47	0.05	5.25	0.015
12. BD (3) C 4- O44	702. RY*(15) O47	0.07	79.25	0.066
13. BD (1) C 4-Ru52	639. RY*(2) H43	0.22	2.36	0.021
13. BD (1) C 4-Ru52	641. RY*(4) H43	0.09	2.66	0.014
13. BD (1) C 4-Ru52	689. RY*(2) O47	0.50	2.88	0.035
13. BD (1) C 4-Ru52	690. RY*(3) O47	0.82	3.08	0.046
13. BD (1) C 4-Ru52	691. RY*(4) O47	0.68	4.25	0.049
13. BD (1) C 4-Ru52	693. RY*(6) O47	0.11	2.65	0.016
13. BD (1) C 4-Ru52	697. RY*(10) O47	0.05	5.34	0.015
13. BD (1) C 4-Ru52	701. RY*(14) O47	0.20	92.83	0.125
13. BD (1) C 4-Ru52	702. RY*(15) O47	0.29	78.69	0.138
20. BD (1) C 7- C 9	688. RY*(1) O47	0.09	2.30	0.013
20. BD (1) C 7- C 9	690. RY*(3) O47	0.08	3.15	0.014
22. BD (2) C 7- N50	691. RY*(4) O47	0.05	4.02	0.014
22. BD (2) C 7- N50	694. RY*(7) O47	0.06	2.84	0.013
27. BD (1) C 9- C11	638. RY*(1) H43	0.13	1.85	0.014
27. BD (1) C 9- C11	688. RY*(1) O47	0.22	2.31	0.020
27. BD (1) C 9- C11	693. RY*(6) O47	0.08	2.73	0.013
27. BD (1) C 9- C11	697. RY*(10) O47	0.05	5.42	0.015
27. BD (1) C 9- C11	934. BD*(1) H43- O47	0.08	1.06	0.008
30. BD (1) C10- O48	638. RY*(1) H43	0.06	1.66	0.009
30. BD (1) C10- O48	640. RY*(3) H43	0.06	2.39	0.011
30. BD (1) C10- O48	641. RY*(4) H43	0.10	2.56	0.014
31. BD (2) C10- O48	641. RY*(4) H43	0.07	2.53	0.012
32. BD (3) C10- O48	638. RY*(1) H43	1.14	2.29	0.046
32. BD (3) C10- O48	639. RY*(2) H43	0.32	2.88	0.027
32. BD (3) C10- O48	640. RY*(3) H43	0.23	3.02	0.024
32. BD (3) C10- O48	641. RY*(4) H43	1.03	3.18	0.051
32. BD (3) C10- O48	642. RY*(5) H43	0.09	3.92	0.016
32. BD (3) C10- O48	688. RY*(1) O47	0.11	2.74	0.015
32. BD (3) C10- O48	689. RY*(2) O47	0.21	3.40	0.024
32. BD (3) C10- O48	690. RY*(3) O47	0.21	3.60	0.025
32. BD (3) C10- O48	692. RY*(5) O47	0.38	3.47	0.033
32. BD (3) C10- O48	693. RY*(6) O47	0.20	3.17	0.022
32. BD (3) C10- O48	698. RY*(11) O47	0.33	5.63	0.039
32. BD (3) C10- O48	934. BD*(1) H43- O47	0.05	1.49	0.008
33. BD (1) C10-Ru52	638. RY*(1) H43	0.31	1.78	0.021
33. BD (1) C10-Ru52	640. RY*(3) H43	0.14	2.50	0.017
33. BD (1) C10-Ru52	689. RY*(2) O47	1.05	2.88	0.050
33. BD (1) C10-Ru52	690. RY*(3) O47	1.97	3.08	0.071
33. BD (1) C10-Ru52	691. RY*(4) O47	0.29	4.25	0.032
33. BD (1) C10-Ru52	692. RY*(5) O47	0.43	2.96	0.033
33. BD (1) C10-Ru52	693. RY*(6) O47	0.18	2.65	0.020
33. BD (1) C10-Ru52	695. RY*(8) O47	0.11	3.04	0.017
33. BD (1) C10-Ru52	696. RY*(9) O47	0.17	3.19	0.021
33. BD (1) C10-Ru52	697. RY*(10) O47	0.22	5.35	0.031
33. BD (1) C10-Ru52	700. RY*(13) O47	0.07	4.70	0.016
33. BD (1) C10-Ru52	702. RY*(15) O47	0.13	78.70	0.091
34. BD (1) C11- C15	638. RY*(1) H43	0.49	1.86	0.027
34. BD (1) C11- C15	639. RY*(2) H43	0.11	2.45	0.014
34. BD (1) C11- C15	640. RY*(3) H43	0.12	2.59	0.016
34. BD (1) C11- C15	641. RY*(4) H43	0.36	2.76	0.028
34. BD (1) C11- C15	642. RY*(5) H43	0.05	3.49	0.012
34. BD (1) C11- C15	689. RY*(2) O47	0.11	2.97	0.016
34. BD (1) C11- C15	692. RY*(5) O47	0.09	3.05	0.015
34. BD (1) C11- C15	698. RY*(11) O47	0.13	5.20	0.023
34. BD (1) C11- C15	934. BD*(1) H43- O47	0.09	1.07	0.009
36. BD (1) C11-Ru52	640. RY*(3) H43	0.12	2.33	0.016
36. BD (1) C11-Ru52	641. RY*(4) H43	0.12	2.50	0.016
36. BD (1) C11-Ru52	642. RY*(5) H43	0.05	3.23	0.012
36. BD (1) C11-Ru52	689. RY*(2) O47	0.65	2.71	0.039
36. BD (1) C11-Ru52	690. RY*(3) O47	1.45	2.91	0.060
36. BD (1) C11-Ru52	691. RY*(4) O47	0.29	4.08	0.032
36. BD (1) C11-Ru52	693. RY*(6) O47	0.21	2.48	0.021
36. BD (1) C11-Ru52	695. RY*(8) O47	0.16	2.87	0.020
36. BD (1) C11-Ru52	696. RY*(9) O47	0.11	3.02	0.017
36. BD (1) C11-Ru52	697. RY*(10) O47	0.07	5.18	0.018
36. BD (1) C11-Ru52	698. RY*(11) O47	0.14	4.95	0.024
36. BD (1) C11-Ru52	700. RY*(13) O47	0.18	4.53	0.026
36. BD (1) C11-Ru52	702. RY*(15) O47	0.11	78.53	0.084
114. CR (4)Ru52	638. RY*(1) H43	0.10	5.85	0.021
120. CR (10)Ru52	934. BD*(1) H43- O47	0.19	2.29	0.018
159. LP (1) N50	693. RY*(6) O47	0.07	2.49	0.013
161. LP (1)Ru52	689. RY*(2) O47	0.11	2.56	0.016
162. LP (2)Ru52	639. RY*(2) H43	0.07	2.04	0.011
162. LP (2)Ru52	641. RY*(4) H43	0.07	2.34	0.012
162. LP (2)Ru52	689. RY*(2) O47	0.56	2.56	0.036
162. LP (2)Ru52	690. RY*(3) O47	0.09	2.76	0.015
162. LP (2)Ru52	691. RY*(4) O47	0.06	3.93	0.015
162. LP (2)Ru52	694. RY*(7) O47	0.06	2.75	0.013
162. LP (2)Ru52	696. RY*(9) O47	0.07	2.86	0.014
162. LP (2)Ru52	934. BD*(1) H43- O47	0.32	0.65	0.014
163. LP (3)Ru52	638. RY*(1) H43	0.17	1.45	0.015
163. LP (3)Ru52	688. RY*(1) O47	1.88	1.91	0.059
163. LP (3)Ru52	689. RY*(2) O47	0.12	2.56	0.018
163. LP (3)Ru52	690. RY*(3) O47	0.09	2.76	0.016
163. LP (3)Ru52	696. RY*(9) O47	0.13	2.87	0.019
163. LP (3)Ru52	698. RY*(11) O47	0.12	4.80	0.023
163. LP (3)Ru52	699. RY*(12) O47	0.12	4.74	0.023
163. LP (3)Ru52	934. BD*(1) H43- O47	0.23	0.66	0.012
from unit 1 to unit 4				
1. BD (1) C 1- C 2	719. RY*(2)Cl49	0.09	2.44	0.014
1. BD (1) C 1- C 2	720. RY*(3)Cl49	0.15	2.54	0.018
1. BD (1) C 1- C 2	721. RY*(4)Cl49	0.14	3.25	0.019
1. BD (1) C 1- C 2	722. RY*(5)Cl49	0.24	2.96	0.024
1. BD (1) C 1- C 2	723. RY*(6)Cl49	0.06	3.69	0.014
5. BD (1) C 2- H27	719. RY*(2)Cl49	0.05	2.26	0.010

5. BD (1) C 2- H27	720. RY*(3)C149	0.13	2.36	0.015
5. BD (1) C 2- H27	721. RY*(4)C149	0.10	3.07	0.016
5. BD (1) C 2- H27	722. RY*(5)C149	0.39	2.78	0.029
5. BD (1) C 2- H27	727. RY*(10)C149	0.07	3.99	0.015
6. BD (1) C 2- N50	719. RY*(2)C149	0.16	2.55	0.018
6. BD (1) C 2- N50	720. RY*(3)C149	0.41	2.65	0.029
6. BD (1) C 2- N50	721. RY*(4)C149	0.22	3.36	0.024
6. BD (1) C 2- N50	722. RY*(5)C149	0.86	3.07	0.046
6. BD (1) C 2- N50	723. RY*(6)C149	0.09	3.81	0.016
6. BD (1) C 2- N50	724. RY*(7)C149	0.08	2.53	0.013
6. BD (1) C 2- N50	726. RY*(9)C149	0.06	2.21	0.010
6. BD (1) C 2- N50	727. RY*(10)C149	0.14	4.28	0.022
6. BD (1) C 2- N50	733. RY*(16)C149	0.07	5.30	0.017
12. BD (3) C 4- O44	719. RY*(2)C149	0.74	2.87	0.041
12. BD (3) C 4- O44	720. RY*(3)C149	3.44	2.97	0.090
12. BD (3) C 4- O44	721. RY*(4)C149	1.27	3.67	0.061
12. BD (3) C 4- O44	722. RY*(5)C149	1.91	3.38	0.072
12. BD (3) C 4- O44	723. RY*(6)C149	0.37	4.12	0.035
12. BD (3) C 4- O44	724. RY*(7)C149	0.53	2.85	0.035
12. BD (3) C 4- O44	725. RY*(8)C149	0.41	6.33	0.046
12. BD (3) C 4- O44	727. RY*(10)C149	0.27	4.60	0.031
12. BD (3) C 4- O44	730. RY*(13)C149	0.09	5.64	0.021
12. BD (3) C 4- O44	733. RY*(16)C149	0.17	5.62	0.027
13. BD (1) C 4-Ru52	719. RY*(2)C149	0.50	2.30	0.031
13. BD (1) C 4-Ru52	721. RY*(4)C149	0.44	3.11	0.034
13. BD (1) C 4-Ru52	722. RY*(5)C149	0.29	2.82	0.026
13. BD (1) C 4-Ru52	723. RY*(6)C149	0.27	3.56	0.028
13. BD (1) C 4-Ru52	724. RY*(7)C149	0.23	2.29	0.021
13. BD (1) C 4-Ru52	725. RY*(8)C149	0.29	5.77	0.037
13. BD (1) C 4-Ru52	726. RY*(9)C149	0.06	1.96	0.010
13. BD (1) C 4-Ru52	732. RY*(15)C149	0.06	26.54	0.036
13. BD (1) C 4-Ru52	735. RY*(18)C149	0.05	41.12	0.043
14. BD (1) C 5- C 7	722. RY*(5)C149	0.05	2.95	0.011
21. BD (1) C 7- N50	719. RY*(2)C149	0.18	2.53	0.019
21. BD (1) C 7- N50	720. RY*(3)C149	0.12	2.64	0.016
21. BD (1) C 7- N50	721. RY*(4)C149	0.17	3.34	0.021
21. BD (1) C 7- N50	722. RY*(5)C149	0.16	3.05	0.020
21. BD (1) C 7- N50	723. RY*(6)C149	0.08	3.79	0.015
21. BD (1) C 7- N50	725. RY*(8)C149	0.06	6.00	0.017
22. BD (2) C 7- N50	722. RY*(5)C149	0.09	2.59	0.015
27. BD (1) C 9- C11	720. RY*(3)C149	0.30	2.49	0.025
27. BD (1) C 9- C11	721. RY*(4)C149	0.12	3.19	0.018
27. BD (1) C 9- C11	722. RY*(5)C149	0.24	2.91	0.024
30. BD (1) C10- O48	720. RY*(3)C149	0.06	2.30	0.010
30. BD (1) C10- O48	721. RY*(4)C149	0.07	3.00	0.013
30. BD (1) C10- O48	722. RY*(5)C149	0.10	2.72	0.015
31. BD (2) C10- O48	721. RY*(4)C149	0.12	2.98	0.017
31. BD (2) C10- O48	722. RY*(5)C149	0.08	2.69	0.013
32. BD (3) C10- O48	718. RY*(1)C149	0.07	1.67	0.010
32. BD (3) C10- O48	719. RY*(2)C149	0.87	2.83	0.044
32. BD (3) C10- O48	720. RY*(3)C149	2.78	2.93	0.081
32. BD (3) C10- O48	721. RY*(4)C149	2.12	3.63	0.078
32. BD (3) C10- O48	722. RY*(5)C149	2.34	3.34	0.079
32. BD (3) C10- O48	723. RY*(6)C149	0.35	4.08	0.034
32. BD (3) C10- O48	724. RY*(7)C149	0.37	2.81	0.029
32. BD (3) C10- O48	725. RY*(8)C149	0.51	6.29	0.051
32. BD (3) C10- O48	727. RY*(10)C149	0.15	4.55	0.023
32. BD (3) C10- O48	730. RY*(13)C149	0.08	5.60	0.019
32. BD (3) C10- O48	733. RY*(16)C149	0.17	5.58	0.027
32. BD (3) C10- O48	736. RY*(19)C149	0.08	5.81	0.019
33. BD (1) C10-Ru52	719. RY*(2)C149	0.15	2.31	0.017
33. BD (1) C10-Ru52	720. RY*(3)C149	0.33	2.41	0.026
33. BD (1) C10-Ru52	721. RY*(4)C149	0.09	3.12	0.015
33. BD (1) C10-Ru52	723. RY*(6)C149	0.43	3.57	0.035
33. BD (1) C10-Ru52	724. RY*(7)C149	0.84	2.29	0.040
33. BD (1) C10-Ru52	725. RY*(8)C149	0.08	5.77	0.020
34. BD (1) C11- C15	719. RY*(2)C149	0.25	2.40	0.022
34. BD (1) C11- C15	720. RY*(3)C149	0.68	2.50	0.037
34. BD (1) C11- C15	721. RY*(4)C149	0.51	3.20	0.036
34. BD (1) C11- C15	722. RY*(5)C149	0.74	2.92	0.042
34. BD (1) C11- C15	723. RY*(6)C149	0.09	3.65	0.016
34. BD (1) C11- C15	725. RY*(8)C149	0.15	5.86	0.027
36. BD (1) C11-Ru52	719. RY*(2)C149	0.07	2.14	0.012
36. BD (1) C11-Ru52	720. RY*(3)C149	0.50	2.25	0.031
36. BD (1) C11-Ru52	721. RY*(4)C149	0.13	2.95	0.018
36. BD (1) C11-Ru52	722. RY*(5)C149	0.30	2.66	0.026
45. BD (1) C15- C19	720. RY*(3)C149	0.08	2.51	0.012
45. BD (1) C15- C19	722. RY*(5)C149	0.07	2.92	0.013
46. BD (1) C15- H33	722. RY*(5)C149	0.05	2.75	0.011
113. CR (3)Ru52	719. RY*(2)C149	0.05	23.67	0.032
113. CR (3)Ru52	720. RY*(3)C149	0.16	23.78	0.055
113. CR (3)Ru52	721. RY*(4)C149	0.11	24.48	0.045
113. CR (3)Ru52	722. RY*(5)C149	0.14	24.19	0.053
114. CR (4)Ru52	720. RY*(3)C149	0.13	6.49	0.026
114. CR (4)Ru52	721. RY*(4)C149	0.16	7.20	0.030
114. CR (4)Ru52	722. RY*(5)C149	0.19	6.91	0.033
114. CR (4)Ru52	723. RY*(6)C149	0.07	7.64	0.020
114. CR (4)Ru52	725. RY*(8)C149	0.07	9.85	0.024
148. LP (1) O44	721. RY*(4)C149	0.07	3.27	0.014
148. LP (1) O44	722. RY*(5)C149	0.09	2.98	0.015
154. LP (1) O48	720. RY*(3)C149	0.06	2.56	0.011
159. LP (1) N50	720. RY*(3)C149	0.11	2.25	0.015
159. LP (1) N50	722. RY*(5)C149	0.12	2.67	0.018
161. LP (1)Ru52	718. RY*(1)C149	0.48	0.83	0.019
162. LP (2)Ru52	721. RY*(4)C149	0.07	2.79	0.014
162. LP (2)Ru52	722. RY*(5)C149	0.15	2.50	0.018
162. LP (2)Ru52	727. RY*(10)C149	0.11	3.71	0.019
162. LP (2)Ru52	735. RY*(18)C149	0.06	40.80	0.047
162. LP (2)Ru52	736. RY*(19)C149	0.05	4.97	0.015
163. LP (3)Ru52	719. RY*(2)C149	0.07	1.99	0.011
163. LP (3)Ru52	720. RY*(3)C149	0.06	2.09	0.011
163. LP (3)Ru52	721. RY*(4)C149	0.09	2.80	0.015
163. LP (3)Ru52	722. RY*(5)C149	0.21	2.51	0.023
163. LP (3)Ru52	723. RY*(6)C149	0.09	3.24	0.017
163. LP (3)Ru52	725. RY*(8)C149	0.06	5.45	0.017

from unit 2 to unit 1

17. BD (2) C 6- O45	169. RY*(2) C 1	0.05	0.96	0.006
17. BD (2) C 6- O45	184. RY*(2) C 2	0.09	1.03	0.008
18. BD (3) C 6- O45	265. RY*(8) C 7	0.06	5.33	0.016
18. BD (3) C 6- O45	560. RY*(3) H27	0.21	2.17	0.019
18. BD (3) C 6- O45	771. RY*(5)Ru52	0.06	7.94	0.019
18. BD (3) C 6- O45	776. RY*(10)Ru52	0.14	9.41	0.033
19. BD (1) C 6-Ru53	184. RY*(2) C 2	0.21	1.16	0.014
19. BD (1) C 6-Ru53	186. RY*(4) C 2	0.06	1.77	0.009
19. BD (1) C 6-Ru53	213. RY*(1) C 4	0.07	2.34	0.012

19. BD (1) C 6-Ru53	216. RY*(4) C 4	0.14	2.71	0.018
19. BD (1) C 6-Ru53	219. RY*(7) C 4	0.12	7.19	0.027
19. BD (1) C 6-Ru53	258. RY*(1) C 7	0.06	2.06	0.010
19. BD (1) C 6-Ru53	319. RY*(2) C11	0.05	1.18	0.007
19. BD (1) C 6-Ru53	320. RY*(3) C11	0.08	1.57	0.010
19. BD (1) C 6-Ru53	383. RY*(6) C15	0.07	3.78	0.015
19. BD (1) C 6-Ru53	706. RY*(4) O48	0.06	1.18	0.008
19. BD (1) C 6-Ru53	767. RY*(1)Ru52	0.13	7.33	0.028
19. BD (1) C 6-Ru53	768. RY*(2)Ru52	0.06	4.06	0.014
19. BD (1) C 6-Ru53	770. RY*(4)Ru52	0.31	2.83	0.027
19. BD (1) C 6-Ru53	773. RY*(7)Ru52	0.30	8.76	0.046
19. BD (1) C 6-Ru53	774. RY*(8)Ru52	0.33	4.16	0.033
19. BD (1) C 6-Ru53	775. RY*(9)Ru52	0.16	10.54	0.038
19. BD (1) C 6-Ru53	776. RY*(10)Ru52	0.27	8.88	0.045
19. BD (1) C 6-Ru53	778. RY*(12)Ru52	0.07	6.43	0.020
19. BD (1) C 6-Ru53	779. RY*(13)Ru52	0.25	15.26	0.056
19. BD (1) C 6-Ru53	783. RY*(17)Ru52	0.14	13.00	0.039
19. BD (1) C 6-Ru53	786. RY*(20)Ru52	0.09	10.78	0.028
19. BD (1) C 6-Ru53	789. RY*(23)Ru52	0.14	10.97	0.036
19. BD (1) C 6-Ru53	790. RY*(24)Ru52	0.1113605.46		1.120
19. BD (1) C 6-Ru53	791. RY*(25)Ru52	0.0633394.90		1.244
19. BD (1) C 6-Ru53	792. RY*(26)Ru52	0.13 1159.92		0.359
19. BD (1) C 6-Ru53	795. RY*(29)Ru52	0.13	53.46	0.076
19. BD (1) C 6-Ru53	796. RY*(30)Ru52	0.10	19.12	0.040
19. BD (1) C 6-Ru53	804. RY*(38)Ru52	0.14	258.83	0.175
19. BD (1) C 6-Ru53	811. RY*(45)Ru52	0.08	51.22	0.057
19. BD (1) C 6-Ru53	875. BD*(1) C 4-Ru52	0.46	0.63	0.016
19. BD (1) C 6-Ru53	876. BD*(1) C10-Ru52	0.05	0.64	0.005
19. BD (1) C 6-Ru53	894. BD*(1) C11-Ru52	0.06	0.54	0.005
23. BD (1) C 8- O46	773. RY*(7)Ru52	0.06	8.61	0.021
23. BD (1) C 8- O46	774. RY*(8)Ru52	0.05	4.01	0.013
23. BD (1) C 8- O46	776. RY*(10)Ru52	0.07	8.73	0.022
23. BD (1) C 8- O46	786. RY*(20)Ru52	0.05	10.63	0.021
25. BD (3) C 8- O46	560. RY*(3) H27	0.07	2.20	0.011
25. BD (3) C 8- O46	776. RY*(10)Ru52	0.08	9.44	0.025
26. BD (1) C 8-Ru53	184. RY*(2) C 2	0.05	1.15	0.007
26. BD (1) C 8-Ru53	770. RY*(4)Ru52	0.05	2.83	0.011
26. BD (1) C 8-Ru53	772. RY*(6)Ru52	0.09	4.92	0.019
39. BD (1) C12- H29	878. BD*(2) C10- O48	0.08	0.48	0.006
40. BD (1) C12- N51	785. RY*(19)Ru52	0.05	7.89	0.018
47. BD (1) C16- C18	773. RY*(7)Ru52	0.05	8.85	0.019
47. BD (1) C16- C18	775. RY*(9)Ru52	0.05	10.64	0.021
49. BD (1) C16-Ru53	770. RY*(4)Ru52	0.09	2.67	0.014
49. BD (1) C16-Ru53	875. BD*(1) C 4-Ru52	0.33	0.47	0.012
49. BD (1) C16-Ru53	894. BD*(1) C11-Ru52	0.14	0.37	0.007
60. BD (2) C20- N51	304. RY*(2) C10	0.06	1.27	0.008
60. BD (2) C20- N51	767. RY*(1)Ru52	0.15	7.10	0.031
60. BD (2) C20- N51	768. RY*(2)Ru52	0.07	3.84	0.016
60. BD (2) C20- N51	771. RY*(5)Ru52	0.06	7.18	0.019
60. BD (2) C20- N51	773. RY*(7)Ru52	0.09	8.54	0.026
60. BD (2) C20- N51	774. RY*(8)Ru52	0.06	3.93	0.014
60. BD (2) C20- N51	775. RY*(9)Ru52	0.07	10.32	0.027
60. BD (2) C20- N51	778. RY*(12)Ru52	0.07	6.20	0.019
60. BD (2) C20- N51	779. RY*(13)Ru52	0.06	15.04	0.029
60. BD (2) C20- N51	780. RY*(14)Ru52	0.05	9.09	0.021
60. BD (2) C20- N51	783. RY*(17)Ru52	0.07	12.77	0.030
60. BD (2) C20- N51	785. RY*(19)Ru52	0.05	7.42	0.019
60. BD (2) C20- N51	789. RY*(23)Ru52	0.10	10.74	0.031
60. BD (2) C20- N51	790. RY*(24)Ru52	0.0713605.24		0.970
60. BD (2) C20- N51	792. RY*(26)Ru52	0.09 1159.69		0.311
60. BD (2) C20- N51	795. RY*(29)Ru52	0.09	53.23	0.065
60. BD (2) C20- N51	796. RY*(30)Ru52	0.07	18.90	0.035
60. BD (2) C20- N51	804. RY*(38)Ru52	0.10	258.60	0.155
131. CR (3)Ru53	776. RY*(10)Ru52	0.05	30.22	0.035
131. CR (3)Ru53	875. BD*(1) C 4-Ru52	0.07	21.97	0.037
131. CR (3)Ru53	876. BD*(1) C10-Ru52	0.05	21.98	0.033
132. CR (4)Ru53	875. BD*(1) C 4-Ru52	0.27	4.72	0.034
132. CR (4)Ru53	876. BD*(1) C10-Ru52	0.14	4.72	0.025
138. CR (10)Ru53	875. BD*(1) C 4-Ru52	0.07	1.95	0.011
160. LP (1) N51	876. BD*(1) C10-Ru52	0.08	0.49	0.005
164. LP (1)Ru53	188. RY*(6) C 2	0.06	3.25	0.013
164. LP (1)Ru53	767. RY*(1)Ru52	0.12	7.00	0.027
164. LP (1)Ru53	768. RY*(2)Ru52	0.20	3.74	0.026
164. LP (1)Ru53	773. RY*(7)Ru52	0.31	8.44	0.048
164. LP (1)Ru53	775. RY*(9)Ru52	0.19	10.22	0.041
164. LP (1)Ru53	776. RY*(10)Ru52	0.17	8.56	0.036
164. LP (1)Ru53	778. RY*(12)Ru52	0.11	6.10	0.024
164. LP (1)Ru53	779. RY*(13)Ru52	0.16	14.94	0.046
164. LP (1)Ru53	780. RY*(14)Ru52	0.05	8.99	0.020
164. LP (1)Ru53	783. RY*(17)Ru52	0.13	12.67	0.038
164. LP (1)Ru53	786. RY*(20)Ru52	0.13	10.45	0.035
164. LP (1)Ru53	789. RY*(23)Ru52	0.18	10.64	0.042
164. LP (1)Ru53	790. RY*(24)Ru52	0.1713605.14		1.418
164. LP (1)Ru53	791. RY*(25)Ru52	0.0933394.58		1.633
164. LP (1)Ru53	792. RY*(26)Ru52	0.20 1159.60		0.456
164. LP (1)Ru53	795. RY*(29)Ru52	0.23	53.14	0.105
164. LP (1)Ru53	796. RY*(30)Ru52	0.18	18.80	0.055
164. LP (1)Ru53	804. RY*(38)Ru52	0.22	258.50	0.226
164. LP (1)Ru53	811. RY*(45)Ru52	0.09	50.90	0.063
164. LP (1)Ru53	812. RY*(46)Ru52	0.05	186.32	0.094
165. LP (2)Ru53	188. RY*(6) C 2	0.07	3.25	0.014
165. LP (2)Ru53	219. RY*(7) C 4	0.06	6.86	0.020
165. LP (2)Ru53	224. RY*(12) C 4	0.05	2.97	0.012
165. LP (2)Ru53	263. RY*(6) C 7	0.05	4.43	0.015
165. LP (2)Ru53	303. RY*(1) C10	0.06	2.14	0.010
165. LP (2)Ru53	305. RY*(3) C10	0.13	2.88	0.018
165. LP (2)Ru53	309. RY*(7) C10	0.07	6.65	0.020
165. LP (2)Ru53	312. RY*(10) C10	0.05	1.91	0.010
165. LP (2)Ru53	315. RY*(13) C10	0.06	3.14	0.014
165. LP (2)Ru53	329. RY*(12) C11	0.06	3.27	0.013
165. LP (2)Ru53	383. RY*(6) C15	0.09	3.46	0.017
165. LP (2)Ru53	646. RY*(4) O44	0.06	0.96	0.007
165. LP (2)Ru53	648. RY*(6) O44	0.05	2.71	0.011
165. LP (2)Ru53	738. RY*(2) N50	0.06	1.09	0.008
165. LP (2)Ru53	740. RY*(4) N50	0.07	5.29	0.019
165. LP (2)Ru53	744. RY*(8) N50	0.06	13.89	0.027
165. LP (2)Ru53	767. RY*(1)Ru52	0.22	7.01	0.038
165. LP (2)Ru53	768. RY*(2)Ru52	0.16	3.74	0.024
165. LP (2)Ru53	772. RY*(6)Ru52	0.13	4.60	0.024
165. LP (2)Ru53	773. RY*(7)Ru52	0.72	8.44	0.075
165. LP (2)Ru53	774. RY*(8)Ru52	0.45	3.84	0.040
165. LP (2)Ru53	775. RY*(9)Ru52	0.40	10.22	0.062
165. LP (2)Ru53	776. RY*(10)Ru52	0.51	8.56	0.064
165. LP (2)Ru53	777. RY*(11)Ru52	0.06	5.18	0.016
165. LP (2)Ru53	778. RY*(12)Ru52	0.22	6.11	0.036
165. LP (2)Ru53	779. RY*(13)Ru52	0.33	14.94	0.067

165. LP (2)Ru53	780. RY*(14)Ru52	0.17	8.99	0.037
165. LP (2)Ru53	781. RY*(15)Ru52	0.06	7.74	0.021
165. LP (2)Ru53	783. RY*(17)Ru52	0.33	12.68	0.062
165. LP (2)Ru53	785. RY*(19)Ru52	0.06	7.32	0.020
165. LP (2)Ru53	786. RY*(20)Ru52	0.59	10.45	0.076
165. LP (2)Ru53	788. RY*(22)Ru52	0.15	9.93	0.037
165. LP (2)Ru53	789. RY*(23)Ru52	0.49	10.64	0.070
165. LP (2)Ru53	790. RY*(24)Ru52	0.37	13605.14	2.149
165. LP (2)Ru53	791. RY*(25)Ru52	0.20	33394.58	2.496
165. LP (2)Ru53	792. RY*(26)Ru52	0.44	1159.60	0.690
165. LP (2)Ru53	795. RY*(29)Ru52	0.53	53.14	0.161
165. LP (2)Ru53	796. RY*(30)Ru52	0.38	18.80	0.081
165. LP (2)Ru53	799. RY*(33)Ru52	0.08	88.41	0.080
165. LP (2)Ru53	804. RY*(38)Ru52	0.49	258.50	0.341
165. LP (2)Ru53	811. RY*(45)Ru52	0.53	50.90	0.159
165. LP (2)Ru53	812. RY*(46)Ru52	0.33	186.32	0.239
165. LP (2)Ru53	875. BD*(1) C 4-Ru52	0.06	0.31	0.004
165. LP (2)Ru53	876. BD*(1) C10-Ru52	0.22	0.32	0.008
166. LP (3)Ru53	769. RY*(3)Ru52	0.12	1.81	0.014
166. LP (3)Ru53	775. RY*(9)Ru52	0.06	10.23	0.025
166. LP (3)Ru53	792. RY*(26)Ru52	0.05	1159.60	0.238
166. LP (3)Ru53	795. RY*(29)Ru52	0.07	53.14	0.062
166. LP (3)Ru53	796. RY*(30)Ru52	0.06	18.81	0.033
166. LP (3)Ru53	804. RY*(38)Ru52	0.06	258.51	0.118
within unit 2				
16. BD (1) C 6- O45	816. RY*(2)Ru53	0.77	2.24	0.037
18. BD (3) C 6- O45	243. RY*(1) C 6	7.17	2.89	0.129
18. BD (3) C 6- O45	245. RY*(3) C 6	1.73	3.66	0.071
18. BD (3) C 6- O45	249. RY*(7) C 6	3.44	7.98	0.148
18. BD (3) C 6- O45	251. RY*(9) C 6	0.64	5.61	0.053
18. BD (3) C 6- O45	256. RY*(14) C 6	0.68	46.68	0.159
18. BD (3) C 6- O45	257. RY*(15) C 6	0.91	26.10	0.138
18. BD (3) C 6- O45	428. RY*(6) C18	1.15	4.05	0.061
18. BD (3) C 6- O45	660. RY*(3) O45	0.89	3.03	0.046
18. BD (3) C 6- O45	661. RY*(4) O45	0.58	1.67	0.028
18. BD (3) C 6- O45	815. RY*(1)Ru53	8.14	8.02	0.228
18. BD (3) C 6- O45	816. RY*(2)Ru53	5.61	2.89	0.114
18. BD (3) C 6- O45	818. RY*(4)Ru53	5.26	3.27	0.117
18. BD (3) C 6- O45	819. RY*(5)Ru53	9.54	7.48	0.239
18. BD (3) C 6- O45	820. RY*(6)Ru53	0.60	4.57	0.047
18. BD (3) C 6- O45	821. RY*(7)Ru53	1.55	4.07	0.071
18. BD (3) C 6- O45	822. RY*(8)Ru53	3.10	5.67	0.118
18. BD (3) C 6- O45	823. RY*(9)Ru53	4.95	10.13	0.200
18. BD (3) C 6- O45	824. RY*(10)Ru53	2.22	8.10	0.120
18. BD (3) C 6- O45	825. RY*(11)Ru53	1.49	7.04	0.091
18. BD (3) C 6- O45	828. RY*(14)Ru53	1.32	9.70	0.101
18. BD (3) C 6- O45	829. RY*(15)Ru53	1.37	8.18	0.094
18. BD (3) C 6- O45	830. RY*(16)Ru53	0.54	7.48	0.057
18. BD (3) C 6- O45	831. RY*(17)Ru53	4.98	13.48	0.232
18. BD (3) C 6- O45	832. RY*(18)Ru53	0.79	6.27	0.063
18. BD (3) C 6- O45	833. RY*(19)Ru53	1.77	8.04	0.107
18. BD (3) C 6- O45	836. RY*(22)Ru53	7.56	11.62	0.265
18. BD (3) C 6- O45	838. RY*(24)Ru53	4.26	35647.87	11.017
18. BD (3) C 6- O45	839. RY*(25)Ru53	5.14	5348.92	4.689
18. BD (3) C 6- O45	840. RY*(26)Ru53	8.49	5744.54	6.241
18. BD (3) C 6- O45	843. RY*(29)Ru53	2.51	11.18	0.150
18. BD (3) C 6- O45	844. RY*(30)Ru53	5.91	33.47	0.398
18. BD (3) C 6- O45	847. RY*(33)Ru53	7.86	278.57	1.323
18. BD (3) C 6- O45	848. RY*(34)Ru53	0.69	51.97	0.169
18. BD (3) C 6- O45	852. RY*(38)Ru53	8.37	356.73	1.545
18. BD (3) C 6- O45	855. RY*(41)Ru53	3.17	141.68	0.599
18. BD (3) C 6- O45	856. RY*(42)Ru53	6.92	3163.49	4.182
18. BD (3) C 6- O45	859. RY*(45)Ru53	0.52	51.64	0.146
19. BD (1) C 6-Ru53	243. RY*(1) C 6	0.68	2.36	0.036
19. BD (1) C 6-Ru53	257. RY*(15) C 6	0.65	25.57	0.117
19. BD (1) C 6-Ru53	274. RY*(2) C 8	1.28	1.63	0.041
19. BD (1) C 6-Ru53	276. RY*(4) C 8	2.31	2.74	0.072
19. BD (1) C 6-Ru53	278. RY*(6) C 8	1.43	2.58	0.055
19. BD (1) C 6-Ru53	279. RY*(7) C 8	1.43	7.11	0.092
19. BD (1) C 6-Ru53	393. RY*(1) C16	1.11	1.57	0.038
19. BD (1) C 6-Ru53	660. RY*(3) O45	1.66	2.50	0.059
19. BD (1) C 6-Ru53	661. RY*(4) O45	0.70	1.14	0.026
19. BD (1) C 6-Ru53	815. RY*(1)Ru53	1.56	7.49	0.098
19. BD (1) C 6-Ru53	816. RY*(2)Ru53	0.64	2.36	0.035
19. BD (1) C 6-Ru53	819. RY*(5)Ru53	0.88	6.95	0.071
19. BD (1) C 6-Ru53	823. RY*(9)Ru53	0.71	9.61	0.075
19. BD (1) C 6-Ru53	828. RY*(14)Ru53	0.90	9.17	0.083
19. BD (1) C 6-Ru53	831. RY*(17)Ru53	0.59	12.95	0.079
19. BD (1) C 6-Ru53	835. RY*(21)Ru53	0.62	12.84	0.081
19. BD (1) C 6-Ru53	836. RY*(22)Ru53	0.60	11.09	0.074
19. BD (1) C 6-Ru53	843. RY*(29)Ru53	0.98	10.65	0.093
19. BD (1) C 6-Ru53	844. RY*(30)Ru53	1.63	32.94	0.211
19. BD (1) C 6-Ru53	847. RY*(33)Ru53	0.81	278.04	0.431
19. BD (1) C 6-Ru53	852. RY*(38)Ru53	0.59	356.21	0.417
19. BD (1) C 6-Ru53	905. BD*(3) C 6- O45	0.71	1.11	0.025
19. BD (1) C 6-Ru53	906. BD*(1) C 6-Ru53	1.08	0.64	0.025
19. BD (1) C 6-Ru53	907. BD*(1) C 8-Ru53	13.06	0.64	0.086
19. BD (1) C 6-Ru53	909. BD*(2) C 8- O46	1.68	0.52	0.027
19. BD (1) C 6-Ru53	910. BD*(3) C 8- O46	2.22	1.13	0.045
19. BD (1) C 6-Ru53	926. BD*(1) C16-Ru53	13.04	0.53	0.079
19. BD (1) C 6-Ru53	927. BD*(1) C16- C22	1.99	1.02	0.041
25. BD (3) C 8- O46	273. RY*(1) C 8	6.60	2.82	0.122
25. BD (3) C 8- O46	276. RY*(4) C 8	0.85	3.30	0.047
25. BD (3) C 8- O46	278. RY*(6) C 8	0.54	3.14	0.037
25. BD (3) C 8- O46	279. RY*(7) C 8	3.38	7.67	0.144
25. BD (3) C 8- O46	281. RY*(9) C 8	0.90	5.45	0.062
25. BD (3) C 8- O46	287. RY*(15) C 8	0.80	27.61	0.133
25. BD (3) C 8- O46	428. RY*(6) C18	0.91	4.09	0.055
25. BD (3) C 8- O46	675. RY*(3) O46	0.69	2.82	0.039
25. BD (3) C 8- O46	676. RY*(4) O46	0.73	1.80	0.032
25. BD (3) C 8- O46	815. RY*(1)Ru53	9.51	8.05	0.247
25. BD (3) C 8- O46	816. RY*(2)Ru53	2.24	2.92	0.072
25. BD (3) C 8- O46	819. RY*(5)Ru53	6.30	7.51	0.194
25. BD (3) C 8- O46	820. RY*(6)Ru53	2.58	4.60	0.097
25. BD (3) C 8- O46	821. RY*(7)Ru53	1.08	4.11	0.060
25. BD (3) C 8- O46	822. RY*(8)Ru53	1.55	5.70	0.084
25. BD (3) C 8- O46	823. RY*(9)Ru53	6.41	10.17	0.228
25. BD (3) C 8- O46	824. RY*(10)Ru53	0.76	8.13	0.070
25. BD (3) C 8- O46	826. RY*(12)Ru53	1.76	3.98	0.075
25. BD (3) C 8- O46	827. RY*(13)Ru53	1.91	14.83	0.150
25. BD (3) C 8- O46	829. RY*(15)Ru53	1.50	8.21	0.099
25. BD (3) C 8- O46	830. RY*(16)Ru53	1.20	7.52	0.085
25. BD (3) C 8- O46	831. RY*(17)Ru53	3.83	13.51	0.203
25. BD (3) C 8- O46	832. RY*(18)Ru53	1.37	6.30	0.083
25. BD (3) C 8- O46	836. RY*(22)Ru53	5.39	11.65	0.224

25. BD (3) C 8- O46	838. RY*(24)Ru53	3.77	35647.90	10.361
25. BD (3) C 8- O46	839. RY*(25)Ru53	4.49	5348.95	4.380
25. BD (3) C 8- O46	840. RY*(26)Ru53	7.47	5744.57	5.856
25. BD (3) C 8- O46	843. RY*(29)Ru53	1.92	11.21	0.131
25. BD (3) C 8- O46	844. RY*(30)Ru53	4.73	33.50	0.356
25. BD (3) C 8- O46	847. RY*(33)Ru53	6.84	278.60	1.234
25. BD (3) C 8- O46	848. RY*(34)Ru53	0.50	52.01	0.144
25. BD (3) C 8- O46	852. RY*(38)Ru53	7.33	356.77	1.445
25. BD (3) C 8- O46	855. RY*(41)Ru53	2.81	141.71	0.564
25. BD (3) C 8- O46	856. RY*(42)Ru53	6.10	3163.52	3.925
25. BD (3) C 8- O46	859. RY*(45)Ru53	0.99	51.67	0.202
25. BD (3) C 8- O46	860. RY*(46)Ru53	0.69	187.22	0.322
26. BD (1) C 8-Ru53	167. LP*(1) C16	0.75	0.43	0.021
26. BD (1) C 8-Ru53	243. RY*(1) C 6	0.74	2.36	0.038
26. BD (1) C 8-Ru53	244. RY*(2) C 6	2.67	1.54	0.058
26. BD (1) C 8-Ru53	245. RY*(3) C 6	3.84	3.13	0.100
26. BD (1) C 8-Ru53	246. RY*(4) C 6	0.90	2.04	0.039
26. BD (1) C 8-Ru53	247. RY*(5) C 6	0.58	2.51	0.035
26. BD (1) C 8-Ru53	249. RY*(7) C 6	1.69	7.45	0.102
26. BD (1) C 8-Ru53	257. RY*(15) C 6	0.73	25.57	0.125
26. BD (1) C 8-Ru53	394. RY*(2) C16	0.60	1.18	0.024
26. BD (1) C 8-Ru53	675. RY*(3) O46	1.16	2.25	0.047
26. BD (1) C 8-Ru53	676. RY*(4) O46	0.54	1.24	0.024
26. BD (1) C 8-Ru53	752. RY*(1) N51	4.17	2.32	0.089
26. BD (1) C 8-Ru53	815. RY*(1)Ru53	1.33	7.49	0.091
26. BD (1) C 8-Ru53	816. RY*(2)Ru53	0.73	2.36	0.038
26. BD (1) C 8-Ru53	818. RY*(4)Ru53	2.43	2.74	0.074
26. BD (1) C 8-Ru53	819. RY*(5)Ru53	1.01	6.95	0.076
26. BD (1) C 8-Ru53	822. RY*(8)Ru53	0.93	5.14	0.063
26. BD (1) C 8-Ru53	823. RY*(9)Ru53	1.59	9.60	0.113
26. BD (1) C 8-Ru53	824. RY*(10)Ru53	0.63	7.57	0.063
26. BD (1) C 8-Ru53	830. RY*(16)Ru53	0.61	6.95	0.059
26. BD (1) C 8-Ru53	831. RY*(17)Ru53	0.73	12.95	0.088
26. BD (1) C 8-Ru53	832. RY*(18)Ru53	0.79	5.74	0.061
26. BD (1) C 8-Ru53	836. RY*(22)Ru53	1.45	11.09	0.115
26. BD (1) C 8-Ru53	839. RY*(25)Ru53	0.70	5348.38	1.756
26. BD (1) C 8-Ru53	840. RY*(26)Ru53	0.71	5744.01	1.838
26. BD (1) C 8-Ru53	843. RY*(29)Ru53	0.97	10.65	0.093
26. BD (1) C 8-Ru53	844. RY*(30)Ru53	2.15	32.94	0.242
26. BD (1) C 8-Ru53	847. RY*(33)Ru53	1.14	278.04	0.512
26. BD (1) C 8-Ru53	852. RY*(38)Ru53	0.89	356.20	0.513
26. BD (1) C 8-Ru53	903. BD*(1) C 6- O45	1.16	0.53	0.023
26. BD (1) C 8-Ru53	904. BD*(2) C 6- O45	2.68	0.52	0.034
26. BD (1) C 8-Ru53	905. BD*(3) C 6- O45	1.91	1.10	0.042
26. BD (1) C 8-Ru53	906. BD*(1) C 6-Ru53	12.38	0.64	0.085
26. BD (1) C 8-Ru53	907. BD*(1) C 8-Ru53	1.25	0.63	0.027
26. BD (1) C 8-Ru53	910. BD*(3) C 8- O46	0.55	1.13	0.023
26. BD (1) C 8-Ru53	913. BD*(1) C12- N51	0.58	0.96	0.021
26. BD (1) C 8-Ru53	921. BD*(1) C20- N51	0.75	0.94	0.024
26. BD (1) C 8-Ru53	926. BD*(1) C16-Ru53	12.46	0.53	0.077
26. BD (1) C 8-Ru53	927. BD*(1) C16- C22	0.54	1.01	0.021
26. BD (1) C 8-Ru53	928. BD*(1) C16- C18	0.71	1.03	0.024
37. BD (1) C12- C14	469. RY*(2) C21	0.97	2.38	0.043
37. BD (1) C12- C14	752. RY*(1) N51	1.41	2.46	0.053
37. BD (1) C12- C14	906. BD*(1) C 6-Ru53	0.52	0.78	0.019
37. BD (1) C12- C14	913. BD*(1) C12- N51	0.51	1.10	0.021
37. BD (1) C12- C14	915. BD*(1) C14- C21	0.72	1.11	0.025
37. BD (1) C12- C14	919. BD*(1) C21- H37	2.45	1.03	0.045
38. BD (2) C12- C14	470. RY*(3) C21	0.91	0.78	0.026
38. BD (2) C12- C14	753. RY*(2) N51	0.78	1.11	0.029
38. BD (2) C12- C14	912. BD*(2) C12- C14	0.62	0.23	0.011
38. BD (2) C12- C14	918. BD*(2) C21- C23	16.58	0.23	0.056
38. BD (2) C12- C14	922. BD*(2) C20- N51	10.77	0.21	0.044
39. BD (1) C12- H29	363. RY*(1) C14	0.89	2.14	0.039
39. BD (1) C12- H29	752. RY*(1) N51	1.40	2.28	0.051
39. BD (1) C12- H29	754. RY*(3) N51	0.50	2.63	0.033
39. BD (1) C12- H29	915. BD*(1) C14- C21	3.32	0.93	0.050
39. BD (1) C12- H29	921. BD*(1) C20- N51	6.76	0.90	0.070
40. BD (1) C12- N51	340. RY*(8) C12	0.53	10.26	0.066
40. BD (1) C12- N51	346. RY*(14) C12	0.62	40.77	0.143
40. BD (1) C12- N51	347. RY*(15) C12	0.91	26.81	0.140
40. BD (1) C12- N51	365. RY*(3) C14	0.84	2.65	0.042
40. BD (1) C12- N51	453. RY*(1) C20	0.67	2.32	0.035
40. BD (1) C12- N51	455. RY*(3) C20	1.57	2.70	0.058
40. BD (1) C12- N51	755. RY*(4) N51	1.30	5.71	0.077
40. BD (1) C12- N51	759. RY*(8) N51	0.51	14.77	0.078
40. BD (1) C12- N51	815. RY*(1)Ru53	0.52	7.74	0.057
40. BD (1) C12- N51	816. RY*(2)Ru53	0.53	2.61	0.033
40. BD (1) C12- N51	820. RY*(6)Ru53	0.52	4.29	0.042
40. BD (1) C12- N51	822. RY*(8)Ru53	1.39	5.39	0.078
40. BD (1) C12- N51	823. RY*(9)Ru53	1.27	9.86	0.100
40. BD (1) C12- N51	824. RY*(10)Ru53	0.51	7.82	0.056
40. BD (1) C12- N51	826. RY*(12)Ru53	0.84	3.67	0.050
40. BD (1) C12- N51	827. RY*(13)Ru53	1.53	14.52	0.134
40. BD (1) C12- N51	828. RY*(14)Ru53	0.58	9.42	0.066
40. BD (1) C12- N51	831. RY*(17)Ru53	0.51	13.20	0.073
40. BD (1) C12- N51	836. RY*(22)Ru53	0.81	11.34	0.086
40. BD (1) C12- N51	838. RY*(24)Ru53	0.56	35647.59	4.019
40. BD (1) C12- N51	839. RY*(25)Ru53	0.68	5348.64	1.704
40. BD (1) C12- N51	840. RY*(26)Ru53	1.12	5744.26	2.267
40. BD (1) C12- N51	844. RY*(30)Ru53	0.72	33.19	0.139
40. BD (1) C12- N51	847. RY*(33)Ru53	1.03	278.29	0.480
40. BD (1) C12- N51	848. RY*(34)Ru53	0.52	51.69	0.146
40. BD (1) C12- N51	852. RY*(38)Ru53	1.10	356.46	0.560
40. BD (1) C12- N51	856. RY*(42)Ru53	0.92	3163.21	1.527
40. BD (1) C12- N51	906. BD*(1) C 6-Ru53	4.24	0.89	0.060
40. BD (1) C12- N51	911. BD*(1) C12- C14	0.80	1.24	0.028
40. BD (1) C12- N51	916. BD*(1) C14- H31	1.57	1.15	0.038
40. BD (1) C12- N51	921. BD*(1) C20- N51	0.62	1.19	0.024
40. BD (1) C12- N51	924. BD*(1) C20- C22	2.75	1.19	0.051
43. BD (1) C14- C21	500. RY*(3) C23	0.94	2.31	0.042
43. BD (1) C14- C21	911. BD*(1) C12- C14	0.76	1.12	0.026
43. BD (1) C14- C21	914. BD*(1) C12- H29	2.38	1.03	0.044
43. BD (1) C14- C21	917. BD*(1) C21- C23	0.81	1.12	0.027
43. BD (1) C14- C21	920. BD*(1) C23- H38	2.50	1.03	0.045
44. BD (1) C14- H31	333. RY*(1) C12	0.64	2.03	0.032
44. BD (1) C14- H31	468. RY*(1) C21	0.84	2.22	0.039
44. BD (1) C14- H31	913. BD*(1) C12- N51	5.34	0.92	0.063
44. BD (1) C14- H31	917. BD*(1) C21- C23	3.39	0.95	0.051
47. BD (1) C16- C18	395. RY*(3) C16	0.73	1.63	0.031
47. BD (1) C16- C18	396. RY*(4) C16	1.89	2.79	0.065
47. BD (1) C16- C18	401. RY*(9) C16	0.52	13.50	0.075
47. BD (1) C16- C18	428. RY*(6) C18	1.03	3.62	0.055
47. BD (1) C16- C18	435. RY*(13) C18	0.60	40.65	0.141
47. BD (1) C16- C18	437. RY*(15) C18	0.71	27.51	0.126
47. BD (1) C16- C18	483. RY*(1) C22	1.13	1.97	0.042

47. BD (1) C16- C18	485. RY*(3) C22	0.91	2.40	0.042
47. BD (1) C16- C18	515. RY*(3) C24	1.36	2.50	0.052
47. BD (1) C16- C18	815. RY*(1)Ru53	1.56	7.58	0.097
47. BD (1) C16- C18	816. RY*(2)Ru53	2.42	2.45	0.069
47. BD (1) C16- C18	819. RY*(5)Ru53	2.82	7.04	0.126
47. BD (1) C16- C18	821. RY*(7)Ru53	1.24	3.64	0.060
47. BD (1) C16- C18	822. RY*(8)Ru53	2.27	5.24	0.098
47. BD (1) C16- C18	825. RY*(11)Ru53	1.16	6.60	0.079
47. BD (1) C16- C18	826. RY*(12)Ru53	0.68	3.51	0.044
47. BD (1) C16- C18	827. RY*(13)Ru53	1.16	14.36	0.116
47. BD (1) C16- C18	829. RY*(15)Ru53	1.34	7.74	0.091
47. BD (1) C16- C18	830. RY*(16)Ru53	0.70	7.05	0.063
47. BD (1) C16- C18	831. RY*(17)Ru53	1.27	13.04	0.115
47. BD (1) C16- C18	833. RY*(19)Ru53	1.37	7.60	0.091
47. BD (1) C16- C18	836. RY*(22)Ru53	1.42	11.19	0.113
47. BD (1) C16- C18	838. RY*(24)Ru53	1.17	35647.43	5.784
47. BD (1) C16- C18	839. RY*(25)Ru53	1.28	5348.48	2.346
47. BD (1) C16- C18	840. RY*(26)Ru53	2.25	5744.10	3.225
47. BD (1) C16- C18	841. RY*(27)Ru53	0.74	49.89	0.172
47. BD (1) C16- C18	843. RY*(29)Ru53	0.58	10.74	0.071
47. BD (1) C16- C18	844. RY*(30)Ru53	1.31	33.03	0.187
47. BD (1) C16- C18	847. RY*(33)Ru53	1.99	278.13	0.667
47. BD (1) C16- C18	852. RY*(38)Ru53	2.17	356.30	0.788
47. BD (1) C16- C18	855. RY*(41)Ru53	0.89	141.25	0.318
47. BD (1) C16- C18	856. RY*(42)Ru53	1.84	3163.06	2.163
47. BD (1) C16- C18	924. BD*(1) C20- C22	3.66	1.03	0.055
47. BD (1) C16- C18	927. BD*(1) C16- C22	0.66	1.11	0.024
47. BD (1) C16- C18	930. BD*(1) C24- H36	2.20	1.01	0.042
47. BD (1) C16- C18	931. BD*(1) C18- C24	1.17	1.09	0.032
47. BD (1) C16- C18	933. BD*(1) C18- H32	0.66	1.02	0.023
48. BD (1) C16- C22	425. RY*(3) C18	1.40	2.33	0.051
48. BD (1) C16- C22	453. RY*(1) C20	0.85	2.15	0.038
48. BD (1) C16- C22	487. RY*(5) C22	0.59	4.58	0.047
48. BD (1) C16- C22	491. RY*(9) C22	0.83	15.30	0.101
48. BD (1) C16- C22	496. RY*(14) C22	0.94	25.86	0.140
48. BD (1) C16- C22	497. RY*(15) C22	0.80	42.36	0.166
48. BD (1) C16- C22	530. RY*(3) C25	0.81	2.39	0.039
48. BD (1) C16- C22	531. RY*(4) C25	0.89	2.06	0.038
48. BD (1) C16- C22	533. RY*(6) C25	0.68	6.45	0.059
48. BD (1) C16- C22	822. RY*(8)Ru53	1.37	5.23	0.076
48. BD (1) C16- C22	827. RY*(13)Ru53	0.68	14.36	0.089
48. BD (1) C16- C22	840. RY*(26)Ru53	0.56	5744.09	1.605
48. BD (1) C16- C22	841. RY*(27)Ru53	0.53	49.88	0.146
48. BD (1) C16- C22	852. RY*(38)Ru53	0.53	356.29	0.390
48. BD (1) C16- C22	865. BD*(1) C25- H39	2.30	1.00	0.043
48. BD (1) C16- C22	913. BD*(1) C12- N51	0.51	1.04	0.021
48. BD (1) C16- C22	923. BD*(1) C20- C23	3.55	1.07	0.055
48. BD (1) C16- C22	924. BD*(1) C20- C22	1.01	1.02	0.029
48. BD (1) C16- C22	925. BD*(1) C22- C25	2.11	1.09	0.043
48. BD (1) C16- C22	928. BD*(1) C16- C18	0.52	1.11	0.021
48. BD (1) C16- C22	933. BD*(1) C18- H32	2.84	1.01	0.048
49. BD (1) C16-Ru53	244. RY*(2) C 6	0.61	1.38	0.027
49. BD (1) C16-Ru53	245. RY*(3) C 6	1.54	2.97	0.062
49. BD (1) C16-Ru53	248. RY*(6) C 6	0.57	2.67	0.036
49. BD (1) C16-Ru53	276. RY*(4) C 8	0.70	2.58	0.039
49. BD (1) C16-Ru53	423. RY*(1) C18	0.71	2.00	0.035
49. BD (1) C16-Ru53	425. RY*(3) C18	0.56	2.09	0.032
49. BD (1) C16-Ru53	483. RY*(1) C22	0.71	1.71	0.032
49. BD (1) C16-Ru53	752. RY*(1) N51	2.81	2.16	0.072
49. BD (1) C16-Ru53	815. RY*(1)Ru53	0.73	7.33	0.068
49. BD (1) C16-Ru53	819. RY*(5)Ru53	0.50	6.79	0.054
49. BD (1) C16-Ru53	829. RY*(15)Ru53	0.50	7.49	0.057
49. BD (1) C16-Ru53	836. RY*(22)Ru53	0.76	10.93	0.084
49. BD (1) C16-Ru53	844. RY*(30)Ru53	0.52	32.78	0.121
49. BD (1) C16-Ru53	904. BD*(2) C 6- O45	0.58	0.36	0.013
49. BD (1) C16-Ru53	905. BD*(3) C 6- O45	1.75	0.95	0.037
49. BD (1) C16-Ru53	906. BD*(1) C 6-Ru53	17.70	0.48	0.086
49. BD (1) C16-Ru53	907. BD*(1) C 8-Ru53	16.92	0.48	0.084
49. BD (1) C16-Ru53	908. BD*(1) C 8- O46	0.88	0.35	0.016
49. BD (1) C16-Ru53	910. BD*(3) C 8- O46	0.98	0.97	0.028
49. BD (1) C16-Ru53	913. BD*(1) C12- N51	1.79	0.80	0.035
49. BD (1) C16-Ru53	923. BD*(1) C20- C23	0.63	0.83	0.021
49. BD (1) C16-Ru53	924. BD*(1) C20- C22	0.59	0.78	0.020
49. BD (1) C16-Ru53	925. BD*(1) C22- C25	6.39	0.84	0.067
49. BD (1) C16-Ru53	926. BD*(1) C16-Ru53	2.75	0.37	0.030
49. BD (1) C16-Ru53	931. BD*(1) C18- C24	5.47	0.84	0.062
49. BD (1) C16-Ru53	933. BD*(1) C18- H32	0.85	0.77	0.023
53. BD (1) C18- C24	393. RY*(1) C16	0.92	1.67	0.035
53. BD (1) C18- C24	545. RY*(3) C26	1.00	2.54	0.045
53. BD (1) C18- C24	866. BD*(1) C26- H40	2.36	1.02	0.044
53. BD (1) C18- C24	926. BD*(1) C16-Ru53	3.81	0.63	0.047
53. BD (1) C18- C24	928. BD*(1) C16- C18	1.39	1.13	0.035
53. BD (1) C18- C24	929. BD*(1) C24- C26	0.76	1.09	0.026
54. BD (2) C18- C24	167. LP*(1) C16	39.91	0.13	0.075
54. BD (2) C18- C24	394. RY*(2) C16	0.76	0.87	0.025
54. BD (2) C18- C24	424. RY*(2) C18	0.60	0.71	0.020
54. BD (2) C18- C24	544. RY*(2) C26	0.85	0.74	0.025
54. BD (2) C18- C24	864. BD*(2) C25- C26	14.50	0.22	0.051
55. BD (1) C18- H32	393. RY*(1) C16	1.50	1.49	0.042
55. BD (1) C18- H32	513. RY*(1) C24	0.96	2.04	0.040
55. BD (1) C18- H32	519. RY*(7) C24	0.52	6.66	0.053
55. BD (1) C18- H32	927. BD*(1) C16- C22	3.76	0.94	0.053
55. BD (1) C18- H32	929. BD*(1) C24- C26	3.75	0.92	0.052
57. BD (1) C20- C22	393. RY*(1) C16	0.97	1.65	0.036
57. BD (1) C20- C22	498. RY*(1) C23	0.80	2.14	0.037
57. BD (1) C20- C22	528. RY*(1) C25	0.90	2.15	0.039
57. BD (1) C20- C22	752. RY*(1) N51	0.73	2.40	0.038
57. BD (1) C20- C22	863. BD*(1) C25- C26	2.10	1.09	0.043
57. BD (1) C20- C22	913. BD*(1) C12- N51	4.68	1.04	0.062
57. BD (1) C20- C22	917. BD*(1) C21- C23	2.02	1.06	0.042
57. BD (1) C20- C22	923. BD*(1) C20- C23	0.99	1.06	0.029
57. BD (1) C20- C22	925. BD*(1) C22- C25	0.88	1.08	0.028
57. BD (1) C20- C22	927. BD*(1) C16- C22	1.03	1.09	0.030
57. BD (1) C20- C22	928. BD*(1) C16- C18	2.57	1.11	0.048
58. BD (1) C20- C23	469. RY*(2) C21	1.53	2.37	0.054
58. BD (1) C20- C23	485. RY*(3) C22	0.91	2.44	0.042
58. BD (1) C20- C23	752. RY*(1) N51	0.51	2.45	0.032
58. BD (1) C20- C23	917. BD*(1) C21- C23	0.92	1.11	0.029
58. BD (1) C20- C23	919. BD*(1) C21- H37	2.33	1.02	0.044
58. BD (1) C20- C23	921. BD*(1) C20- N51	0.52	1.07	0.021
58. BD (1) C20- C23	924. BD*(1) C20- C22	1.11	1.07	0.031
58. BD (1) C20- C23	927. BD*(1) C16- C22	2.15	1.15	0.044
59. BD (1) C20- N51	335. RY*(3) C12	2.39	2.56	0.070
59. BD (1) C20- N51	461. RY*(9) C20	0.66	11.43	0.078
59. BD (1) C20- N51	463. RY*(11) C20	0.58	6.21	0.054
59. BD (1) C20- N51	465. RY*(13) C20	1.04	24.19	0.142

59. BD (1) C20- N51	467. RY*(15) C20	0.78	42.98	0.164
59. BD (1) C20- N51	503. RY*(6) C23	0.53	7.31	0.056
59. BD (1) C20- N51	505. RY*(8) C23	0.64	3.95	0.045
59. BD (1) C20- N51	754. RY*(3) N51	1.10	2.90	0.051
59. BD (1) C20- N51	822. RY*(8)Ru53	0.92	5.38	0.063
59. BD (1) C20- N51	826. RY*(12)Ru53	0.57	3.65	0.041
59. BD (1) C20- N51	827. RY*(13)Ru53	0.83	14.50	0.099
59. BD (1) C20- N51	906. BD*(1) C 6-Ru53	4.95	0.87	0.064
59. BD (1) C20- N51	914. BD*(1) C12- H29	1.90	1.13	0.041
59. BD (1) C20- N51	920. BD*(1) C23- H38	1.63	1.13	0.038
59. BD (1) C20- N51	923. BD*(1) C20- C23	1.04	1.22	0.032
59. BD (1) C20- N51	924. BD*(1) C20- C22	0.63	1.17	0.024
59. BD (1) C20- N51	925. BD*(1) C22- C25	2.35	1.24	0.048
60. BD (2) C20- N51	147. LP (1) C22	13.15	0.19	0.057
60. BD (2) C20- N51	334. RY*(2) C12	2.60	0.95	0.048
60. BD (2) C20- N51	484. RY*(2) C22	0.75	0.83	0.024
60. BD (2) C20- N51	499. RY*(2) C23	0.92	0.77	0.026
60. BD (2) C20- N51	817. RY*(3)Ru53	0.96	1.42	0.036
60. BD (2) C20- N51	912. BD*(2) C12- C14	20.03	0.28	0.067
60. BD (2) C20- N51	918. BD*(2) C21- C23	7.52	0.27	0.041
61. BD (1) C21- C23	365. RY*(3) C14	0.87	2.54	0.042
61. BD (1) C21- C23	453. RY*(1) C20	0.69	2.21	0.035
61. BD (1) C21- C23	915. BD*(1) C14- C21	0.77	1.11	0.026
61. BD (1) C21- C23	916. BD*(1) C14- H31	2.45	1.04	0.045
61. BD (1) C21- C23	923. BD*(1) C20- C23	1.08	1.13	0.031
61. BD (1) C21- C23	924. BD*(1) C20- C22	3.57	1.08	0.056
62. BD (2) C21- C23	364. RY*(2) C14	1.07	0.81	0.029
62. BD (2) C21- C23	912. BD*(2) C12- C14	12.37	0.23	0.048
62. BD (2) C21- C23	922. BD*(2) C20- N51	22.54	0.21	0.064
63. BD (1) C21- H37	363. RY*(1) C14	0.87	2.15	0.039
63. BD (1) C21- H37	498. RY*(1) C23	0.89	2.03	0.038
63. BD (1) C21- H37	911. BD*(1) C12- C14	3.37	0.95	0.051
63. BD (1) C21- H37	923. BD*(1) C20- C23	3.87	0.95	0.054
64. BD (1) C22- C25	395. RY*(3) C16	0.68	1.63	0.030
64. BD (1) C22- C25	455. RY*(3) C20	1.23	2.54	0.050
64. BD (1) C22- C25	545. RY*(3) C26	1.70	2.54	0.059
64. BD (1) C22- C25	863. BD*(1) C25- C26	1.02	1.11	0.030
64. BD (1) C22- C25	866. BD*(1) C26- H40	2.32	1.02	0.043
64. BD (1) C22- C25	921. BD*(1) C20- N51	2.81	1.04	0.048
64. BD (1) C22- C25	924. BD*(1) C20- C22	1.00	1.04	0.029
64. BD (1) C22- C25	926. BD*(1) C16-Ru53	3.40	0.63	0.044
64. BD (1) C22- C25	927. BD*(1) C16- C22	2.14	1.12	0.044
65. BD (1) C23- H38	453. RY*(1) C20	1.01	2.04	0.041
65. BD (1) C23- H38	468. RY*(1) C21	0.89	2.23	0.040
65. BD (1) C23- H38	915. BD*(1) C14- C21	3.48	0.94	0.051
65. BD (1) C23- H38	921. BD*(1) C20- N51	5.74	0.91	0.065
66. BD (1) C24- C26	426. RY*(4) C18	0.66	1.64	0.029
66. BD (1) C24- C26	530. RY*(3) C25	0.97	2.40	0.043
66. BD (1) C24- C26	863. BD*(1) C25- C26	0.95	1.11	0.029
66. BD (1) C24- C26	865. BD*(1) C25- H39	2.54	1.01	0.045
66. BD (1) C24- C26	931. BD*(1) C18- C24	0.81	1.10	0.027
66. BD (1) C24- C26	933. BD*(1) C18- H32	2.17	1.03	0.042
67. BD (1) C24- H36	423. RY*(1) C18	0.93	2.09	0.040
67. BD (1) C24- H36	543. RY*(1) C26	0.92	2.14	0.040
67. BD (1) C24- H36	863. BD*(1) C25- C26	3.66	0.94	0.053
67. BD (1) C24- H36	928. BD*(1) C16- C18	4.78	0.96	0.061
68. BD (1) C25- C26	483. RY*(1) C22	0.71	1.98	0.034
68. BD (1) C25- C26	515. RY*(3) C24	1.01	2.52	0.045
68. BD (1) C25- C26	924. BD*(1) C20- C22	3.44	1.05	0.054
68. BD (1) C25- C26	925. BD*(1) C22- C25	1.27	1.11	0.034
68. BD (1) C25- C26	929. BD*(1) C24- C26	0.87	1.10	0.028
68. BD (1) C25- C26	930. BD*(1) C24- H36	2.31	1.03	0.044
69. BD (2) C25- C26	147. LP (1) C22	34.72	0.12	0.073
69. BD (2) C25- C26	484. RY*(2) C22	0.62	0.76	0.021
69. BD (2) C25- C26	514. RY*(2) C24	0.80	0.75	0.024
69. BD (2) C25- C26	932. BD*(2) C18- C24	15.14	0.23	0.053
70. BD (1) C25- H39	483. RY*(1) C22	1.19	1.82	0.042
70. BD (1) C25- H39	543. RY*(1) C26	0.97	2.15	0.041
70. BD (1) C25- H39	927. BD*(1) C16- C22	4.94	0.96	0.062
70. BD (1) C25- H39	929. BD*(1) C24- C26	3.56	0.94	0.052
71. BD (1) C26- H40	513. RY*(1) C24	0.96	2.05	0.040
71. BD (1) C26- H40	528. RY*(1) C25	0.96	2.01	0.039
71. BD (1) C26- H40	925. BD*(1) C22- C25	4.05	0.94	0.055
71. BD (1) C26- H40	931. BD*(1) C18- C24	3.73	0.94	0.053
78. CR (1) C 6	661. RY*(4) O45	0.91	10.50	0.087
80. CR (1) C 8	676. RY*(4) O46	0.88	10.60	0.086
84. CR (1) C12	363. RY*(1) C14	0.71	11.48	0.080
84. CR (1) C12	365. RY*(3) C14	0.66	11.70	0.078
84. CR (1) C12	921. BD*(1) C20- N51	1.04	10.24	0.093
86. CR (1) C14	335. RY*(3) C12	0.63	11.59	0.076
86. CR (1) C14	336. RY*(4) C12	0.86	11.08	0.087
86. CR (1) C14	469. RY*(2) C21	1.02	11.51	0.097
86. CR (1) C14	913. BD*(1) C12- N51	0.70	10.23	0.076
88. CR (1) C16	423. RY*(1) C18	0.53	11.42	0.069
88. CR (1) C16	425. RY*(3) C18	0.98	11.51	0.095
88. CR (1) C16	483. RY*(1) C22	0.55	11.13	0.070
88. CR (1) C16	485. RY*(3) C22	0.86	11.57	0.089
88. CR (1) C16	924. BD*(1) C20- C22	0.67	10.20	0.074
88. CR (1) C16	925. BD*(1) C22- C25	0.73	10.26	0.078
88. CR (1) C16	926. BD*(1) C16-Ru53	0.54	9.79	0.070
88. CR (1) C16	931. BD*(1) C18- C24	0.58	10.26	0.069
90. CR (1) C18	395. RY*(3) C16	1.00	10.77	0.093
90. CR (1) C18	515. RY*(3) C24	0.93	11.65	0.093
90. CR (1) C18	926. BD*(1) C16-Ru53	0.82	9.77	0.087
92. CR (1) C20	483. RY*(1) C22	0.53	11.19	0.069
92. CR (1) C20	498. RY*(1) C23	0.60	11.37	0.074
92. CR (1) C20	754. RY*(3) N51	0.53	11.98	0.071
92. CR (1) C20	913. BD*(1) C12- N51	0.91	10.27	0.087
92. CR (1) C20	925. BD*(1) C22- C25	0.61	10.32	0.072
92. CR (1) C20	927. BD*(1) C16- C22	0.59	10.33	0.071
93. CR (1) C21	365. RY*(3) C14	1.35	11.68	0.112
93. CR (1) C21	500. RY*(3) C23	1.33	11.45	0.110
93. CR (1) C21	923. BD*(1) C20- C23	0.50	10.26	0.065
94. CR (1) C22	395. RY*(3) C16	0.74	10.79	0.080
94. CR (1) C22	453. RY*(1) C20	0.55	11.32	0.070
94. CR (1) C22	528. RY*(1) C25	0.52	11.32	0.068
94. CR (1) C22	530. RY*(3) C25	0.62	11.55	0.075
94. CR (1) C22	921. BD*(1) C20- N51	0.51	10.19	0.065
94. CR (1) C22	923. BD*(1) C20- C23	0.78	10.24	0.081
94. CR (1) C22	926. BD*(1) C16-Ru53	0.62	9.78	0.075
95. CR (1) C23	455. RY*(3) C20	1.17	11.72	0.104
95. CR (1) C23	469. RY*(2) C21	1.19	11.51	0.105
95. CR (1) C23	921. BD*(1) C20- N51	0.69	10.21	0.076
95. CR (1) C23	924. BD*(1) C20- C22	0.91	10.21	0.087
96. CR (1) C24	425. RY*(3) C18	0.86	11.50	0.089
96. CR (1) C24	426. RY*(4) C18	0.61	10.79	0.072

96. CR (1) C24	545. RY*(3) C26	0.85	11.68	0.089
96. CR (1) C24	928. BD*(1) C16- C18	0.83	10.27	0.083
97. CR (1) C25	485. RY*(3) C22	0.95	11.56	0.094
97. CR (1) C25	545. RY*(3) C26	1.27	11.69	0.109
97. CR (1) C25	924. BD*(1) C20- C22	0.77	10.19	0.080
97. CR (1) C25	927. BD*(1) C16- C22	0.89	10.27	0.086
98. CR (1) C26	515. RY*(3) C24	1.26	11.65	0.108
98. CR (1) C26	530. RY*(3) C25	1.29	11.54	0.109
98. CR (1) C26	925. BD*(1) C22- C25	0.58	10.25	0.069
100. CR (1) O45	243. RY*(1) C 6	4.93	20.42	0.284
100. CR (1) O45	906. BD*(1) C 6-Ru53	0.62	18.70	0.105
101. CR (1) O46	273. RY*(1) C 8	4.88	20.31	0.282
101. CR (1) O46	907. BD*(1) C 8-Ru53	0.66	18.69	0.107
110. CR (1) N51	333. RY*(1) C12	0.94	15.43	0.108
110. CR (1) N51	335. RY*(3) C12	0.94	15.69	0.109
110. CR (1) N51	453. RY*(1) C20	1.00	15.43	0.111
110. CR (1) N51	455. RY*(3) C20	0.93	15.81	0.108
110. CR (1) N51	906. BD*(1) C 6-Ru53	4.42	14.00	0.242
129. CR (1)Ru53	847. RY*(33)Ru53	0.67	904.54	0.693
130. CR (2)Ru53	847. RY*(33)Ru53	0.90	590.36	0.649
130. CR (2)Ru53	852. RY*(38)Ru53	0.54	668.53	0.537
130. CR (2)Ru53	905. BD*(3) C 6- O45	0.73	313.43	0.431
130. CR (2)Ru53	910. BD*(3) C 8- O46	0.70	313.45	0.419
131. CR (3)Ru53	815. RY*(1)Ru53	1.33	28.83	0.175
131. CR (3)Ru53	819. RY*(5)Ru53	0.81	28.29	0.135
131. CR (3)Ru53	822. RY*(8)Ru53	0.59	26.49	0.111
131. CR (3)Ru53	823. RY*(9)Ru53	1.51	30.95	0.193
131. CR (3)Ru53	827. RY*(13)Ru53	0.84	35.61	0.154
131. CR (3)Ru53	831. RY*(17)Ru53	1.16	34.29	0.178
131. CR (3)Ru53	836. RY*(22)Ru53	2.16	32.43	0.236
131. CR (3)Ru53	840. RY*(26)Ru53	1.66	5765.35	2.764
131. CR (3)Ru53	843. RY*(29)Ru53	0.69	31.99	0.132
131. CR (3)Ru53	844. RY*(30)Ru53	4.25	54.28	0.429
131. CR (3)Ru53	847. RY*(33)Ru53	5.11	299.38	1.104
131. CR (3)Ru53	852. RY*(38)Ru53	1.48	377.55	0.668
131. CR (3)Ru53	855. RY*(41)Ru53	1.13	162.49	0.383
131. CR (3)Ru53	905. BD*(3) C 6- O45	3.84	22.45	0.264
131. CR (3)Ru53	910. BD*(3) C 8- O46	3.62	22.47	0.255
131. CR (3)Ru53	913. BD*(1) C12- N51	0.82	22.30	0.121
131. CR (3)Ru53	921. BD*(1) C20- N51	0.64	22.28	0.108
131. CR (3)Ru53	926. BD*(1) C16-Ru53	0.86	21.87	0.132
131. CR (3)Ru53	927. BD*(1) C16- C22	0.65	22.36	0.108
131. CR (3)Ru53	928. BD*(1) C16- C18	1.45	22.37	0.162
132. CR (4)Ru53	243. RY*(1) C 6	3.49	6.44	0.134
132. CR (4)Ru53	273. RY*(1) C 8	3.06	6.34	0.124
132. CR (4)Ru53	393. RY*(1) C16	0.62	5.65	0.053
132. CR (4)Ru53	815. RY*(1)Ru53	0.79	11.57	0.086
132. CR (4)Ru53	819. RY*(5)Ru53	0.73	11.04	0.081
132. CR (4)Ru53	822. RY*(8)Ru53	0.51	9.23	0.062
132. CR (4)Ru53	823. RY*(9)Ru53	0.86	13.69	0.097
132. CR (4)Ru53	827. RY*(13)Ru53	0.58	18.36	0.093
132. CR (4)Ru53	831. RY*(17)Ru53	0.86	17.03	0.108
132. CR (4)Ru53	836. RY*(22)Ru53	1.38	15.18	0.130
132. CR (4)Ru53	840. RY*(26)Ru53	0.91	5748.09	2.053
132. CR (4)Ru53	844. RY*(30)Ru53	1.44	37.03	0.207
132. CR (4)Ru53	847. RY*(33)Ru53	1.51	282.12	0.584
132. CR (4)Ru53	852. RY*(38)Ru53	1.04	360.29	0.547
132. CR (4)Ru53	905. BD*(3) C 6- O45	10.85	5.19	0.212
132. CR (4)Ru53	910. BD*(3) C 8- O46	10.45	5.22	0.208
132. CR (4)Ru53	913. BD*(1) C12- N51	2.44	5.04	0.099
132. CR (4)Ru53	921. BD*(1) C20- N51	1.95	5.03	0.089
132. CR (4)Ru53	926. BD*(1) C16-Ru53	2.61	4.61	0.106
132. CR (4)Ru53	927. BD*(1) C16- C22	1.63	5.10	0.082
132. CR (4)Ru53	928. BD*(1) C16- C18	3.96	5.11	0.127
135. CR (7)Ru53	905. BD*(3) C 6- O45	1.90	2.42	0.061
135. CR (7)Ru53	906. BD*(1) C 6-Ru53	3.59	1.95	0.081
135. CR (7)Ru53	907. BD*(1) C 8-Ru53	1.73	1.95	0.056
135. CR (7)Ru53	910. BD*(3) C 8- O46	1.00	2.44	0.044
138. CR (10)Ru53	904. BD*(2) C 6- O45	1.00	1.84	0.040
138. CR (10)Ru53	906. BD*(1) C 6-Ru53	1.61	1.95	0.054
138. CR (10)Ru53	907. BD*(1) C 8-Ru53	4.22	1.95	0.088
138. CR (10)Ru53	910. BD*(3) C 8- O46	1.31	2.44	0.051
138. CR (10)Ru53	926. BD*(1) C16-Ru53	2.01	1.84	0.059
141. CR (13)Ru53	903. BD*(1) C 6- O45	0.91	1.84	0.039
141. CR (13)Ru53	906. BD*(1) C 6-Ru53	0.96	1.95	0.042
141. CR (13)Ru53	907. BD*(1) C 8-Ru53	0.58	1.95	0.032
141. CR (13)Ru53	926. BD*(1) C16-Ru53	5.29	1.84	0.095
147. LP (1) C22	167. LP*(1) C16	1023.10	0.02	0.114
147. LP (1) C22	394. RY*(2) C16	0.96	0.76	0.033
147. LP (1) C22	457. RY*(5) C20	0.79	1.86	0.047
147. LP (1) C22	484. RY*(2) C22	2.53	0.64	0.049
147. LP (1) C22	529. RY*(2) C25	2.87	0.61	0.051
147. LP (1) C22	864. BD*(2) C25- C26	57.10	0.11	0.085
147. LP (1) C22	922. BD*(2) C20- N51	124.88	0.06	0.088
147. LP (1) C22	932. BD*(2) C18- C24	0.74	0.12	0.010
149. LP (1) O45	243. RY*(1) C 6	9.23	2.51	0.136
149. LP (1) O45	250. RY*(8) C 6	1.75	3.68	0.072
149. LP (1) O45	906. BD*(1) C 6-Ru53	3.18	0.79	0.049
150. LP (1) O46	273. RY*(1) C 8	9.31	2.41	0.134
150. LP (1) O46	280. RY*(8) C 8	1.17	3.07	0.054
150. LP (1) O46	283. RY*(11) C 8	0.90	3.02	0.047
150. LP (1) O46	907. BD*(1) C 8-Ru53	3.28	0.79	0.049
160. LP (1) N51	333. RY*(1) C12	2.26	1.91	0.064
160. LP (1) N51	335. RY*(3) C12	0.58	2.17	0.034
160. LP (1) N51	453. RY*(1) C20	2.10	1.92	0.062
160. LP (1) N51	455. RY*(3) C20	0.98	2.29	0.046
160. LP (1) N51	906. BD*(1) C 6-Ru53	71.52	0.49	0.167
160. LP (1) N51	909. BD*(2) C 8- O46	0.81	0.36	0.016
160. LP (1) N51	910. BD*(3) C 8- O46	0.83	0.98	0.028
160. LP (1) N51	911. BD*(1) C12- C14	7.07	0.83	0.074
160. LP (1) N51	914. BD*(1) C12- H29	2.60	0.74	0.043
160. LP (1) N51	923. BD*(1) C20- C23	7.49	0.83	0.076
160. LP (1) N51	924. BD*(1) C20- C22	1.67	0.79	0.035
160. LP (1) N51	925. BD*(1) C22- C25	0.56	0.85	0.021
160. LP (1) N51	926. BD*(1) C16-Ru53	1.74	0.38	0.023
160. LP (1) N51	928. BD*(1) C16- C18	1.45	0.88	0.035
164. LP (1)Ru53	167. LP*(1) C16	3.41	0.11	0.021
164. LP (1)Ru53	246. RY*(4) C 6	1.65	1.72	0.050
164. LP (1)Ru53	395. RY*(3) C16	0.61	1.21	0.026
164. LP (1)Ru53	754. RY*(3) N51	1.81	2.35	0.062
164. LP (1)Ru53	903. BD*(1) C 6- O45	17.41	0.21	0.054
164. LP (1)Ru53	904. BD*(2) C 6- O45	4.15	0.20	0.026
164. LP (1)Ru53	908. BD*(1) C 8- O46	3.66	0.19	0.024
164. LP (1)Ru53	909. BD*(2) C 8- O46	0.55	0.19	0.009
164. LP (1)Ru53	913. BD*(1) C12- N51	0.57	0.64	0.018
164. LP (1)Ru53	921. BD*(1) C20- N51	0.57	0.62	0.018

164. LP (1)Ru53	928. BD*(1) C16- C18	0.80	0.71	0.022
165. LP (2)Ru53	167. LP*(1) C16	14.68	0.11	0.043
165. LP (2)Ru53	246. RY*(4) C 6	0.50	1.72	0.028
165. LP (2)Ru53	275. RY*(3) C 8	2.10	1.98	0.062
165. LP (2)Ru53	394. RY*(2) C16	1.61	0.86	0.036
165. LP (2)Ru53	832. RY*(18)Ru53	0.51	5.42	0.051
165. LP (2)Ru53	903. BD*(1) C 6- O45	3.01	0.21	0.023
165. LP (2)Ru53	904. BD*(2) C 6- O45	1.37	0.20	0.015
165. LP (2)Ru53	908. BD*(1) C 8- O46	18.88	0.19	0.055
165. LP (2)Ru53	909. BD*(2) C 8- O46	5.06	0.19	0.028
165. LP (2)Ru53	926. BD*(1) C16-Ru53	0.98	0.21	0.013
166. LP (3)Ru53	244. RY*(2) C 6	2.70	1.23	0.056
166. LP (3)Ru53	245. RY*(3) C 6	0.61	2.81	0.041
166. LP (3)Ru53	274. RY*(2) C 8	2.33	1.32	0.054
166. LP (3)Ru53	753. RY*(2) N51	1.92	1.07	0.044
166. LP (3)Ru53	903. BD*(1) C 6- O45	4.17	0.22	0.028
166. LP (3)Ru53	904. BD*(2) C 6- O45	17.61	0.21	0.056
166. LP (3)Ru53	908. BD*(1) C 8- O46	4.95	0.20	0.029
166. LP (3)Ru53	909. BD*(2) C 8- O46	18.64	0.20	0.056
166. LP (3)Ru53	922. BD*(2) C20- N51	3.77	0.16	0.023

from unit 2 to unit 3

18. BD (3) C 6- O45	638. RY*(1) H43	0.08	2.30	0.012
18. BD (3) C 6- O45	639. RY*(2) H43	0.13	2.89	0.017
18. BD (3) C 6- O45	641. RY*(4) H43	0.09	3.19	0.015
18. BD (3) C 6- O45	688. RY*(1) O47	0.13	2.75	0.017
18. BD (3) C 6- O45	689. RY*(2) O47	0.29	3.41	0.028
18. BD (3) C 6- O45	692. RY*(5) O47	0.08	3.48	0.015
18. BD (3) C 6- O45	694. RY*(7) O47	0.06	3.60	0.013
18. BD (3) C 6- O45	695. RY*(8) O47	0.09	3.57	0.016
19. BD (1) C 6-Ru53	638. RY*(1) H43	0.23	1.77	0.018
19. BD (1) C 6-Ru53	640. RY*(3) H43	0.14	2.50	0.017
19. BD (1) C 6-Ru53	641. RY*(4) H43	0.05	2.67	0.011
19. BD (1) C 6-Ru53	689. RY*(2) O47	0.77	2.88	0.043
19. BD (1) C 6-Ru53	690. RY*(3) O47	2.14	3.08	0.074
19. BD (1) C 6-Ru53	691. RY*(4) O47	0.31	4.25	0.033
19. BD (1) C 6-Ru53	692. RY*(5) O47	0.43	2.96	0.032
19. BD (1) C 6-Ru53	695. RY*(8) O47	0.24	3.04	0.025
19. BD (1) C 6-Ru53	696. RY*(9) O47	0.16	3.19	0.020
19. BD (1) C 6-Ru53	697. RY*(10) O47	0.11	5.34	0.022
19. BD (1) C 6-Ru53	700. RY*(13) O47	0.10	4.69	0.019
19. BD (1) C 6-Ru53	702. RY*(15) O47	0.12	78.69	0.087
19. BD (1) C 6-Ru53	934. BD*(1) H43- O47	0.12	0.98	0.010
23. BD (1) C 8- O46	641. RY*(4) H43	0.05	2.52	0.010
25. BD (3) C 8- O46	638. RY*(1) H43	0.07	2.33	0.012
25. BD (3) C 8- O46	688. RY*(1) O47	0.05	2.79	0.011
25. BD (3) C 8- O46	689. RY*(2) O47	0.06	3.44	0.013
25. BD (3) C 8- O46	692. RY*(5) O47	0.16	3.52	0.021
25. BD (3) C 8- O46	702. RY*(15) O47	0.07	79.25	0.065
26. BD (1) C 8-Ru53	639. RY*(2) H43	0.21	2.36	0.020
26. BD (1) C 8-Ru53	641. RY*(4) H43	0.16	2.66	0.019
26. BD (1) C 8-Ru53	689. RY*(2) O47	0.50	2.88	0.034
26. BD (1) C 8-Ru53	690. RY*(3) O47	0.97	3.08	0.050
26. BD (1) C 8-Ru53	691. RY*(4) O47	0.83	4.25	0.054
26. BD (1) C 8-Ru53	694. RY*(7) O47	0.10	3.07	0.016
26. BD (1) C 8-Ru53	695. RY*(8) O47	0.16	3.04	0.020
26. BD (1) C 8-Ru53	701. RY*(14) O47	0.22	92.83	0.130
26. BD (1) C 8-Ru53	702. RY*(15) O47	0.32	78.69	0.145
47. BD (1) C16- C18	638. RY*(1) H43	0.11	1.86	0.013
47. BD (1) C16- C18	639. RY*(2) H43	0.06	2.46	0.011
47. BD (1) C16- C18	640. RY*(3) H43	0.06	2.59	0.012
47. BD (1) C16- C18	688. RY*(1) O47	0.06	2.32	0.011
47. BD (1) C16- C18	689. RY*(2) O47	0.10	2.97	0.016
47. BD (1) C16- C18	690. RY*(3) O47	0.08	3.17	0.014
47. BD (1) C16- C18	934. BD*(1) H43- O47	0.05	1.07	0.007
48. BD (1) C16- C22	641. RY*(4) H43	0.05	2.75	0.011
48. BD (1) C16- C22	934. BD*(1) H43- O47	0.16	1.06	0.012
49. BD (1) C16-Ru53	638. RY*(1) H43	0.15	1.61	0.014
49. BD (1) C16-Ru53	689. RY*(2) O47	0.57	2.72	0.036
49. BD (1) C16-Ru53	690. RY*(3) O47	1.35	2.92	0.058
49. BD (1) C16-Ru53	691. RY*(4) O47	0.29	4.09	0.032
49. BD (1) C16-Ru53	695. RY*(8) O47	0.25	2.88	0.025
49. BD (1) C16-Ru53	696. RY*(9) O47	0.09	3.03	0.016
49. BD (1) C16-Ru53	697. RY*(10) O47	0.12	5.18	0.023
49. BD (1) C16-Ru53	700. RY*(13) O47	0.26	4.53	0.032
49. BD (1) C16-Ru53	702. RY*(15) O47	0.11	78.53	0.086
55. BD (1) C18- H32	689. RY*(2) O47	0.06	2.80	0.011
57. BD (1) C20- C22	934. BD*(1) H43- O47	0.11	1.05	0.010
59. BD (1) C20- N51	640. RY*(3) H43	0.05	2.73	0.011
59. BD (1) C20- N51	641. RY*(4) H43	0.10	2.90	0.015
59. BD (1) C20- N51	934. BD*(1) H43- O47	0.11	1.21	0.010
135. CR (7)Ru53	934. BD*(1) H43- O47	0.06	2.29	0.010
138. CR (10)Ru53	934. BD*(1) H43- O47	0.07	2.29	0.012
160. LP (1) N51	934. BD*(1) H43- O47	0.10	0.82	0.009
164. LP (1)Ru53	638. RY*(1) H43	0.07	1.45	0.009
164. LP (1)Ru53	639. RY*(2) H43	0.10	2.04	0.014
164. LP (1)Ru53	641. RY*(4) H43	0.07	2.34	0.012
164. LP (1)Ru53	689. RY*(2) O47	0.10	2.56	0.015
164. LP (1)Ru53	690. RY*(3) O47	0.06	2.75	0.013
164. LP (1)Ru53	934. BD*(1) H43- O47	0.07	0.65	0.007
165. LP (2)Ru53	639. RY*(2) H43	0.07	2.04	0.012
165. LP (2)Ru53	641. RY*(4) H43	0.25	2.34	0.023
165. LP (2)Ru53	689. RY*(2) O47	0.79	2.56	0.043
165. LP (2)Ru53	690. RY*(3) O47	0.09	2.76	0.016
165. LP (2)Ru53	691. RY*(4) O47	0.11	3.93	0.020
165. LP (2)Ru53	694. RY*(7) O47	0.11	2.75	0.017
165. LP (2)Ru53	696. RY*(9) O47	0.12	2.87	0.018
165. LP (2)Ru53	698. RY*(11) O47	0.07	4.79	0.018
165. LP (2)Ru53	934. BD*(1) H43- O47	0.26	0.65	0.013
166. LP (3)Ru53	638. RY*(1) H43	0.07	1.45	0.010
166. LP (3)Ru53	688. RY*(1) O47	1.48	1.91	0.052
166. LP (3)Ru53	690. RY*(3) O47	0.12	2.76	0.018
166. LP (3)Ru53	691. RY*(4) O47	0.09	3.93	0.018
166. LP (3)Ru53	695. RY*(8) O47	0.07	2.72	0.013
166. LP (3)Ru53	699. RY*(12) O47	0.12	4.74	0.023
166. LP (3)Ru53	934. BD*(1) H43- O47	0.19	0.66	0.011

from unit 2 to unit 4

16. BD (1) C 6- O45	722. RY*(5)Cl49	0.06	2.71	0.011
17. BD (2) C 6- O45	721. RY*(4)Cl49	0.12	2.98	0.017
17. BD (2) C 6- O45	722. RY*(5)Cl49	0.07	2.70	0.013
18. BD (3) C 6- O45	719. RY*(2)Cl49	0.55	2.83	0.035
18. BD (3) C 6- O45	720. RY*(3)Cl49	1.31	2.94	0.055
18. BD (3) C 6- O45	721. RY*(4)Cl49	1.12	3.64	0.057
18. BD (3) C 6- O45	722. RY*(5)Cl49	0.85	3.35	0.048
18. BD (3) C 6- O45	723. RY*(6)Cl49	0.15	4.09	0.022

18. BD (3) C 6- O45	724. RY*(7)Cl49	0.23	2.82	0.023
18. BD (3) C 6- O45	725. RY*(8)Cl49	0.19	6.30	0.031
18. BD (3) C 6- O45	726. RY*(9)Cl49	0.16	2.49	0.018
18. BD (3) C 6- O45	727. RY*(10)Cl49	0.07	4.56	0.016
18. BD (3) C 6- O45	730. RY*(13)Cl49	0.11	5.61	0.022
19. BD (1) C 6-Ru53	719. RY*(2)Cl49	0.32	2.31	0.025
19. BD (1) C 6-Ru53	720. RY*(3)Cl49	0.51	2.41	0.032
19. BD (1) C 6-Ru53	721. RY*(4)Cl49	0.26	3.11	0.026
19. BD (1) C 6-Ru53	723. RY*(6)Cl49	0.62	3.56	0.043
19. BD (1) C 6-Ru53	724. RY*(7)Cl49	0.94	2.29	0.042
19. BD (1) C 6-Ru53	725. RY*(8)Cl49	0.16	5.77	0.028
25. BD (3) C 8- O46	719. RY*(2)Cl49	0.47	2.87	0.033
25. BD (3) C 8- O46	720. RY*(3)Cl49	1.63	2.97	0.062
25. BD (3) C 8- O46	721. RY*(4)Cl49	0.61	3.67	0.042
25. BD (3) C 8- O46	722. RY*(5)Cl49	0.70	3.39	0.043
25. BD (3) C 8- O46	723. RY*(6)Cl49	0.19	4.12	0.025
25. BD (3) C 8- O46	724. RY*(7)Cl49	0.32	2.85	0.027
25. BD (3) C 8- O46	725. RY*(8)Cl49	0.19	6.33	0.031
25. BD (3) C 8- O46	727. RY*(10)Cl49	0.15	4.60	0.024
25. BD (3) C 8- O46	730. RY*(13)Cl49	0.12	5.64	0.023
26. BD (1) C 8-Ru53	719. RY*(2)Cl49	0.68	2.30	0.036
26. BD (1) C 8-Ru53	720. RY*(3)Cl49	0.18	2.41	0.019
26. BD (1) C 8-Ru53	721. RY*(4)Cl49	0.62	3.11	0.040
26. BD (1) C 8-Ru53	722. RY*(5)Cl49	0.48	2.82	0.034
26. BD (1) C 8-Ru53	723. RY*(6)Cl49	0.36	3.56	0.032
26. BD (1) C 8-Ru53	724. RY*(7)Cl49	0.34	2.29	0.025
26. BD (1) C 8-Ru53	725. RY*(8)Cl49	0.36	5.77	0.042
26. BD (1) C 8-Ru53	732. RY*(15)Cl49	0.05	26.54	0.034
37. BD (1) C12- C14	719. RY*(2)Cl49	0.07	2.44	0.012
37. BD (1) C12- C14	720. RY*(3)Cl49	0.06	2.55	0.011
37. BD (1) C12- C14	721. RY*(4)Cl49	0.07	3.25	0.014
37. BD (1) C12- C14	722. RY*(5)Cl49	0.12	2.96	0.017
39. BD (1) C12- H29	721. RY*(4)Cl49	0.06	3.07	0.012
39. BD (1) C12- H29	722. RY*(5)Cl49	0.24	2.78	0.023
40. BD (1) C12- N51	719. RY*(2)Cl49	0.10	2.56	0.014
40. BD (1) C12- N51	720. RY*(3)Cl49	0.14	2.66	0.017
40. BD (1) C12- N51	721. RY*(4)Cl49	0.09	3.36	0.016
40. BD (1) C12- N51	722. RY*(5)Cl49	0.45	3.08	0.033
40. BD (1) C12- N51	727. RY*(10)Cl49	0.08	4.29	0.017
47. BD (1) C16- C18	719. RY*(2)Cl49	0.15	2.40	0.017
47. BD (1) C16- C18	720. RY*(3)Cl49	0.16	2.50	0.018
47. BD (1) C16- C18	721. RY*(4)Cl49	0.27	3.21	0.027
47. BD (1) C16- C18	722. RY*(5)Cl49	0.32	2.92	0.027
47. BD (1) C16- C18	725. RY*(8)Cl49	0.09	5.86	0.020
48. BD (1) C16- C22	720. RY*(3)Cl49	0.16	2.49	0.018
49. BD (1) C16-Ru53	720. RY*(3)Cl49	0.08	2.25	0.012
59. BD (1) C20- N51	719. RY*(2)Cl49	0.13	2.54	0.017
59. BD (1) C20- N51	720. RY*(3)Cl49	0.07	2.64	0.013
59. BD (1) C20- N51	721. RY*(4)Cl49	0.09	3.35	0.015
60. BD (2) C20- N51	720. RY*(3)Cl49	0.06	2.18	0.011
60. BD (2) C20- N51	722. RY*(5)Cl49	0.09	2.60	0.014
131. CR (3)Ru53	719. RY*(2)Cl49	0.07	23.65	0.036
131. CR (3)Ru53	720. RY*(3)Cl49	0.15	23.75	0.054
131. CR (3)Ru53	721. RY*(4)Cl49	0.12	24.45	0.048
131. CR (3)Ru53	722. RY*(5)Cl49	0.13	24.17	0.050
132. CR (4)Ru53	719. RY*(2)Cl49	0.05	6.39	0.016
132. CR (4)Ru53	720. RY*(3)Cl49	0.09	6.49	0.021
132. CR (4)Ru53	721. RY*(4)Cl49	0.14	7.20	0.028
132. CR (4)Ru53	722. RY*(5)Cl49	0.14	6.91	0.028
132. CR (4)Ru53	723. RY*(6)Cl49	0.06	7.65	0.019
132. CR (4)Ru53	725. RY*(8)Cl49	0.06	9.85	0.022
164. LP (1)Ru53	718. RY*(1)Cl49	0.53	0.83	0.020
164. LP (1)Ru53	720. RY*(3)Cl49	0.07	2.09	0.012
164. LP (1)Ru53	721. RY*(4)Cl49	0.08	2.79	0.014
164. LP (1)Ru53	722. RY*(5)Cl49	0.05	2.50	0.011
165. LP (2)Ru53	721. RY*(4)Cl49	0.14	2.79	0.019
165. LP (2)Ru53	722. RY*(5)Cl49	0.24	2.50	0.023
165. LP (2)Ru53	727. RY*(10)Cl49	0.12	3.71	0.020
165. LP (2)Ru53	735. RY*(18)Cl49	0.06	40.80	0.048
165. LP (2)Ru53	736. RY*(19)Cl49	0.07	4.97	0.018
166. LP (3)Ru53	727. RY*(10)Cl49	0.08	3.72	0.017
from unit 3 to unit 1				
72. BD (1) H43- O47	193. RY*(11) C 2	0.06	5.74	0.016
72. BD (1) H43- O47	213. RY*(1) C 4	0.19	2.44	0.019
72. BD (1) H43- O47	219. RY*(7) C 4	0.24	7.28	0.037
72. BD (1) H43- O47	261. RY*(4) C 7	0.07	2.11	0.011
72. BD (1) H43- O47	263. RY*(6) C 7	0.13	4.85	0.022
72. BD (1) H43- O47	268. RY*(11) C 7	0.06	5.93	0.017
72. BD (1) H43- O47	271. RY*(14) C 7	0.06	42.63	0.045
72. BD (1) H43- O47	272. RY*(15) C 7	0.10	24.32	0.044
72. BD (1) H43- O47	288. RY*(1) C 9	0.12	2.01	0.014
72. BD (1) H43- O47	291. RY*(4) C 9	0.09	1.79	0.012
72. BD (1) H43- O47	303. RY*(1) C10	0.26	2.56	0.023
72. BD (1) H43- O47	304. RY*(2) C10	0.10	1.60	0.011
72. BD (1) H43- O47	305. RY*(3) C10	0.12	3.30	0.018
72. BD (1) H43- O47	309. RY*(7) C10	0.13	7.07	0.027
72. BD (1) H43- O47	310. RY*(8) C10	0.07	3.94	0.015
72. BD (1) H43- O47	318. RY*(1) C11	0.28	1.69	0.020
72. BD (1) H43- O47	320. RY*(3) C11	0.15	1.66	0.014
72. BD (1) H43- O47	321. RY*(4) C11	0.21	2.90	0.022
72. BD (1) H43- O47	378. RY*(1) C15	0.06	2.26	0.010
72. BD (1) H43- O47	379. RY*(2) C15	0.06	1.11	0.007
72. BD (1) H43- O47	383. RY*(6) C15	0.21	3.88	0.025
72. BD (1) H43- O47	384. RY*(7) C15	0.08	8.61	0.024
72. BD (1) H43- O47	588. RY*(1) H33	0.11	1.97	0.013
72. BD (1) H43- O47	646. RY*(4) O44	0.07	1.38	0.009
72. BD (1) H43- O47	648. RY*(6) O44	0.06	3.13	0.013
72. BD (1) H43- O47	705. RY*(3) O48	0.09	2.63	0.014
72. BD (1) H43- O47	738. RY*(2) N50	0.41	1.51	0.022
72. BD (1) H43- O47	739. RY*(3) N50	0.17	2.75	0.020
72. BD (1) H43- O47	740. RY*(4) N50	0.32	5.71	0.038
72. BD (1) H43- O47	743. RY*(7) N50	0.05	3.02	0.011
72. BD (1) H43- O47	744. RY*(8) N50	0.32	14.31	0.061
72. BD (1) H43- O47	749. RY*(13) N50	0.13	6.72	0.026
72. BD (1) H43- O47	750. RY*(14) N50	0.13	48.38	0.072
72. BD (1) H43- O47	751. RY*(15) N50	0.23	26.67	0.070
72. BD (1) H43- O47	767. RY*(1)Ru52	0.69	7.43	0.064
72. BD (1) H43- O47	768. RY*(2)Ru52	0.14	4.16	0.022
72. BD (1) H43- O47	769. RY*(3)Ru52	0.99	2.23	0.042
72. BD (1) H43- O47	770. RY*(4)Ru52	0.99	2.93	0.048
72. BD (1) H43- O47	771. RY*(5)Ru52	0.28	7.51	0.041
72. BD (1) H43- O47	772. RY*(6)Ru52	0.65	5.02	0.051
72. BD (1) H43- O47	773. RY*(7)Ru52	0.62	8.86	0.066
72. BD (1) H43- O47	774. RY*(8)Ru52	0.11	4.26	0.019
72. BD (1) H43- O47	775. RY*(9)Ru52	0.67	10.64	0.076

72. BD (1) H43- O47	776. RY*(10)Ru52	0.19	8.98	0.037
72. BD (1) H43- O47	778. RY*(12)Ru52	0.35	6.53	0.043
72. BD (1) H43- O47	779. RY*(13)Ru52	0.31	15.36	0.061
72. BD (1) H43- O47	780. RY*(14)Ru52	0.30	9.42	0.048
72. BD (1) H43- O47	781. RY*(15)Ru52	0.16	8.17	0.033
72. BD (1) H43- O47	783. RY*(17)Ru52	0.47	13.10	0.070
72. BD (1) H43- O47	785. RY*(19)Ru52	0.67	7.74	0.065
72. BD (1) H43- O47	787. RY*(21)Ru52	0.21	13.11	0.047
72. BD (1) H43- O47	789. RY*(23)Ru52	0.80	11.06	0.084
72. BD (1) H43- O47	790. RY*(24)Ru52	0.49	13605.56	2.313
72. BD (1) H43- O47	791. RY*(25)Ru52	0.26	33395.00	2.660
72. BD (1) H43- O47	792. RY*(26)Ru52	0.58	1160.02	0.731
72. BD (1) H43- O47	793. RY*(27)Ru52	0.29	50.90	0.108
72. BD (1) H43- O47	794. RY*(28)Ru52	0.19	186.76	0.169
72. BD (1) H43- O47	795. RY*(29)Ru52	0.54	53.56	0.152
72. BD (1) H43- O47	796. RY*(30)Ru52	0.32	19.22	0.071
72. BD (1) H43- O47	799. RY*(33)Ru52	0.10	88.83	0.085
72. BD (1) H43- O47	804. RY*(38)Ru52	0.65	258.93	0.366
72. BD (1) H43- O47	875. BD*(1) C 4-Ru52	6.36	0.73	0.066
72. BD (1) H43- O47	879. BD*(3) C10- O48	0.07	1.20	0.008
72. BD (1) H43- O47	896. BD*(2) C11- C15	0.17	0.65	0.010
102. CR (1) O47	875. BD*(1) C 4-Ru52	5.17	18.70	0.301
151. LP (1) O47	188. RY*(6) C 2	0.17	3.42	0.022
151. LP (1) O47	189. RY*(7) C 2	0.05	9.90	0.021
151. LP (1) O47	213. RY*(1) C 4	0.06	2.19	0.010
151. LP (1) O47	219. RY*(7) C 4	0.10	7.03	0.024
151. LP (1) O47	260. RY*(3) C 7	0.06	2.31	0.010
151. LP (1) O47	263. RY*(6) C 7	0.06	4.60	0.015
151. LP (1) O47	290. RY*(3) C 9	0.06	2.17	0.010
151. LP (1) O47	292. RY*(5) C 9	0.07	3.58	0.014
151. LP (1) O47	293. RY*(6) C 9	0.06	3.13	0.013
151. LP (1) O47	303. RY*(1) C10	0.08	2.31	0.012
151. LP (1) O47	309. RY*(7) C10	0.11	6.82	0.024
151. LP (1) O47	310. RY*(8) C10	0.11	3.69	0.019
151. LP (1) O47	311. RY*(9) C10	0.08	4.94	0.018
151. LP (1) O47	313. RY*(11) C10	0.07	2.45	0.012
151. LP (1) O47	318. RY*(1) C11	0.08	1.44	0.009
151. LP (1) O47	321. RY*(4) C11	0.12	2.65	0.016
151. LP (1) O47	326. RY*(9) C11	0.06	13.18	0.024
151. LP (1) O47	383. RY*(6) C15	0.08	3.63	0.015
151. LP (1) O47	646. RY*(4) O44	0.09	1.13	0.009
151. LP (1) O47	648. RY*(6) O44	0.07	2.88	0.013
151. LP (1) O47	706. RY*(4) O48	0.06	1.03	0.007
151. LP (1) O47	767. RY*(1)Ru52	0.39	7.18	0.047
151. LP (1) O47	768. RY*(2)Ru52	0.17	3.91	0.023
151. LP (1) O47	770. RY*(4)Ru52	0.11	2.68	0.016
151. LP (1) O47	773. RY*(7)Ru52	0.98	8.61	0.083
151. LP (1) O47	774. RY*(8)Ru52	0.10	4.01	0.018
151. LP (1) O47	775. RY*(9)Ru52	0.93	10.39	0.088
151. LP (1) O47	776. RY*(10)Ru52	0.67	8.73	0.069
151. LP (1) O47	778. RY*(12)Ru52	0.30	6.28	0.039
151. LP (1) O47	779. RY*(13)Ru52	0.55	15.11	0.082
151. LP (1) O47	780. RY*(14)Ru52	1.49	9.16	0.105
151. LP (1) O47	781. RY*(15)Ru52	0.10	7.92	0.025
151. LP (1) O47	782. RY*(16)Ru52	0.07	6.77	0.019
151. LP (1) O47	783. RY*(17)Ru52	0.32	12.85	0.057
151. LP (1) O47	784. RY*(18)Ru52	0.08	6.33	0.020
151. LP (1) O47	785. RY*(19)Ru52	0.10	7.49	0.024
151. LP (1) O47	786. RY*(20)Ru52	0.23	10.62	0.044
151. LP (1) O47	787. RY*(21)Ru52	0.05	12.86	0.023
151. LP (1) O47	789. RY*(23)Ru52	0.46	10.81	0.064
151. LP (1) O47	790. RY*(24)Ru52	0.49	13605.31	2.314
151. LP (1) O47	791. RY*(25)Ru52	0.26	33394.75	2.656
151. LP (1) O47	792. RY*(26)Ru52	0.57	1159.77	0.731
151. LP (1) O47	795. RY*(29)Ru52	0.55	53.31	0.155
151. LP (1) O47	796. RY*(30)Ru52	0.39	18.97	0.078
151. LP (1) O47	797. RY*(31)Ru52	0.12	19.41	0.043
151. LP (1) O47	798. RY*(32)Ru52	0.08	54.23	0.057
151. LP (1) O47	799. RY*(33)Ru52	0.10	88.58	0.086
151. LP (1) O47	800. RY*(34)Ru52	0.12	49.94	0.071
151. LP (1) O47	801. RY*(35)Ru52	0.07	19.11	0.034
151. LP (1) O47	803. RY*(37)Ru52	0.08	186.46	0.110
151. LP (1) O47	804. RY*(38)Ru52	0.63	258.67	0.364
151. LP (1) O47	805. RY*(39)Ru52	0.15	17.65	0.046
151. LP (1) O47	806. RY*(40)Ru52	0.09	54.32	0.063
151. LP (1) O47	809. RY*(43)Ru52	0.10	18.37	0.038
151. LP (1) O47	810. RY*(44)Ru52	0.06	54.41	0.050
151. LP (1) O47	811. RY*(45)Ru52	0.14	51.07	0.077
151. LP (1) O47	812. RY*(46)Ru52	0.09	186.49	0.115
151. LP (1) O47	873. BD*(2) C 4- O44	0.23	0.36	0.008
151. LP (1) O47	875. BD*(1) C 4-Ru52	9.81	0.48	0.066
151. LP (1) O47	876. BD*(1) C10-Ru52	0.79	0.49	0.019
151. LP (1) O47	884. BD*(1) C 2- N50	0.11	0.81	0.008
151. LP (1) O47	887. BD*(2) C 7- N50	0.08	0.33	0.005
151. LP (1) O47	895. BD*(1) C11- C15	0.21	0.88	0.012
151. LP (1) O47	896. BD*(2) C11- C15	0.18	0.39	0.008
152. LP (2) O47	221. RY*(9) C 4	0.09	4.86	0.020
152. LP (2) O47	226. RY*(14) C 4	0.06	45.98	0.050
152. LP (2) O47	326. RY*(9) C11	0.06	13.37	0.026
152. LP (2) O47	332. RY*(15) C11	0.05	27.42	0.035
152. LP (2) O47	768. RY*(2)Ru52	0.09	4.10	0.018
152. LP (2) O47	769. RY*(3)Ru52	0.14	2.17	0.016
152. LP (2) O47	775. RY*(9)Ru52	0.33	10.58	0.056
152. LP (2) O47	777. RY*(11)Ru52	0.07	5.54	0.019
152. LP (2) O47	780. RY*(14)Ru52	0.17	9.35	0.038
152. LP (2) O47	783. RY*(17)Ru52	0.08	13.03	0.031
152. LP (2) O47	784. RY*(18)Ru52	0.14	6.51	0.029
152. LP (2) O47	785. RY*(19)Ru52	0.11	7.68	0.028
152. LP (2) O47	789. RY*(23)Ru52	0.06	11.00	0.025
152. LP (2) O47	805. RY*(39)Ru52	0.13	17.84	0.047
152. LP (2) O47	806. RY*(40)Ru52	0.07	54.51	0.058
152. LP (2) O47	809. RY*(43)Ru52	0.10	18.55	0.041
152. LP (2) O47	810. RY*(44)Ru52	0.06	54.60	0.053
152. LP (2) O47	872. BD*(1) C 4- O44	0.10	0.55	0.007
152. LP (2) O47	875. BD*(1) C 4-Ru52	43.98	0.67	0.156
152. LP (2) O47	876. BD*(1) C10-Ru52	0.05	0.67	0.005
152. LP (2) O47	878. BD*(2) C10- O48	0.19	0.55	0.009
152. LP (2) O47	879. BD*(3) C10- O48	0.43	1.13	0.021
152. LP (2) O47	884. BD*(1) C 2- N50	0.07	1.00	0.008
152. LP (2) O47	886. BD*(1) C 7- N50	0.10	0.98	0.009
152. LP (2) O47	887. BD*(2) C 7- N50	0.12	0.52	0.007
152. LP (2) O47	895. BD*(1) C11- C15	0.19	1.06	0.013
152. LP (2) O47	896. BD*(2) C11- C15	0.27	0.58	0.011
153. LP (3) O47	216. RY*(4) C 4	0.16	2.45	0.019
153. LP (3) O47	219. RY*(7) C 4	0.16	6.93	0.033
153. LP (3) O47	226. RY*(14) C 4	0.07	45.69	0.055

153. LP (3) O47	383. RY*(6) C15	0.06	3.52	0.014
153. LP (3) O47	743. RY*(7) N50	0.05	2.66	0.011
153. LP (3) O47	767. RY*(1)Ru52	0.31	7.07	0.046
153. LP (3) O47	768. RY*(2)Ru52	0.08	3.80	0.017
153. LP (3) O47	770. RY*(4)Ru52	0.37	2.57	0.030
153. LP (3) O47	772. RY*(6)Ru52	0.05	4.67	0.015
153. LP (3) O47	773. RY*(7)Ru52	0.58	8.50	0.068
153. LP (3) O47	775. RY*(9)Ru52	0.55	10.28	0.073
153. LP (3) O47	776. RY*(10)Ru52	0.28	8.62	0.047
153. LP (3) O47	778. RY*(12)Ru52	0.16	6.17	0.031
153. LP (3) O47	779. RY*(13)Ru52	0.19	15.00	0.052
153. LP (3) O47	780. RY*(14)Ru52	0.31	9.06	0.051
153. LP (3) O47	781. RY*(15)Ru52	0.10	7.81	0.027
153. LP (3) O47	783. RY*(17)Ru52	0.10	12.74	0.035
153. LP (3) O47	785. RY*(19)Ru52	0.09	7.39	0.025
153. LP (3) O47	786. RY*(20)Ru52	0.07	10.52	0.026
153. LP (3) O47	788. RY*(22)Ru52	0.06	10.00	0.023
153. LP (3) O47	789. RY*(23)Ru52	0.20	10.71	0.045
153. LP (3) O47	790. RY*(24)Ru52	0.22	13605.21	1.678
153. LP (3) O47	791. RY*(25)Ru52	0.13	33394.64	2.010
153. LP (3) O47	792. RY*(26)Ru52	0.27	1159.66	0.545
153. LP (3) O47	795. RY*(29)Ru52	0.28	53.20	0.118
153. LP (3) O47	796. RY*(30)Ru52	0.24	18.86	0.066
153. LP (3) O47	804. RY*(38)Ru52	0.31	258.57	0.273
153. LP (3) O47	874. BD*(3) C 4- O44	0.10	0.87	0.009
153. LP (3) O47	875. BD*(1) C 4-Ru52	26.41	0.37	0.089
153. LP (3) O47	877. BD*(1) C10- O48	0.11	0.28	0.005
153. LP (3) O47	879. BD*(3) C10- O48	0.52	0.84	0.020
153. LP (3) O47	884. BD*(1) C 2- N50	0.16	0.71	0.010
153. LP (3) O47	887. BD*(2) C 7- N50	0.11	0.23	0.005
153. LP (3) O47	894. BD*(1) C11-Ru52	1.11	0.28	0.016
153. LP (3) O47	895. BD*(1) C11- C15	0.21	0.77	0.012
153. LP (3) O47	896. BD*(2) C11- C15	0.82	0.29	0.014
from unit 3 to unit 2				
72. BD (1) H43- O47	167. LP*(1) C16	0.35	0.53	0.016
72. BD (1) H43- O47	243. RY*(1) C 6	0.11	2.46	0.014
72. BD (1) H43- O47	245. RY*(3) C 6	0.16	3.23	0.020
72. BD (1) H43- O47	249. RY*(7) C 6	0.29	7.55	0.042
72. BD (1) H43- O47	273. RY*(1) C 8	0.16	2.36	0.017
72. BD (1) H43- O47	274. RY*(2) C 8	0.05	1.73	0.009
72. BD (1) H43- O47	279. RY*(7) C 8	0.17	7.21	0.031
72. BD (1) H43- O47	338. RY*(6) C12	0.09	3.49	0.016
72. BD (1) H43- O47	393. RY*(1) C16	0.31	1.67	0.020
72. BD (1) H43- O47	395. RY*(3) C16	0.09	1.63	0.011
72. BD (1) H43- O47	396. RY*(4) C16	0.11	2.80	0.016
72. BD (1) H43- O47	398. RY*(6) C16	0.07	3.25	0.014
72. BD (1) H43- O47	399. RY*(7) C16	0.07	5.22	0.017
72. BD (1) H43- O47	403. RY*(11) C16	0.07	3.69	0.014
72. BD (1) H43- O47	423. RY*(1) C18	0.05	2.26	0.010
72. BD (1) H43- O47	424. RY*(2) C18	0.05	1.11	0.007
72. BD (1) H43- O47	428. RY*(6) C18	0.14	3.62	0.020
72. BD (1) H43- O47	429. RY*(7) C18	0.06	8.56	0.021
72. BD (1) H43- O47	458. RY*(6) C20	0.07	3.49	0.014
72. BD (1) H43- O47	459. RY*(7) C20	0.10	3.72	0.017
72. BD (1) H43- O47	465. RY*(13) C20	0.05	24.05	0.032
72. BD (1) H43- O47	483. RY*(1) C22	0.10	1.97	0.013
72. BD (1) H43- O47	486. RY*(4) C22	0.11	1.77	0.013
72. BD (1) H43- O47	487. RY*(5) C22	0.08	4.59	0.017
72. BD (1) H43- O47	570. RY*(3) H29	0.05	1.77	0.008
72. BD (1) H43- O47	676. RY*(4) O46	0.05	1.34	0.007
72. BD (1) H43- O47	679. RY*(7) O46	0.07	2.67	0.013
72. BD (1) H43- O47	753. RY*(2) N51	0.12	1.48	0.012
72. BD (1) H43- O47	755. RY*(4) N51	0.16	5.56	0.027
72. BD (1) H43- O47	759. RY*(8) N51	0.05	14.62	0.024
72. BD (1) H43- O47	815. RY*(1)Ru53	0.43	7.59	0.051
72. BD (1) H43- O47	816. RY*(2)Ru53	0.31	2.46	0.025
72. BD (1) H43- O47	817. RY*(3)Ru53	1.64	1.75	0.048
72. BD (1) H43- O47	818. RY*(4)Ru53	0.23	2.84	0.023
72. BD (1) H43- O47	819. RY*(5)Ru53	0.38	7.05	0.047
72. BD (1) H43- O47	820. RY*(6)Ru53	0.05	4.14	0.013
72. BD (1) H43- O47	821. RY*(7)Ru53	0.29	3.65	0.029
72. BD (1) H43- O47	822. RY*(8)Ru53	0.96	5.24	0.063
72. BD (1) H43- O47	823. RY*(9)Ru53	1.03	9.71	0.089
72. BD (1) H43- O47	824. RY*(10)Ru53	0.10	7.67	0.025
72. BD (1) H43- O47	825. RY*(11)Ru53	0.13	6.61	0.027
72. BD (1) H43- O47	826. RY*(12)Ru53	0.40	3.52	0.033
72. BD (1) H43- O47	827. RY*(13)Ru53	0.79	14.37	0.095
72. BD (1) H43- O47	829. RY*(15)Ru53	0.09	7.75	0.024
72. BD (1) H43- O47	830. RY*(16)Ru53	0.22	7.06	0.036
72. BD (1) H43- O47	831. RY*(17)Ru53	0.65	13.05	0.082
72. BD (1) H43- O47	832. RY*(18)Ru53	0.39	5.84	0.043
72. BD (1) H43- O47	833. RY*(19)Ru53	0.13	7.61	0.028
72. BD (1) H43- O47	834. RY*(20)Ru53	0.23	12.02	0.047
72. BD (1) H43- O47	835. RY*(21)Ru53	0.12	12.94	0.036
72. BD (1) H43- O47	836. RY*(22)Ru53	0.71	11.19	0.080
72. BD (1) H43- O47	838. RY*(24)Ru53	0.59	35647.44	4.090
72. BD (1) H43- O47	839. RY*(25)Ru53	0.67	5348.49	1.694
72. BD (1) H43- O47	840. RY*(26)Ru53	1.14	5744.11	2.292
72. BD (1) H43- O47	841. RY*(27)Ru53	0.31	49.90	0.111
72. BD (1) H43- O47	842. RY*(28)Ru53	0.20	186.73	0.173
72. BD (1) H43- O47	843. RY*(29)Ru53	0.20	10.75	0.042
72. BD (1) H43- O47	844. RY*(30)Ru53	0.65	33.04	0.131
72. BD (1) H43- O47	847. RY*(33)Ru53	1.01	278.14	0.474
72. BD (1) H43- O47	852. RY*(38)Ru53	1.10	356.31	0.561
72. BD (1) H43- O47	855. RY*(41)Ru53	0.44	141.25	0.223
72. BD (1) H43- O47	856. RY*(42)Ru53	0.94	3163.06	1.541
72. BD (1) H43- O47	906. BD*(1) C 6-Ru53	0.17	0.74	0.011
72. BD (1) H43- O47	907. BD*(1) C 8-Ru53	6.11	0.74	0.065
72. BD (1) H43- O47	928. BD*(1) C16- C18	0.05	1.13	0.007
102. CR (1) O47	907. BD*(1) C 8-Ru53	5.19	18.71	0.301
151. LP (1) O47	167. LP*(1) C16	0.17	0.28	0.008
151. LP (1) O47	243. RY*(1) C 6	0.05	2.21	0.010
151. LP (1) O47	244. RY*(2) C 6	0.06	1.39	0.008
151. LP (1) O47	245. RY*(3) C 6	0.09	2.98	0.014
151. LP (1) O47	396. RY*(4) C16	0.06	2.55	0.011
151. LP (1) O47	401. RY*(9) C16	0.06	13.26	0.025
151. LP (1) O47	815. RY*(1)Ru53	0.18	7.34	0.033
151. LP (1) O47	816. RY*(2)Ru53	0.35	2.21	0.025
151. LP (1) O47	819. RY*(5)Ru53	0.23	6.80	0.036
151. LP (1) O47	820. RY*(6)Ru53	0.38	3.89	0.035
151. LP (1) O47	822. RY*(8)Ru53	0.07	4.99	0.017
151. LP (1) O47	823. RY*(9)Ru53	0.28	9.45	0.046
151. LP (1) O47	824. RY*(10)Ru53	0.14	7.42	0.029
151. LP (1) O47	825. RY*(11)Ru53	0.07	6.36	0.018
151. LP (1) O47	827. RY*(13)Ru53	0.07	14.12	0.029

151. LP (1) O47	828. RY*(14)Ru53	0.33	9.02	0.049
151. LP (1) O47	831. RY*(17)Ru53	0.19	12.80	0.045
151. LP (1) O47	832. RY*(18)Ru53	0.18	5.59	0.029
151. LP (1) O47	833. RY*(19)Ru53	0.37	7.36	0.047
151. LP (1) O47	834. RY*(20)Ru53	0.18	11.77	0.041
151. LP (1) O47	836. RY*(22)Ru53	0.19	10.94	0.041
151. LP (1) O47	838. RY*(24)Ru53	0.18	35647.19	2.264
151. LP (1) O47	839. RY*(25)Ru53	0.20	5348.23	0.932
151. LP (1) O47	840. RY*(26)Ru53	0.34	5743.86	1.257
151. LP (1) O47	843. RY*(29)Ru53	0.05	10.50	0.021
151. LP (1) O47	844. RY*(30)Ru53	0.17	32.79	0.067
151. LP (1) O47	845. RY*(31)Ru53	0.17	18.43	0.050
151. LP (1) O47	846. RY*(32)Ru53	0.12	54.21	0.072
151. LP (1) O47	847. RY*(33)Ru53	0.28	277.89	0.251
151. LP (1) O47	848. RY*(34)Ru53	0.15	51.29	0.078
151. LP (1) O47	851. RY*(37)Ru53	0.09	186.63	0.119
151. LP (1) O47	852. RY*(38)Ru53	0.32	356.05	0.305
151. LP (1) O47	855. RY*(41)Ru53	0.14	141.00	0.124
151. LP (1) O47	856. RY*(42)Ru53	0.29	3162.81	0.856
151. LP (1) O47	904. BD*(2) C 6- O45	0.10	0.37	0.006
151. LP (1) O47	905. BD*(3) C 6- O45	0.15	0.95	0.011
151. LP (1) O47	907. BD*(1) C 8-Ru53	9.45	0.48	0.065
151. LP (1) O47	908. BD*(1) C 8- O46	0.07	0.36	0.005
151. LP (1) O47	909. BD*(2) C 8- O46	0.14	0.36	0.007
151. LP (1) O47	927. BD*(1) C16- C22	0.13	0.86	0.009
152. LP (2) O47	167. LP*(1) C16	0.54	0.47	0.017
152. LP (2) O47	281. RY*(9) C 8	0.12	4.93	0.023
152. LP (2) O47	286. RY*(14) C 8	0.07	46.13	0.053
152. LP (2) O47	818. RY*(4)Ru53	0.07	2.77	0.013
152. LP (2) O47	823. RY*(9)Ru53	0.16	9.64	0.038
152. LP (2) O47	825. RY*(11)Ru53	0.14	6.55	0.029
152. LP (2) O47	828. RY*(14)Ru53	0.24	9.20	0.045
152. LP (2) O47	831. RY*(17)Ru53	0.06	12.98	0.027
152. LP (2) O47	832. RY*(18)Ru53	0.06	5.78	0.017
152. LP (2) O47	845. RY*(31)Ru53	0.11	18.62	0.044
152. LP (2) O47	846. RY*(32)Ru53	0.07	54.40	0.059
152. LP (2) O47	857. RY*(43)Ru53	0.07	19.48	0.036
152. LP (2) O47	904. BD*(2) C 6- O45	0.21	0.56	0.010
152. LP (2) O47	905. BD*(3) C 6- O45	0.45	1.14	0.021
152. LP (2) O47	906. BD*(1) C 6-Ru53	0.08	0.67	0.007
152. LP (2) O47	907. BD*(1) C 8-Ru53	47.32	0.67	0.162
152. LP (2) O47	908. BD*(1) C 8- O46	0.09	0.55	0.006
152. LP (2) O47	913. BD*(1) C12- N51	0.09	0.99	0.009
152. LP (2) O47	921. BD*(1) C20- N51	0.12	0.98	0.010
152. LP (2) O47	922. BD*(2) C20- N51	0.09	0.51	0.007
152. LP (2) O47	927. BD*(1) C16- C22	0.05	1.05	0.007
152. LP (2) O47	928. BD*(1) C16- C18	0.20	1.06	0.014
153. LP (3) O47	167. LP*(1) C16	1.34	0.18	0.016
153. LP (3) O47	276. RY*(4) C 8	0.12	2.49	0.017
153. LP (3) O47	279. RY*(7) C 8	0.10	6.85	0.025
153. LP (3) O47	286. RY*(14) C 8	0.08	45.84	0.060
153. LP (3) O47	287. RY*(15) C 8	0.06	26.79	0.038
153. LP (3) O47	815. RY*(1)Ru53	0.13	7.23	0.030
153. LP (3) O47	816. RY*(2)Ru53	0.12	2.10	0.016
153. LP (3) O47	819. RY*(5)Ru53	0.14	6.69	0.030
153. LP (3) O47	820. RY*(6)Ru53	0.35	3.78	0.035
153. LP (3) O47	821. RY*(7)Ru53	0.07	3.29	0.014
153. LP (3) O47	823. RY*(9)Ru53	0.22	9.35	0.044
153. LP (3) O47	824. RY*(10)Ru53	0.19	7.31	0.036
153. LP (3) O47	828. RY*(14)Ru53	0.06	8.91	0.022
153. LP (3) O47	829. RY*(15)Ru53	0.06	7.39	0.020
153. LP (3) O47	832. RY*(18)Ru53	0.06	5.48	0.018
153. LP (3) O47	833. RY*(19)Ru53	0.06	7.25	0.020
153. LP (3) O47	836. RY*(22)Ru53	0.09	10.84	0.031
153. LP (3) O47	837. RY*(23)Ru53	0.07	8.80	0.024
153. LP (3) O47	838. RY*(24)Ru53	0.10	35647.08	1.841
153. LP (3) O47	839. RY*(25)Ru53	0.09	5348.13	0.665
153. LP (3) O47	840. RY*(26)Ru53	0.18	5743.75	0.999
153. LP (3) O47	844. RY*(30)Ru53	0.06	32.68	0.042
153. LP (3) O47	847. RY*(33)Ru53	0.13	277.78	0.187
153. LP (3) O47	848. RY*(34)Ru53	0.09	51.19	0.065
153. LP (3) O47	851. RY*(37)Ru53	0.06	186.53	0.099
153. LP (3) O47	852. RY*(38)Ru53	0.16	355.95	0.234
153. LP (3) O47	855. RY*(41)Ru53	0.08	140.90	0.101
153. LP (3) O47	856. RY*(42)Ru53	0.15	3162.71	0.662
153. LP (3) O47	903. BD*(1) C 6- O45	0.07	0.27	0.004
153. LP (3) O47	904. BD*(2) C 6- O45	0.09	0.27	0.004
153. LP (3) O47	905. BD*(3) C 6- O45	0.48	0.85	0.019
153. LP (3) O47	907. BD*(1) C 8-Ru53	21.15	0.38	0.080
153. LP (3) O47	908. BD*(1) C 8- O46	0.07	0.26	0.004
153. LP (3) O47	910. BD*(3) C 8- O46	0.09	0.87	0.008
153. LP (3) O47	913. BD*(1) C12- N51	0.13	0.70	0.009
153. LP (3) O47	922. BD*(2) C20- N51	0.05	0.22	0.003
153. LP (3) O47	926. BD*(1) C16-Ru53	1.18	0.27	0.016
153. LP (3) O47	928. BD*(1) C16- C18	0.15	0.77	0.010
within unit 3				
152. LP (2) O47	640. RY*(3) H43	0.58	2.53	0.036
153. LP (3) O47	641. RY*(4) H43	0.74	2.41	0.041
from unit 3 to unit 4				
72. BD (1) H43- O47	719. RY*(2)C149	0.42	2.41	0.028
72. BD (1) H43- O47	721. RY*(4)C149	0.48	3.21	0.035
72. BD (1) H43- O47	722. RY*(5)C149	0.62	2.92	0.038
72. BD (1) H43- O47	723. RY*(6)C149	0.12	3.66	0.018
72. BD (1) H43- O47	725. RY*(8)C149	0.20	5.87	0.031
151. LP (1) O47	719. RY*(2)C149	0.34	2.15	0.024
151. LP (1) O47	720. RY*(3)C149	0.07	2.26	0.011
151. LP (1) O47	721. RY*(4)C149	0.42	2.96	0.032
151. LP (1) O47	722. RY*(5)C149	0.58	2.67	0.035
151. LP (1) O47	723. RY*(6)C149	0.13	3.41	0.019
151. LP (1) O47	725. RY*(8)C149	0.12	5.62	0.023
153. LP (3) O47	720. RY*(3)C149	0.14	2.15	0.017
from unit 4 to unit 1				
104. CR (1)C149	894. BD*(1) C11-Ru52	0.47	100.11	0.211
105. CR (2)C149	767. RY*(1)Ru52	0.05	17.03	0.026
105. CR (2)C149	894. BD*(1) C11-Ru52	3.75	10.24	0.189
106. CR (3)C149	894. BD*(1) C11-Ru52	0.08	6.95	0.023
107. CR (4)C149	894. BD*(1) C11-Ru52	0.19	6.95	0.035
108. CR (5)C149	894. BD*(1) C11-Ru52	0.08	6.95	0.022
155. LP (1)C149	767. RY*(1)Ru52	0.25	7.53	0.039
155. LP (1)C149	768. RY*(2)Ru52	0.09	4.26	0.018
155. LP (1)C149	771. RY*(5)Ru52	0.05	7.61	0.018
155. LP (1)C149	773. RY*(7)Ru52	0.11	8.96	0.028
155. LP (1)C149	776. RY*(10)Ru52	0.05	9.08	0.020

155. LP (1)Cl49	779. RY*(13)Ru52	0.16	15.46	0.044
155. LP (1)Cl49	781. RY*(15)Ru52	0.20	8.27	0.036
155. LP (1)Cl49	782. RY*(16)Ru52	0.20	7.12	0.034
155. LP (1)Cl49	789. RY*(23)Ru52	0.15	11.16	0.037
155. LP (1)Cl49	790. RY*(24)Ru52	0.09	13605.66	1.007
155. LP (1)Cl49	792. RY*(26)Ru52	0.10	1160.12	0.311
155. LP (1)Cl49	795. RY*(29)Ru52	0.11	53.66	0.070
155. LP (1)Cl49	796. RY*(30)Ru52	0.07	19.32	0.033
155. LP (1)Cl49	801. RY*(35)Ru52	0.05	19.47	0.028
155. LP (1)Cl49	804. RY*(38)Ru52	0.12	259.03	0.157
155. LP (1)Cl49	872. BD*(1) C 4- O44	0.08	0.72	0.007
155. LP (1)Cl49	877. BD*(1) C10- O48	0.09	0.74	0.008
155. LP (1)Cl49	881. BD*(1) C 1- C 2	0.12	1.19	0.011
155. LP (1)Cl49	886. BD*(1) C 7- N50	0.07	1.15	0.008
155. LP (1)Cl49	894. BD*(1) C11-Ru52	8.71	0.73	0.077
156. LP (2)Cl49	558. RY*(1) H27	0.13	1.71	0.014
156. LP (2)Cl49	767. RY*(1)Ru52	0.05	7.04	0.017
156. LP (2)Cl49	768. RY*(2)Ru52	0.10	3.78	0.018
156. LP (2)Cl49	771. RY*(5)Ru52	0.06	7.13	0.019
156. LP (2)Cl49	781. RY*(15)Ru52	0.14	7.78	0.029
156. LP (2)Cl49	782. RY*(16)Ru52	0.11	6.64	0.024
156. LP (2)Cl49	792. RY*(26)Ru52	0.06	1159.64	0.229
156. LP (2)Cl49	795. RY*(29)Ru52	0.06	53.18	0.051
156. LP (2)Cl49	796. RY*(30)Ru52	0.05	18.84	0.028
156. LP (2)Cl49	804. RY*(38)Ru52	0.06	258.54	0.114
156. LP (2)Cl49	873. BD*(2) C 4- O44	0.06	0.23	0.004
156. LP (2)Cl49	876. BD*(1) C10-Ru52	0.23	0.36	0.009
156. LP (2)Cl49	881. BD*(1) C 1- C 2	0.26	0.71	0.012
156. LP (2)Cl49	882. BD*(2) C 1- C 2	0.06	0.22	0.003
156. LP (2)Cl49	885. BD*(1) C 2- H27	1.78	0.61	0.030
156. LP (2)Cl49	886. BD*(1) C 7- N50	0.14	0.66	0.009
157. LP (3)Cl49	176. RY*(9) C 1	0.11	3.49	0.019
157. LP (3)Cl49	185. RY*(3) C 2	0.08	2.08	0.013
157. LP (3)Cl49	188. RY*(6) C 2	0.43	3.29	0.036
157. LP (3)Cl49	189. RY*(7) C 2	0.25	9.77	0.047
157. LP (3)Cl49	190. RY*(8) C 2	0.11	3.70	0.019
157. LP (3)Cl49	213. RY*(1) C 4	0.91	2.06	0.041
157. LP (3)Cl49	215. RY*(3) C 4	0.11	2.07	0.014
157. LP (3)Cl49	216. RY*(4) C 4	0.24	2.42	0.023
157. LP (3)Cl49	218. RY*(6) C 4	0.10	2.35	0.014
157. LP (3)Cl49	219. RY*(7) C 4	1.19	6.90	0.086
157. LP (3)Cl49	224. RY*(12) C 4	0.06	3.01	0.013
157. LP (3)Cl49	258. RY*(1) C 7	0.12	1.77	0.014
157. LP (3)Cl49	263. RY*(6) C 7	0.28	4.47	0.034
157. LP (3)Cl49	288. RY*(1) C 9	0.08	1.62	0.011
157. LP (3)Cl49	290. RY*(3) C 9	0.20	2.04	0.019
157. LP (3)Cl49	292. RY*(5) C 9	0.36	3.45	0.033
157. LP (3)Cl49	293. RY*(6) C 9	0.21	3.00	0.024
157. LP (3)Cl49	303. RY*(1) C10	0.45	2.18	0.030
157. LP (3)Cl49	306. RY*(4) C10	0.07	1.70	0.010
157. LP (3)Cl49	309. RY*(7) C10	0.22	6.68	0.036
157. LP (3)Cl49	310. RY*(8) C10	0.47	3.56	0.039
157. LP (3)Cl49	314. RY*(12) C10	0.13	2.91	0.019
157. LP (3)Cl49	318. RY*(1) C11	0.18	1.31	0.015
157. LP (3)Cl49	321. RY*(4) C11	0.58	2.52	0.036
157. LP (3)Cl49	323. RY*(6) C11	0.16	2.51	0.019
157. LP (3)Cl49	324. RY*(7) C11	0.23	4.67	0.031
157. LP (3)Cl49	326. RY*(9) C11	0.47	13.05	0.075
157. LP (3)Cl49	328. RY*(11) C11	0.08	3.36	0.015
157. LP (3)Cl49	329. RY*(12) C11	0.08	3.31	0.015
157. LP (3)Cl49	330. RY*(13) C11	0.08	3.56	0.016
157. LP (3)Cl49	331. RY*(14) C11	0.10	40.38	0.059
157. LP (3)Cl49	332. RY*(15) C11	0.23	27.10	0.076
157. LP (3)Cl49	378. RY*(1) C15	0.05	1.88	0.009
157. LP (3)Cl49	380. RY*(3) C15	0.11	1.98	0.014
157. LP (3)Cl49	381. RY*(4) C15	0.10	1.26	0.010
157. LP (3)Cl49	383. RY*(6) C15	0.95	3.50	0.055
157. LP (3)Cl49	384. RY*(7) C15	0.16	8.23	0.034
157. LP (3)Cl49	417. RY*(10) C17	0.05	4.02	0.014
157. LP (3)Cl49	558. RY*(1) H27	0.06	1.71	0.010
157. LP (3)Cl49	560. RY*(3) H27	0.16	1.35	0.014
157. LP (3)Cl49	561. RY*(4) H27	0.18	2.14	0.018
157. LP (3)Cl49	562. RY*(5) H27	0.06	3.70	0.014
157. LP (3)Cl49	565. RY*(3) H28	0.06	1.87	0.010
157. LP (3)Cl49	575. RY*(3) H30	0.07	2.06	0.012
157. LP (3)Cl49	592. RY*(5) H33	0.05	4.33	0.014
157. LP (3)Cl49	595. RY*(3) H34	0.13	1.63	0.014
157. LP (3)Cl49	630. RY*(3) H41	0.15	1.45	0.014
157. LP (3)Cl49	645. RY*(3) O44	0.15	1.99	0.016
157. LP (3)Cl49	646. RY*(4) O44	0.47	0.99	0.021
157. LP (3)Cl49	647. RY*(5) O44	0.12	2.13	0.015
157. LP (3)Cl49	648. RY*(6) O44	0.32	2.75	0.028
157. LP (3)Cl49	649. RY*(7) O44	0.13	1.95	0.015
157. LP (3)Cl49	653. RY*(11) O44	0.05	11.48	0.024
157. LP (3)Cl49	705. RY*(3) O48	0.13	2.25	0.016
157. LP (3)Cl49	706. RY*(4) O48	0.71	0.89	0.024
157. LP (3)Cl49	707. RY*(5) O48	0.25	2.41	0.024
157. LP (3)Cl49	709. RY*(7) O48	0.07	3.08	0.014
157. LP (3)Cl49	713. RY*(11) O48	0.06	9.60	0.023
157. LP (3)Cl49	737. RY*(1) N50	0.26	2.08	0.022
157. LP (3)Cl49	740. RY*(4) N50	0.08	5.33	0.020
157. LP (3)Cl49	745. RY*(9) N50	0.13	4.94	0.024
157. LP (3)Cl49	767. RY*(1)Ru52	5.02	7.04	0.178
157. LP (3)Cl49	768. RY*(2)Ru52	3.57	3.78	0.110
157. LP (3)Cl49	769. RY*(3)Ru52	1.37	1.85	0.048
157. LP (3)Cl49	770. RY*(4)Ru52	0.63	2.55	0.038
157. LP (3)Cl49	771. RY*(5)Ru52	2.50	7.13	0.127
157. LP (3)Cl49	773. RY*(7)Ru52	3.14	8.48	0.155
157. LP (3)Cl49	775. RY*(9)Ru52	3.55	10.26	0.181
157. LP (3)Cl49	776. RY*(10)Ru52	2.02	8.60	0.125
157. LP (3)Cl49	777. RY*(11)Ru52	0.17	5.22	0.028
157. LP (3)Cl49	778. RY*(12)Ru52	1.38	6.14	0.088
157. LP (3)Cl49	779. RY*(13)Ru52	3.09	14.98	0.204
157. LP (3)Cl49	780. RY*(14)Ru52	0.36	9.03	0.054
157. LP (3)Cl49	781. RY*(15)Ru52	1.77	7.78	0.111
157. LP (3)Cl49	782. RY*(16)Ru52	0.56	6.64	0.058
157. LP (3)Cl49	783. RY*(17)Ru52	1.90	12.71	0.148
157. LP (3)Cl49	784. RY*(18)Ru52	0.23	6.19	0.036
157. LP (3)Cl49	785. RY*(19)Ru52	0.85	7.36	0.075
157. LP (3)Cl49	786. RY*(20)Ru52	0.09	10.49	0.030
157. LP (3)Cl49	787. RY*(21)Ru52	0.49	12.73	0.075
157. LP (3)Cl49	788. RY*(22)Ru52	0.06	9.97	0.024
157. LP (3)Cl49	789. RY*(23)Ru52	4.07	10.68	0.198
157. LP (3)Cl49	790. RY*(24)Ru52	3.04	13605.18	6.108
157. LP (3)Cl49	791. RY*(25)Ru52	1.66	33394.62	7.080
157. LP (3)Cl49	792. RY*(26)Ru52	3.63	1159.64	1.948

157. LP (3)C149	793. RY*(27)Ru52	0.11	50.52	0.071
157. LP (3)C149	794. RY*(28)Ru52	0.06	186.38	0.103
157. LP (3)C149	795. RY*(29)Ru52	3.83	53.18	0.429
157. LP (3)C149	796. RY*(30)Ru52	3.09	18.84	0.229
157. LP (3)C149	799. RY*(33)Ru52	0.64	88.45	0.226
157. LP (3)C149	801. RY*(35)Ru52	0.07	18.98	0.035
157. LP (3)C149	802. RY*(36)Ru52	0.06	54.13	0.053
157. LP (3)C149	804. RY*(38)Ru52	4.07	258.54	0.975
157. LP (3)C149	806. RY*(40)Ru52	0.06	54.19	0.052
157. LP (3)C149	807. RY*(41)Ru52	0.29	81.24	0.146
157. LP (3)C149	808. RY*(42)Ru52	0.10	2110.88	0.438
157. LP (3)C149	872. BD*(1) C 4- O44	0.81	0.23	0.012
157. LP (3)C149	874. BD*(3) C 4- O44	0.50	0.85	0.020
157. LP (3)C149	876. BD*(1) C10-Ru52	0.50	0.36	0.012
157. LP (3)C149	877. BD*(1) C10- O48	0.59	0.26	0.011
157. LP (3)C149	879. BD*(3) C10- O48	0.40	0.81	0.017
157. LP (3)C149	885. BD*(1) C 2- H27	0.07	0.61	0.006
157. LP (3)C149	886. BD*(1) C 7- N50	0.18	0.66	0.010
157. LP (3)C149	894. BD*(1) C11-Ru52	26.88	0.25	0.075
157. LP (3)C149	895. BD*(1) C11- C15	0.06	0.75	0.006
158. LP (4)C149	326. RY*(9) C11	0.07	13.21	0.029
158. LP (4)C149	331. RY*(14) C11	0.05	40.54	0.045
158. LP (4)C149	332. RY*(15) C11	0.07	27.26	0.041
158. LP (4)C149	767. RY*(1)Ru52	0.31	7.21	0.045
158. LP (4)C149	778. RY*(12)Ru52	0.10	6.31	0.024
158. LP (4)C149	781. RY*(15)Ru52	0.27	7.95	0.045
158. LP (4)C149	782. RY*(16)Ru52	0.19	6.80	0.035
158. LP (4)C149	783. RY*(17)Ru52	0.10	12.88	0.034
158. LP (4)C149	789. RY*(23)Ru52	0.07	10.84	0.026
158. LP (4)C149	796. RY*(30)Ru52	0.05	19.00	0.030
158. LP (4)C149	797. RY*(31)Ru52	0.13	19.44	0.048
158. LP (4)C149	798. RY*(32)Ru52	0.07	54.26	0.060
158. LP (4)C149	805. RY*(39)Ru52	0.06	17.68	0.032
158. LP (4)C149	872. BD*(1) C 4- O44	0.29	0.40	0.010
158. LP (4)C149	874. BD*(3) C 4- O44	0.14	1.01	0.011
158. LP (4)C149	875. BD*(1) C 4-Ru52	0.98	0.51	0.020
158. LP (4)C149	876. BD*(1) C10-Ru52	0.22	0.52	0.010
158. LP (4)C149	877. BD*(1) C10- O48	0.25	0.42	0.009
158. LP (4)C149	878. BD*(2) C10- O48	0.24	0.40	0.009
158. LP (4)C149	879. BD*(3) C10- O48	0.27	0.98	0.016
158. LP (4)C149	881. BD*(1) C 1- C 2	0.07	0.87	0.007
158. LP (4)C149	886. BD*(1) C 7- N50	0.24	0.83	0.013
158. LP (4)C149	894. BD*(1) C11-Ru52	27.58	0.41	0.096
158. LP (4)C149	895. BD*(1) C11- C15	0.06	0.91	0.007
158. LP (4)C149	896. BD*(2) C11- C15	0.09	0.42	0.006

from unit 4 to unit 2

104. CR (1)C149	926. BD*(1) C16-Ru53	0.49	100.11	0.214
105. CR (2)C149	926. BD*(1) C16-Ru53	3.87	10.23	0.193
107. CR (4)C149	926. BD*(1) C16-Ru53	0.20	6.94	0.036
108. CR (5)C149	926. BD*(1) C16-Ru53	0.16	6.94	0.032
155. LP (1)C149	815. RY*(1)Ru53	0.18	7.69	0.033
155. LP (1)C149	822. RY*(8)Ru53	0.06	5.34	0.016
155. LP (1)C149	828. RY*(14)Ru53	0.11	9.37	0.028
155. LP (1)C149	829. RY*(15)Ru53	0.16	7.85	0.031
155. LP (1)C149	830. RY*(16)Ru53	0.15	7.16	0.030
155. LP (1)C149	836. RY*(22)Ru53	0.07	11.29	0.025
155. LP (1)C149	838. RY*(24)Ru53	0.06	35647.54	1.287
155. LP (1)C149	839. RY*(25)Ru53	0.07	5348.59	0.528
155. LP (1)C149	840. RY*(26)Ru53	0.11	5744.21	0.709
155. LP (1)C149	844. RY*(30)Ru53	0.05	33.14	0.038
155. LP (1)C149	847. RY*(33)Ru53	0.09	278.24	0.140
155. LP (1)C149	852. RY*(38)Ru53	0.10	356.41	0.171
155. LP (1)C149	853. RY*(39)Ru53	0.06	18.63	0.031
155. LP (1)C149	856. RY*(42)Ru53	0.09	3163.16	0.489
155. LP (1)C149	903. BD*(1) C 6- O45	0.11	0.73	0.009
155. LP (1)C149	908. BD*(1) C 8- O46	0.06	0.72	0.006
155. LP (1)C149	911. BD*(1) C12- C14	0.11	1.19	0.010
155. LP (1)C149	921. BD*(1) C20- N51	0.06	1.14	0.008
155. LP (1)C149	926. BD*(1) C16-Ru53	8.91	0.73	0.078
156. LP (2)C149	568. RY*(1) H29	0.12	1.76	0.013
156. LP (2)C149	816. RY*(2)Ru53	0.09	2.08	0.012
156. LP (2)C149	829. RY*(15)Ru53	0.15	7.37	0.029
156. LP (2)C149	830. RY*(16)Ru53	0.08	6.67	0.021
156. LP (2)C149	906. BD*(1) C 6-Ru53	0.25	0.36	0.009
156. LP (2)C149	911. BD*(1) C12- C14	0.28	0.70	0.012
156. LP (2)C149	914. BD*(1) C12- H29	1.90	0.61	0.030
156. LP (2)C149	921. BD*(1) C20- N51	0.15	0.66	0.009
157. LP (3)C149	243. RY*(1) C 6	0.15	2.08	0.017
157. LP (3)C149	249. RY*(7) C 6	0.09	7.17	0.024
157. LP (3)C149	250. RY*(8) C 6	0.12	3.24	0.019
157. LP (3)C149	252. RY*(10) C 6	0.06	2.20	0.011
157. LP (3)C149	254. RY*(12) C 6	0.08	2.78	0.014
157. LP (3)C149	273. RY*(1) C 8	0.40	1.98	0.027
157. LP (3)C149	275. RY*(3) C 8	0.07	2.02	0.011
157. LP (3)C149	276. RY*(4) C 8	0.17	2.46	0.020
157. LP (3)C149	278. RY*(6) C 8	0.09	2.29	0.014
157. LP (3)C149	279. RY*(7) C 8	0.57	6.83	0.059
157. LP (3)C149	340. RY*(8) C12	0.14	9.72	0.035
157. LP (3)C149	364. RY*(2) C14	0.08	0.80	0.007
157. LP (3)C149	371. RY*(9) C14	0.05	3.37	0.013
157. LP (3)C149	396. RY*(4) C16	0.22	2.41	0.022
157. LP (3)C149	397. RY*(5) C16	0.10	2.75	0.016
157. LP (3)C149	398. RY*(6) C16	0.05	2.87	0.012
157. LP (3)C149	399. RY*(7) C16	0.15	4.84	0.025
157. LP (3)C149	401. RY*(9) C16	0.23	13.13	0.053
157. LP (3)C149	403. RY*(11) C16	0.05	3.31	0.013
157. LP (3)C149	406. RY*(14) C16	0.13	26.48	0.057
157. LP (3)C149	407. RY*(15) C16	0.07	40.26	0.049
157. LP (3)C149	426. RY*(4) C18	0.06	1.26	0.008
157. LP (3)C149	428. RY*(6) C18	0.42	3.24	0.035
157. LP (3)C149	429. RY*(7) C18	0.07	8.18	0.023
157. LP (3)C149	453. RY*(1) C20	0.12	1.79	0.014
157. LP (3)C149	458. RY*(6) C20	0.05	3.11	0.012
157. LP (3)C149	459. RY*(7) C20	0.05	3.34	0.012
157. LP (3)C149	460. RY*(8) C20	0.06	5.49	0.018
157. LP (3)C149	485. RY*(3) C22	0.10	2.03	0.014
157. LP (3)C149	487. RY*(5) C22	0.18	4.21	0.026
157. LP (3)C149	570. RY*(3) H29	0.45	1.39	0.024
157. LP (3)C149	571. RY*(4) H29	0.10	2.09	0.014
157. LP (3)C149	610. RY*(3) H37	0.06	1.37	0.009
157. LP (3)C149	625. RY*(3) H40	0.05	1.60	0.009
157. LP (3)C149	661. RY*(4) O45	0.35	0.86	0.016
157. LP (3)C149	662. RY*(5) O45	0.16	2.42	0.018
157. LP (3)C149	675. RY*(3) O46	0.06	1.97	0.010
157. LP (3)C149	676. RY*(4) O46	0.13	0.96	0.011

157. LP (3)Cl49	679. RY*(7) O46	0.14	2.28	0.017
157. LP (3)Cl49	752. RY*(1) N51	0.13	2.04	0.015
157. LP (3)Cl49	760. RY*(9) N51	0.11	4.82	0.022
157. LP (3)Cl49	815. RY*(1)Ru53	2.52	7.21	0.128
157. LP (3)Cl49	816. RY*(2)Ru53	0.90	2.08	0.041
157. LP (3)Cl49	818. RY*(4)Ru53	0.56	2.45	0.035
157. LP (3)Cl49	819. RY*(5)Ru53	1.26	6.67	0.087
157. LP (3)Cl49	820. RY*(6)Ru53	0.13	3.76	0.021
157. LP (3)Cl49	822. RY*(8)Ru53	0.86	4.86	0.061
157. LP (3)Cl49	823. RY*(9)Ru53	2.02	9.32	0.130
157. LP (3)Cl49	824. RY*(10)Ru53	1.22	7.29	0.089
157. LP (3)Cl49	825. RY*(11)Ru53	0.50	6.23	0.053
157. LP (3)Cl49	827. RY*(13)Ru53	0.90	13.99	0.107
157. LP (3)Cl49	828. RY*(14)Ru53	0.75	8.88	0.078
157. LP (3)Cl49	829. RY*(15)Ru53	0.99	7.37	0.081
157. LP (3)Cl49	830. RY*(16)Ru53	0.55	6.67	0.058
157. LP (3)Cl49	831. RY*(17)Ru53	0.51	12.66	0.076
157. LP (3)Cl49	832. RY*(18)Ru53	0.15	5.46	0.027
157. LP (3)Cl49	835. RY*(21)Ru53	0.28	12.56	0.056
157. LP (3)Cl49	836. RY*(22)Ru53	2.30	10.81	0.150
157. LP (3)Cl49	837. RY*(23)Ru53	0.10	8.77	0.029
157. LP (3)Cl49	838. RY*(24)Ru53	1.59	35647.06	7.156
157. LP (3)Cl49	839. RY*(25)Ru53	1.71	5348.10	2.871
157. LP (3)Cl49	840. RY*(26)Ru53	3.06	5743.72	3.980
157. LP (3)Cl49	841. RY*(27)Ru53	0.10	49.51	0.066
157. LP (3)Cl49	842. RY*(28)Ru53	0.06	186.34	0.102
157. LP (3)Cl49	843. RY*(29)Ru53	0.88	10.37	0.091
157. LP (3)Cl49	844. RY*(30)Ru53	1.77	32.66	0.228
157. LP (3)Cl49	847. RY*(33)Ru53	2.63	277.76	0.812
157. LP (3)Cl49	852. RY*(38)Ru53	2.91	355.92	0.967
157. LP (3)Cl49	855. RY*(41)Ru53	1.21	140.87	0.392
157. LP (3)Cl49	856. RY*(42)Ru53	2.49	3162.68	2.667
157. LP (3)Cl49	861. RY*(47)Ru53	0.07	19.28	0.036
157. LP (3)Cl49	862. RY*(48)Ru53	0.06	54.12	0.053
157. LP (3)Cl49	903. BD*(1) C 6- O45	0.40	0.25	0.009
157. LP (3)Cl49	905. BD*(3) C 6- O45	0.20	0.82	0.012
157. LP (3)Cl49	906. BD*(1) C 6-Ru53	0.28	0.36	0.009
157. LP (3)Cl49	908. BD*(1) C 8- O46	0.39	0.23	0.009
157. LP (3)Cl49	909. BD*(2) C 8- O46	0.12	0.23	0.005
157. LP (3)Cl49	910. BD*(3) C 8- O46	0.33	0.85	0.016
157. LP (3)Cl49	914. BD*(1) C12- H29	0.06	0.61	0.006
157. LP (3)Cl49	921. BD*(1) C20- N51	0.11	0.66	0.008
157. LP (3)Cl49	926. BD*(1) C16-Ru53	14.42	0.25	0.054
158. LP (4)Cl49	167. LP*(1) C16	0.16	0.31	0.008
158. LP (4)Cl49	401. RY*(9) C16	0.12	13.29	0.038
158. LP (4)Cl49	406. RY*(14) C16	0.11	26.64	0.052
158. LP (4)Cl49	407. RY*(15) C16	0.09	40.42	0.057
158. LP (4)Cl49	815. RY*(1)Ru53	0.51	7.37	0.058
158. LP (4)Cl49	817. RY*(3)Ru53	0.18	1.53	0.016
158. LP (4)Cl49	818. RY*(4)Ru53	0.08	2.62	0.014
158. LP (4)Cl49	822. RY*(8)Ru53	0.09	5.02	0.021
158. LP (4)Cl49	826. RY*(12)Ru53	0.09	3.30	0.016
158. LP (4)Cl49	827. RY*(13)Ru53	0.07	14.15	0.031
158. LP (4)Cl49	829. RY*(15)Ru53	0.36	7.53	0.050
158. LP (4)Cl49	830. RY*(16)Ru53	0.41	6.84	0.051
158. LP (4)Cl49	836. RY*(22)Ru53	0.11	10.97	0.034
158. LP (4)Cl49	838. RY*(24)Ru53	0.16	35647.22	2.304
158. LP (4)Cl49	839. RY*(25)Ru53	0.14	5348.27	0.819
158. LP (4)Cl49	840. RY*(26)Ru53	0.28	5743.89	1.220
158. LP (4)Cl49	843. RY*(29)Ru53	0.06	10.53	0.025
158. LP (4)Cl49	847. RY*(33)Ru53	0.18	277.92	0.214
158. LP (4)Cl49	852. RY*(38)Ru53	0.24	356.09	0.280
158. LP (4)Cl49	853. RY*(39)Ru53	0.24	18.31	0.064
158. LP (4)Cl49	854. RY*(40)Ru53	0.14	54.25	0.084
158. LP (4)Cl49	855. RY*(41)Ru53	0.13	141.03	0.129
158. LP (4)Cl49	856. RY*(42)Ru53	0.24	3162.84	0.837
158. LP (4)Cl49	857. RY*(43)Ru53	0.09	19.32	0.039
158. LP (4)Cl49	903. BD*(1) C 6- O45	0.51	0.41	0.013
158. LP (4)Cl49	904. BD*(2) C 6- O45	0.14	0.40	0.007
158. LP (4)Cl49	905. BD*(3) C 6- O45	0.34	0.99	0.017
158. LP (4)Cl49	906. BD*(1) C 6-Ru53	0.35	0.52	0.012
158. LP (4)Cl49	907. BD*(1) C 8-Ru53	1.09	0.52	0.021
158. LP (4)Cl49	908. BD*(1) C 8- O46	0.34	0.39	0.010
158. LP (4)Cl49	909. BD*(2) C 8- O46	0.06	0.39	0.005
158. LP (4)Cl49	910. BD*(3) C 8- O46	0.22	1.01	0.014
158. LP (4)Cl49	911. BD*(1) C12- C14	0.10	0.86	0.009
158. LP (4)Cl49	921. BD*(1) C20- N51	0.33	0.82	0.016
158. LP (4)Cl49	926. BD*(1) C16-Ru53	35.12	0.41	0.108
158. LP (4)Cl49	928. BD*(1) C16- C18	0.08	0.91	0.008
from unit 4 to unit 3				
157. LP (3)Cl49	638. RY*(1) H43	0.33	1.49	0.021
157. LP (3)Cl49	641. RY*(4) H43	0.38	2.38	0.029
157. LP (3)Cl49	688. RY*(1) O47	0.06	1.94	0.010
157. LP (3)Cl49	690. RY*(3) O47	0.07	2.79	0.013
157. LP (3)Cl49	692. RY*(5) O47	0.83	2.67	0.045
157. LP (3)Cl49	698. RY*(11) O47	0.08	4.83	0.019
157. LP (3)Cl49	699. RY*(12) O47	0.05	4.77	0.015
157. LP (3)Cl49	700. RY*(13) O47	0.07	4.41	0.016
158. LP (4)Cl49	934. BD*(1) H43- O47	0.09	0.85	0.008
within unit 4				
157. LP (3)Cl49	720. RY*(3)Cl49	8.16	2.13	0.125
158. LP (4)Cl49	723. RY*(6)Cl49	1.13	3.44	0.060
158. LP (4)Cl49	725. RY*(8)Cl49	0.97	5.65	0.071
158. LP (4)Cl49	727. RY*(10)Cl49	0.62	3.91	0.047
158. LP (4)Cl49	732. RY*(15)Cl49	0.54	26.42	0.114
158. LP (4)Cl49	735. RY*(18)Cl49	0.53	41.00	0.141

(3) Analytical Frequencies

```
============================================================
=== CALCULATE ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ===
============================================================

                 -------------------------------------------------

                 This Analytical Second Derivatives Progam
                          was written for ADF by

                              Stephen K. Wolff
```

```
                    Scientific Computing & Modelling

                          Vrije University
                       Theoretical Chemistry
                         De Boelelaan 1083
                         1081 HV Amsterdam
                          The Netherlands

                 ------------------------------------------------
                          Date last modified:
                               JUNE 2006


                              References:
                              ===========

                  Attila Berces, Ross M. Dickson, Liangyou Fan
                  Heiko Jacobsen, David Swerhone, Tom Ziegler,
                  Computer Physics Communications 100 (1997) 247.

                  Heiko Jacobsen, Attila Berces
                  David Swerhone, Tom Ziegler,
                  Computer Physics Communications 100 (1997) 263.

                  Stephen K. Wolff
                  Int. J. Quantum Chem. 104 (2005) 645.

                 ------------------------------------------------

            <><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>

               SECOND DERIVATIVES INFORMATION:
               -------------------------------

               === PRINT

                 EIGS,  lprint_eigbas =  F
                 U1,    lprint_u1     =  F
                 PARTS, lprint_parts  =  F

               === DEBUG

                 ALL        =  F
                 B1         =  F
                 DENSITIES  =  F
                 FIT        =  F
                 HESSIAN    =  F
                 NUMBERS    =  F
                 SYMMETRY   =  F
                 U1         =  F

               === CPKS

                 MAX_CPKS_ITERATIONS    =    20
                 U1_ACCURACY PARAMETER  =     5.00
                 U1 ACCURACY            =     0.0000100

            <><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><><>

 Number of elements of the density matrix on this node (used, total):    219716    436645


                                  ****************************************
                                  *  F R E Q U E N C Y    A N A L Y S I S  *
                                  ****************************************


 Atomic Masses:
 ----------------
    1. C              12.00000000
    2. H               1.00782500
    3. O              15.99491400
    4. C              12.00000000
    5. C              12.00000000
    6. Cl             34.96885200
    7. C              12.00000000
    8. N              14.00307400
    9. O              15.99491400
   10. C              12.00000000
   11. O              15.99491400
   12. H               1.00782500
   13. C              12.00000000
   14. C              12.00000000
   15. C              12.00000000
   16. Ru            101.90434800
   17. H               1.00782500
   18. Ru            101.90434800
   19. C              12.00000000
   20. C              12.00000000
   21. C              12.00000000
   22. C              12.00000000
   23. O              15.99491400
   24. H               1.00782500
   25. H               1.00782500
   26. C              12.00000000
   27. O              15.99491400
   28. N              14.00307400
   29. H               1.00782500
   30. C              12.00000000
   31. C              12.00000000
   32. H               1.00782500
   33. C              12.00000000
   34. C              12.00000000
   35. C              12.00000000
   36. C              12.00000000
   37. H               1.00782500
   38. C              12.00000000
   39. C              12.00000000
   40. H               1.00782500
   41. C              12.00000000
   42. C              12.00000000
   43. C              12.00000000
   44. H               1.00782500
   45. H               1.00782500
   46. C              12.00000000
```

```
  47. H              1.00782500
  48. C             12.00000000
  49. H              1.00782500
  50. H              1.00782500
  51. H              1.00782500
  52. H              1.00782500
  53. H              1.00782500


List of All Frequencies:


Intensities
===========
```

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
20.839274	151.359926	0.790627
23.876753	23.594531	0.141210
30.758388	158.155115	1.219340
34.583377	10.130875	0.087820
41.674115	6.094410	0.063661
59.217620	1.773600	0.026326
60.720663	1.513349	0.023033
66.758289	5.578553	0.093348
75.712172	1.263282	0.023974
84.088910	33.412740	0.704253
84.661933	38.347641	0.813776
87.493418	6.772418	0.148524
90.867337	19.291553	0.439393
93.159736	16.073810	0.375340
97.658980	49.147368	1.203069
116.097538	27.403538	0.797458
116.854650	1.838064	0.053837
125.555344	1.377887	0.043364
142.552929	72.737798	2.599048
168.836756	5.806893	0.245747
183.520403	45.059731	2.072770
187.727870	125.097964	5.886499
189.994830	39.047014	1.859549
191.479947	234.657240	11.262514
210.148877	155.872135	8.210576
225.247810	18.281526	1.032170
249.766503	104.476000	6.540769
252.161902	56.006212	3.539922
259.946908	7.481246	0.487457
266.263737	5.347589	0.356901
282.857557	51.005030	3.616253
285.358174	40.926244	2.927320
347.582798	147.112416	12.816979
365.160739	29.142749	2.667428
366.088872	33.768117	3.098642
413.449119	27.088315	2.807257
414.304965	61.164786	6.351842
424.929248	5.103759	0.543607
425.522277	24.688125	2.633228
450.708643	59.360433	6.706115
461.379988	515.976025	59.671416
465.814611	23.549736	2.749649
467.595645	110.177614	12.913438
470.441732	23.133935	2.727931
478.313802	18.213655	2.183675
483.722778	47.123761	5.713662
488.746966	136.146055	16.678892
508.911546	17.761634	2.265705
511.323752	8.662587	1.110252
527.127864	160.711336	21.234428
531.516980	63.713786	8.488455
547.446212	39.456629	5.414265
549.005997	8.971641	1.234602
556.421974	14.134162	1.971299
558.804730	0.844948	0.118350
598.119194	52.542589	7.877298
605.487246	121.308238	18.410830
626.660681	33.235099	5.220445
626.980836	45.613414	7.168444
636.884675	76.939875	12.282601
638.088129	96.491965	15.432983
643.340784	18.128614	2.923370
644.378636	24.401183	3.941215
660.692654	10.806683	1.789658
661.787726	15.961060	2.647637
714.113512	25.058709	4.485429
714.484705	11.022762	1.974065
722.782500	173.606628	31.452270
723.017755	92.707299	16.801226
740.891992	523.417657	97.203374
741.245948	165.553426	30.759451
756.634334	2.818596	0.534561
756.770075	2.850659	0.540738
782.616623	6.554664	1.285812
782.738313	21.069110	4.133718
842.374829	2.720766	0.574480
843.222279	4.397367	0.929422
862.353739	6.953723	1.503076
862.451185	1.434141	0.310031
914.403675	196.428645	45.021593
920.136878	3.991119	0.920503
920.604580	0.091742	0.021170
958.661633	4.318336	1.037671
960.181966	3.818128	0.918929
960.662868	3.410602	0.821259
962.312099	2.603723	0.628042
974.428099	2.642529	0.645428
975.135424	1.509105	0.368861
1000.645668	15.796226	3.961975
1001.932197	13.972826	3.509140
1008.212140	109.537282	27.681649
1008.680842	113.756141	28.761180
1017.874651	19.444363	4.960964
1018.993698	22.527760	5.753970
1046.931287	7.253722	1.903519
1047.501809	3.202254	0.840792
1053.971117	76.516751	20.214514

1054.309066	21.891476	5.785236
1098.509537	5.353221	1.473999
1098.834886	5.263543	1.449735
1116.949120	2.117258	0.592769
1117.835882	2.149417	0.602250
1151.325576	12.540440	3.619004
1151.825152	14.301587	4.129038
1158.549743	24.132012	7.007874
1158.623150	14.277488	4.146408
1235.732837	16.459858	5.098339
1236.696576	21.609687	6.698687
1270.473590	86.356300	27.500320
1272.035574	33.023315	10.529263
1284.747355	4.291431	1.381968
1286.070746	4.753503	1.532346
1299.660493	54.254864	17.674481
1299.995053	29.999489	9.775379
1312.890062	4.795634	1.578165
1313.150629	8.092158	2.663526
1412.260996	51.059745	18.074724
1412.583933	75.808265	26.841630
1427.619424	8.685866	3.108162
1427.868109	13.062329	4.675056
1442.748416	29.839800	10.791072
1443.771383	20.517482	7.425070
1467.811833	197.125791	72.525696
1469.107942	165.640084	60.995419
1540.512305	23.969639	9.255603
1541.849356	23.760712	9.182892
1555.432860	67.028310	26.132900
1556.618691	79.834610	31.149532
1570.104101	90.615831	35.662402
1571.525071	112.875989	44.463224
1593.180672	153.284928	61.212844
1593.524587	88.370167	35.297384
1933.150912	1121.230843	543.298949
1937.419903	1514.255977	735.361898
1995.885194	1890.349968	945.705339
1999.950190	897.251630	449.791771
3082.634649	1.677293	1.296012
3083.694263	1.656892	1.280689
3091.884412	8.362062	6.480592
3091.919601	11.784616	9.133173
3100.725232	25.703542	19.977186
3101.356726	14.465106	11.244791
3104.968367	7.182775	5.590202
3105.728437	13.340119	10.384875
3105.899246	2.106759	1.640138
3106.961040	11.075122	8.625066
3117.144297	39.188288	30.619019
3117.853556	40.438793	31.603266
3130.376920	3.386417	2.657144
3131.734300	2.736987	2.148502
3135.767003	9.035771	7.102104
3137.239403	7.517094	5.911201
3660.841677	29.066365	26.671641

```
 ============================
 Statistical Thermal Analysis  ***  ideal gas assumed  ***
 ============================

 Pressure:                  1.000000 atm.
 Temperature:             298.150000 K


 Moments of Inertia (and direction vectors)
 ==========================================

       14042.1321      22703.2328      24687.7366
 ------------------------------------------------
          -0.5979          0.6127          0.5168
          -0.7205         -0.6934         -0.0115
           0.3513         -0.3792          0.8560


 The rotational contribution to the molecular entropy includes
 a term, dependent on the symmetry number sigma. The results
 reported below were computed using sigma = 1, determined
 from the point group symmetry of the input geometry (NOSYM).
 If this is not the correct symmetry, please contact SCM to
 report a bug.

     Temp                                                  Transl     Rotat    Vibrat     Total
     ----                                                  ------     -----    ------     -----

     298.15   Entropy (cal/mole-K):                        45.414    37.307   133.240   215.961
              Internal Energy (Kcal/mole):                  0.889     0.889   245.996   247.774
              Constant Volume Heat Capacity (cal/mole-K):   2.981     2.981   122.539   128.500

 ********************************************************************************************


================================================================
*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
================================================================



 ============================================================
 SCAN POTENTIAL ENERGY SURFACE ALONG A RANGE OF NORMAL MODES  ***  with IR intensities  ***
 ============================================================

 RANGE OF FREQUENCIES: from  -1000.000 to      0.000


 ===================
 Vibration symmetry:  ***  A  ***
 ===================
```

Total number of frequencies of this symmetry: 153
Frequencies, cm^(-1):

20.839	23.877	30.758	34.583	41.674	59.218	60.721	66.758
75.712	84.089	84.662	87.493	90.867	93.160	97.659	116.098
116.855	125.555	142.553	168.837	183.520	187.728	189.995	191.480
210.149	225.248	249.767	252.162	259.947	266.264	282.858	285.358
347.583	365.161	366.089	413.449	414.305	424.929	425.522	450.709
461.380	465.815	467.596	470.442	478.314	483.723	488.747	508.912
511.324	527.128	531.517	547.446	549.006	556.422	558.805	598.119
605.487	626.661	626.981	636.885	638.088	643.341	644.379	660.693
661.788	714.114	714.485	722.783	723.018	740.892	741.246	756.634
756.770	782.617	782.738	842.375	843.222	862.354	862.451	914.404
920.137	920.605	958.662	960.182	960.663	962.312	974.428	975.135
1000.646	1001.932	1008.212	1008.681	1017.875	1018.994	1046.931	1047.502
1053.971	1054.309	1098.510	1098.835	1116.949	1117.836	1151.326	1151.825
1158.550	1158.623	1235.733	1236.697	1270.474	1272.036	1284.747	1286.071
1299.660	1299.995	1312.890	1313.151	1412.261	1412.584	1427.619	1427.868
1442.748	1443.771	1467.812	1469.108	1540.512	1541.849	1555.433	1556.619
1570.104	1571.525	1593.181	1593.525	1933.151	1937.420	1995.885	1999.950
3082.635	3083.694	3091.884	3091.920	3100.725	3101.357	3104.968	3105.728
3105.899	3106.961	3117.144	3117.854	3130.377	3131.734	3135.767	3137.239
3660.842							

Number of frequencies in the requested range: 0

b) ax-eq-3c

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007    *
*  ------------------------------------                                     *
*                                             Build 200711141748            *
*                                                                           *
*                                                                           *
*                                 =================                         *
*                                 |               |                         *
*                                 |     A D F     |                         *
*                                 |               |                         *
*                                 =================                         *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*****************************  pentium64_linux  *****************************

ADF 2007.01  RunTime: Sep09-2008 13:09:32
equatorial-parallel-OH


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                              VWN
   Gradient Corrections:             Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                         Restricted
   Fragments:                        Restricted

OTHER ASPECTS
   Relativistic Corrections:         scalar (ZORA,SAPA)                   *** SPECIAL ***
   Core Treatment:                   Frozen Orbital(s)

   Electric Field:                   ---

   Hyperfine or Zeeman Interaction:  ---


Fragment File(s)
----------------
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Sep09-2008 13:09:31
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Sep09-2008 13:09:29
        title: Hydrogen (TZP)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Sep09-2008 13:09:31
        title: Chlorine (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Sep09-2008 13:09:30
        title: Nitrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Sep09-2008 13:09:31
        title: Oxygen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Sep09-2008 13:09:30
        title: Ruthenium (TZP, all electron)


                                  ********************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ********************************************


==========================
Geometry Convergence Tests
==========================

Energy  old :        -13.28923765
        new :        -13.28924215

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value          Criterion    Conv.        Ratio
-----------------------------------------------------------------------------
change in energy      -0.00000450     0.00050000    YES        1.28392598
gradient max           0.00077498     0.00100000    YES        0.71396132
gradient rms           0.00016666     0.00066667    YES        0.82479934
cart. step max         0.00541567     0.01000000    YES        3.80676792
cart. step rms         0.00158959     0.00666667    YES        3.65243209

prediction dE :       -0.00001118
```

```
**********************************************************************************************
                          Geometry CONVERGED
**********************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************


Coordinates (Cartesian)
=======================

    Atom                  bohr                                angstrom                Geometric Variables
                 X           Y           Z           X           Y           Z       (0:frozen, *:LT par.)
-----------------------------------------------------------------------------------------------------------
    1 C       6.619659   -1.713833   -6.443456    3.502973   -0.906921   -3.409730      1       2       3
    2 H       5.444274   -0.671788   -2.642710    2.880986   -0.355495   -1.398462      4       5       6
    3 C       5.160235   -0.439159   -4.669721    2.730679   -0.232393   -2.471110      7       8       9
    4 C       6.101893   -1.329048   -9.005793    3.228983   -0.703302   -4.765660     10      11      12
    5 Cl      2.299019    0.465714    1.051626    1.216588    0.246445    0.556497     13      14      15
    6 N       3.277647    1.145757   -5.331339    1.734456    0.606308   -2.821223     16      17      18
    7 O       3.340096   -6.116458   -2.553502    1.767502   -3.236690   -1.351255     19      20      21
    8 C       4.182702    0.325309   -9.695679    2.213390    0.172146   -5.130732     22      23      24
    9 O      -4.483356   -6.999124   -1.797187   -2.372490   -3.703777   -0.951030     25      26      27
   10 H       3.769851    0.662091  -11.681317    1.994919    0.350364   -6.181487     28      29      30
   11 C       1.769982   -4.797559   -1.739162    0.936634   -2.538759   -0.920325     31      32      33
   12 C       2.776091    1.585995   -7.827817    1.469044    0.839272   -4.142302     34      35      36
   13 C      -3.097271   -5.415860   -1.152095   -1.639005   -2.865950   -0.609662     37      38      39
   14 Ru      0.878654    3.185242   -2.719874    0.464964    1.685558   -1.439296     40      41      42
   15 H      -5.151633    0.982447   -0.696890   -2.726127    0.519889   -0.368778     43      44      45
   16 Ru     -0.795220   -2.941152   -0.162740   -0.420812   -1.556391   -0.086118     46      47      48
   17 C       0.782720    3.439429   -8.301549    0.414198    1.820067   -4.392991     49      50      51
   18 C      -1.393117    5.170025   -0.861411   -0.737206    2.735859   -0.455839     52      53      54
   19 C      -0.345445    4.587157   -6.145501   -0.182801    2.427419   -3.252059     55      56      57
   20 C      -5.306091    0.544887    1.311746   -2.807862    0.288342    0.694146     58      59      60
   21 H       0.913809    3.254574  -12.405846    0.483567    1.722247   -6.564891     61      62      63
   22 H      -8.448142    2.992444    2.123993   -4.470564    1.583533    1.123969     64      65      66
   23 C       0.042346    4.142653  -10.762944    0.022409    2.192197   -5.695505     67      68      69
   24 O      -2.792132    6.530980    0.159274   -1.477533    3.456046    0.084284     70      71      72
   25 N      -3.593029   -1.132582    2.168914   -1.901349   -0.599337    1.147740     73      74      75
   26 H       2.701803   -7.484451    2.376555    1.429733   -3.960601    1.257619     76      77      78
   27 C      -7.100451    1.638170    2.887783   -3.757397    0.866882    1.528149     79      80      81
   28 C      -2.187523    6.456595   -6.576765   -1.157587    3.416683   -3.480274     82      83      84
   29 H      -3.081567    7.413704   -4.986133   -1.630695    3.923163   -2.638548     85      86      87
   30 C      -0.212954   -4.743671    3.275486   -0.112690   -2.510243    1.733312     88      89      90
   31 C      -1.791537    5.989752  -11.129820   -0.948041    3.169640   -5.889647     91      92      93
   32 C       1.532851   -6.659268    3.859620    0.811150   -3.523933    2.042423     94      95      96
   33 C      -2.901700    7.150304   -9.024206   -1.535513    3.783778   -4.775404     97      98      99
   34 H      -2.345069    6.536954  -13.037328   -1.240957    3.459207   -6.899057    100     101     102
   35 C      -3.582958   -1.849136    4.646317   -1.896020   -0.978521    2.458725    103     104     105
   36 C      -7.102858    0.963896    5.443864   -3.758671    0.510072    2.880769    106     107     108
   37 H      -4.327831    8.616850   -9.291813   -2.290190    4.559841   -4.917015    109     110     111
   38 C      -1.707380   -3.771662    5.289510   -0.903507   -1.995878    2.799088    112     113     114
   39 C      -5.344965   -0.778798    6.321210   -2.828433   -0.412122    3.345040    115     116     117
   40 C       1.829467   -7.549408    6.330954    0.968112   -3.994975    3.350197    118     119     120
   41 H       3.209541   -9.032389    6.720058    1.698416   -4.779734    3.556101    121     122     123
   42 H      -8.476633    1.787722    6.741089   -4.485641    0.946022    3.567231    124     125     126
   43 C      -1.389667   -4.672202    7.775151   -0.735380   -2.472423    4.114433    127     128     129
   44 H      -5.338021   -1.336820    8.299518   -2.824759   -0.707415    4.391916    130     131     132
   45 C       0.372537   -6.551215    8.302408    0.197138   -3.466754    4.393445    133     134     135
   46 H      -2.522464   -3.898293    9.312779   -1.334830   -2.062888    4.928111    136     137     138
   47 H       0.610094   -7.238124   10.230288    0.322848   -3.830250    5.413635    139     140     141
   48 H       7.194381   -2.307935  -10.454188    3.807103   -1.221307   -5.532118    142     143     144
   49 H       8.106206   -2.990877   -5.818110    4.289619   -1.582704   -3.078811    145     146     147
   50 O      -1.719859    0.068592   -2.958268   -0.910110    0.036297   -1.565448    148     149     150
   51 H      -1.723495   -0.542114   -4.698881   -0.912034   -0.286874   -2.486541    151     152     153
   52 C       3.298364    5.760634   -2.377577    1.745419    3.048396   -1.258160    154     155     156
   53 O       4.797703    7.351654   -2.144499    2.538835    3.890328   -1.134820    157     158     159
-----------------------------------------------------------------------------------------------------------

Number of elements of the density matrix on this node (used, total):     54137    436645


=====================================================
Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
=====================================================

General Accuracy Parameter :                          4.50

Symmetry used in the points section:  NOSYM


Summary of the Symmetry Unique Points:
--------------------------------------
   Nr. of used Symmetry Operators                     1

   Points in the Atomic Spheres                   34100
   Points in the Atomic Polyhedra                339680
   Points in the Outer Region                     30352
   ------------------------------------------------------
   Total                                         404132

   Sum of Weights                                161131.617951

Total nr. of points:     404132
Nr. of blocks:             3158
Block length:               128
Nr. of dummy points:         92


Test of Precision of the Numerical Integration Grid
===================================================

Integral of the Total Core Density:                   0.00000000000000

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B O N D I N G   E N E R G Y  ***  (decomposition)  ***
===========================

*** WARNING ***
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The bond energy is computed as an energy difference between molecule and fragments. In particular when the fragments are single atoms, they are usually computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied for the true (multiplet) fragment ground state. See ref: E.J.Baerends, V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make the direct connection to that paper, where detailed explanations can be found on the meaning of the various terms.

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	155.556827901289495	4232.9167	97613.39	408414.39
Delta V^Pauli Coulomb:	-81.100290116244167	-2206.8512	-50891.21	-212928.78
Delta V^Pauli LDA-XC:	-19.213422501629786	-522.8238	-12056.61	-50444.83
Delta V^Pauli GGA-Exchange:	1.116502332138559	30.3816	700.62	2931.38
Delta V^Pauli GGA-Correlation:	-0.313061885045533	-8.5188	-196.45	-821.94
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	56.046555730508565	1525.1044	35169.75	147150.21
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	56.046555730508565	1525.1044	35169.75	147150.21
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-11.931714335313194	-324.6785	-7487.26	-31326.71
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	44.114841395195370	1200.4259	27682.48	115823.50
Orbital Interactions				
A:	-57.397406466159850	-1561.8629	-36017.42	-150696.87
Total Orbital Interactions:	-57.404079740144894	-1562.0445	-36021.61	-150714.39
Alternative Decomposition Orb.Int.				
Kinetic:	-142.948573281015030	-3889.8286	-89701.59	-375311.43
Coulomb:	78.807551953418923	2144.4626	49452.49	206909.20
XC:	6.736941587451834	183.3215	4227.50	17687.84
Total Orbital Interactions:	-57.404079740144276	-1562.0445	-36021.61	-150714.39
Residu (E=Steric+OrbInt+Res):	-0.000009861326231	-0.0003	-0.01	-0.03
Total Bonding Energy:	-13.289248206275754	-361.6188	-8339.13	-34890.92

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.931714335313194	-324.6785	-7487.26	-31326.71
Kinetic Energy:	12.608254620274465	343.0881	7911.80	33102.97
Coulomb (Steric+OrbInt) Energy:	-2.292748024151479	-62.3888	-1438.72	-6019.61
XC Energy:	-11.673040467084929	-317.6396	-7324.94	-30647.56
Total Bonding Energy:	-13.289248206275136	-361.6188	-8339.13	-34890.92

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): -0.0122970627
2. Electrostatic (Fit correction): 0.0000000000

Scaled ZORA energy correction, not included in bonding energy (hartree): -0.0009435279
WARNING: This scaled ZORA energy correction should only be used to compare two calculations in which the only difference in the calculation is the electron configuration. Then the difference in energy of this term should be added to the difference in energy of the two electron configurations. This term should not be used otherwise. In practice it is useful only for core excitation energy calculations.

F R A G M E N T E N E R G Y T E R M S * (summed over all fragments) ***

The energy terms below are (parts of) the Total Energy of the fragments from which the molecule is built.

Exchange and Correlation				
Exchange LDA:	-441.224207759349497	-12006.3216	-276872.40	-1158433.99
Exchange GGA:	-37.432176164100696	-1018.5813	-23489.05	-98278.16
Correlation LDA:	-23.634119862018686	-643.1171	-14830.64	-62051.37
Correlation GGA:	11.032323784875590	300.2048	6922.89	28965.36
Total XC:	-491.258180000593313	-13367.8152	-308269.19	-1289798.17

(1) Analytical frequency

=== CALCULATE ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ===

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 This Analytical Second Derivatives Progam
           was written for ADF by

              Stephen K. Wolff

        Scientific Computing & Modelling

              Vrije University
            Theoretical Chemistry
             De Boelelaan 1083
             1081 HV Amsterdam
              The Netherlands

 -----------------------------------------------
             Date last modified:
                  JUNE 2006

                 References:
                 ===========

  Attila Berces, Ross M. Dickson, Liangyou Fan
  Heiko Jacobsen, David Swerhone, Tom Ziegler,
  Computer Physics Communications 100 (1997) 247.

  Heiko Jacobsen, Attila Berces
  David Swerhone, Tom Ziegler,
  Computer Physics Communications 100 (1997) 263.

  Stephen K. Wolff
  Int. J. Quantum Chem. 104 (2005) 645.

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  SECOND DERIVATIVES INFORMATION:
  -------------------------------

  === PRINT

    EIGS,  lprint_eigbas =  F
    U1,    lprint_u1     =  F
    PARTS, lprint_parts  =  F

  === DEBUG

    ALL        =  F
    B1         =  F
    DENSITIES  =  F
    FIT        =  F
    HESSIAN    =  F
    NUMBERS    =  F
    SYMMETRY   =  F
    U1         =  F

  === CPKS

    MAX_CPKS_ITERATIONS    =    20
    U1_ACCURACY PARAMETER  =     5.00
    U1 ACCURACY            =     0.0000100

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 Number of elements of the density matrix on this node (used, total):     54137    436645
```

Intensities
===========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
17.040740	126.946191	0.542233
26.438172	156.655852	1.038140
33.277392	137.376168	1.145879
37.135346	0.409233	0.003809
45.483137	9.692732	0.110503
67.493496	0.116196	0.001966
68.886486	5.891394	0.101726
70.801018	1.968734	0.034939
78.200688	1.863950	0.036536
87.302592	91.062159	1.992706
88.529409	23.061764	0.511750
92.790726	7.947372	0.184844
93.964024	7.475873	0.176077
97.530334	0.329488	0.008055
104.063886	33.582665	0.875978
115.017015	3.170330	0.091400
117.821466	3.041649	0.089828
127.008548	1.263247	0.040216
132.650004	38.135338	1.267982
178.572130	4.583738	0.205169
186.165005	1.751567	0.081734
189.285488	5.602052	0.265792
196.559531	6.135820	0.302305
206.680805	238.924685	12.377680
227.062068	46.637618	2.654355
244.674778	7.978691	0.489327
249.716085	132.778361	8.310973
253.364876	59.943866	3.806880
261.492923	17.002436	1.114421
263.662617	15.934385	1.053081
285.351592	55.239138	3.950984
286.235572	16.430491	1.178833
348.785885	313.520715	27.409632
365.689417	50.727570	4.649803
366.209449	13.725556	1.259904
413.962491	103.821211	10.772715
415.716332	24.960470	2.600926
422.869179	611.613177	64.827748
424.036080	32.595351	3.464468
426.155995	312.829631	33.416007
465.696301	29.212102	3.409916

467.034370	13.675612	1.600935
469.624448	9.310525	1.095981
470.216868	1.141507	0.134541
482.896056	8.887546	1.075755
483.444607	12.856908	1.557978
504.883653	36.819938	4.659641
507.807623	9.355799	1.190853
522.530639	33.724403	4.417068
524.153006	140.736095	18.490202
527.154446	95.921431	12.674522
544.700861	42.885542	5.855271
550.093614	22.312875	3.076594
557.548973	4.357022	0.608907
558.094574	1.608828	0.225059
594.813068	29.661087	4.422274
599.000477	196.010878	29.429671
626.447255	25.662997	4.029674
627.419381	59.842353	9.411193
637.213596	80.032462	12.782897
638.489782	101.179831	16.192950
643.114502	15.351590	2.474684
644.174346	27.853025	4.497321
660.266988	4.365773	0.722535
660.580028	14.610644	2.419206
714.348259	33.448197	5.989089
715.965835	26.170824	4.696645
723.424121	57.865807	10.492840
723.900660	152.313244	27.637243
741.370819	160.649065	29.853260
741.598184	564.815457	104.991297
755.986082	3.746835	0.709997
757.805645	4.462179	0.847584
783.242606	9.736013	1.911417
783.952646	14.334916	2.816846
844.224181	7.778876	1.646087
844.312307	0.988467	0.209191
863.520137	12.362203	2.675755
863.783285	0.040831	0.008840
877.387055	159.944591	35.175384
921.341680	0.338847	0.078253
921.640942	0.191616	0.044266
960.281403	1.112020	0.267663
961.229535	1.089729	0.262557
965.002859	4.363812	1.055535
966.710404	2.954318	0.715866
977.224419	3.571169	0.874748
986.831088	15.758801	3.898020
1000.796363	17.696533	4.439274
1002.894943	21.625067	5.436144
1007.296949	212.226065	53.583899
1007.606595	21.280562	5.374674
1017.732989	17.647608	4.501920
1018.825667	14.551174	3.716002
1045.359487	8.637767	2.263316
1046.157078	5.765163	1.511773
1053.060116	53.377860	14.089397
1053.928247	41.010280	10.833826
1097.561764	6.035138	1.660329
1098.331210	5.780453	1.591378
1116.935682	1.691179	0.473474
1117.331770	1.802195	0.504733
1150.827312	18.790640	5.420381
1151.527247	16.640031	4.802932
1157.881614	22.912397	6.649864
1158.874311	19.950828	5.795292
1235.092756	18.995903	5.880816
1237.613081	13.390915	4.154064
1269.077402	76.312062	24.275007
1270.488808	37.136759	11.826410
1284.349674	5.010608	1.613065
1288.716728	7.839993	2.532510
1299.142819	57.217024	18.632032
1300.501719	42.745415	13.934088
1311.724375	12.040688	3.958877
1311.811374	3.273681	1.076430
1411.722515	16.715005	5.914716
1411.861137	125.810812	44.523369
1427.450207	8.885498	3.179222
1428.273210	5.735058	2.053181
1441.709880	11.142139	4.026471
1442.295996	36.369995	13.148485
1466.758436	114.318932	42.029558
1468.608501	236.301105	86.986100
1539.792178	22.851811	8.819842
1541.146080	27.464689	10.609540
1554.774124	79.594112	31.018895
1555.875699	91.299100	35.605695
1570.687567	128.551915	50.611176
1571.825615	98.449366	38.787818
1592.638019	113.507303	45.312597
1593.486147	138.550934	55.339575
1928.160009	981.296587	474.265387
1937.661284	1438.862482	698.835922
1992.541235	1971.804422	984.802685
2000.225298	711.828113	356.888145
3082.211969	3.810019	2.943525
3082.231424	0.325237	0.251271
3090.937378	9.541068	7.392056
3091.285066	7.985863	6.187839
3097.433604	33.718256	26.178525
3101.302540	19.727941	15.335713
3102.452310	6.667091	5.184651
3103.428626	11.373410	8.847295
3104.655306	6.570633	5.113270
3105.111832	12.964345	10.090342
3116.821260	53.602023	41.876574
3117.328151	35.852047	28.013963
3130.233618	3.720951	2.919502
3131.199112	3.453674	2.710629
3136.534712	9.758270	7.671866
3137.366934	5.933573	4.666161
3669.446341	26.525230	24.397076

Zero-Point Energy : 0.361010 a.u.

========== 9.823583 eV

List of All Frequencies:

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
17.040740	0.000000	0.000000
26.438172	156.655852	1.038140
33.277392	137.376168	1.145879
37.135346	0.409233	0.003809
45.483137	9.692732	0.110503
67.493496	0.116196	0.001966
68.886486	5.891394	0.101726
70.801018	1.968734	0.034939
78.200688	1.863950	0.036536
87.302592	91.062159	1.992706
88.529409	23.061764	0.511750
92.790726	7.947372	0.184844
93.964024	7.475873	0.176077
97.530334	0.329488	0.008055
104.063886	33.582665	0.875978
115.017015	3.170330	0.091400
117.821466	3.041649	0.089828
127.008548	1.263247	0.040216
132.650004	38.135338	1.267982
178.572130	4.583738	0.205169
186.165005	1.751567	0.081734
189.285488	5.602052	0.265792
196.559531	6.135820	0.302305
206.680805	238.924685	12.377680
227.062068	46.637618	2.654355
244.674778	7.978691	0.489327
249.716085	132.778361	8.310973
253.364876	59.943866	3.806880
261.492923	17.002436	1.114421
263.662617	15.934385	1.053081
285.351592	55.239138	3.950984
286.235572	16.430491	1.178833
348.785885	313.520715	27.409632
365.689417	50.727570	4.649803
366.209449	13.725556	1.259904
413.962491	103.821211	10.772715
415.716332	24.960470	2.600926
422.869179	611.613177	64.827748
424.036080	32.595351	3.464468
426.155995	312.829631	33.416007
465.696301	29.212102	3.409916
467.034370	13.675612	1.600935
469.624448	9.310525	1.095981
470.216868	1.141507	0.134541
482.896056	8.887546	1.075755
483.444607	12.856908	1.557978
504.883653	36.819938	4.659641
507.807623	9.355799	1.190853
522.530639	33.724403	4.417068
524.153006	140.736095	18.490202
527.154446	95.921431	12.674522
544.700861	42.885542	5.855271
550.093614	22.312875	3.076594
557.548973	4.357022	0.608907
558.094574	1.608828	0.225059
594.813068	29.661087	4.422274
599.000477	196.010878	29.429671
626.447255	25.662997	4.029674
627.419381	59.842353	9.411193
637.213596	80.032462	12.782897
638.489782	101.179831	16.192950
643.114502	15.351590	2.474684
644.174346	27.853025	4.497321
660.266988	4.365773	0.722535
660.580028	14.610644	2.419206
714.348259	33.448197	5.989089
715.965835	26.170824	4.696645
723.424121	57.865807	10.492840
723.900660	152.313244	27.637243
741.370819	160.649065	29.853260
741.598184	564.815457	104.991297
755.986082	3.746835	0.709997
757.805645	4.462179	0.847584
783.242606	9.736013	1.911417
783.952646	14.334916	2.816846
844.224181	7.778876	1.646087
844.312307	0.988467	0.209191
863.520137	12.362203	2.675755
863.783285	0.040831	0.008840
877.387055	159.944591	35.175384
921.341680	0.338847	0.078253
921.640942	0.191616	0.044266
960.281403	1.112020	0.267663
961.229535	1.089729	0.262557
965.002859	4.363812	1.055535
966.710404	2.954318	0.715866
977.224419	3.571169	0.874748
986.831088	15.758801	3.898020
1000.796363	17.696533	4.439274
1002.894943	21.625067	5.436144
1007.296949	212.226065	53.583899
1007.606595	21.280562	5.374674
1017.732989	17.647608	4.501920
1018.825667	14.551174	3.716002
1045.359487	8.637767	2.263316
1046.157078	5.765163	1.511773
1053.060116	53.377860	14.089397
1053.928247	41.010280	10.833826
1097.561764	6.035138	1.660329
1098.331210	5.780453	1.591378
1116.935682	1.691179	0.473474
1117.331770	1.802195	0.504733
1150.827312	18.790640	5.420381
1151.527247	16.640031	4.802932

1157.881614	22.912397	6.649864
1158.874311	19.950828	5.795292
1235.092756	18.995903	5.880816
1237.613081	13.390915	4.154064
1269.077402	76.312062	24.275007
1270.488808	37.136759	11.826410
1284.349674	5.010608	1.613065
1288.716728	7.839993	2.532510
1299.142819	57.217024	18.632032
1300.501719	42.745415	13.934088
1311.724375	12.040688	3.958877
1311.811374	3.273681	1.076430
1411.722515	16.715005	5.914716
1411.861137	125.810812	44.523369
1427.450207	8.885498	3.179222
1428.273210	5.735058	2.053181
1441.709880	11.142139	4.026471
1442.295996	36.369995	13.148485
1466.758436	114.318932	42.029558
1468.608501	236.301105	86.986100
1539.792178	22.851811	8.819842
1541.146080	27.464689	10.609540
1554.774124	79.594112	31.018895
1555.875699	91.299100	35.605695
1570.687567	128.551915	50.611176
1571.825615	98.449366	38.787818
1592.638019	113.507303	45.312597
1593.486147	138.550934	55.339575
1928.160009	981.296587	474.265387
1937.661284	1438.862482	698.835922
1992.541235	1971.804422	984.802685
2000.225298	711.828113	356.888145
3082.211969	3.810019	2.943525
3082.231424	0.325237	0.251271
3090.937378	9.541068	7.392056
3091.285066	7.985863	6.187839
3097.433604	33.718256	26.178525
3101.302540	19.727941	15.335713
3102.452310	6.667091	5.184651
3103.428626	11.373410	8.847295
3104.655306	6.570633	5.113270
3105.111832	12.964345	10.090342
3116.821260	53.602023	41.876574
3117.328151	35.852047	28.013963
3130.233618	3.720951	2.919502
3131.199112	3.453674	2.710629
3136.534712	9.758270	7.671866
3137.366934	5.933573	4.666161
3669.446341	26.525230	24.397076

```
============================
Statistical Thermal Analysis  ***  ideal gas assumed  ***
============================

Pressure:                  1.000000 atm.
Temperature:             298.150000 K


Moments of Inertia (and direction vectors)
==========================================

      11787.9551      24336.9248      28798.3976
-------------------------------------------------
         -0.2203          0.6547         -0.7230
         -0.5769         -0.6852         -0.4446
          0.7865         -0.3192         -0.5287


The rotational contribution to the molecular entropy includes
a term, dependent on the symmetry number sigma. The results
reported below were computed using sigma = 1, determined
from the point group symmetry of the input geometry (NOSYM).
If this is not the correct symmetry, please contact SCM to
report a bug.

    Temp                                                    Transl     Rotat    Vibrat     Total
    ----                                                    ------     -----    ------     -----

    298.15   Entropy (cal/mole-K):                          45.414    37.355   124.249   207.019
             Internal Energy (Kcal/mole):                    0.889     0.889   245.397   247.174
             Constant Volume Heat Capacity (cal/mole-K):     2.981     2.981   120.440   126.402


*****************************************************************************************************


=====================================================================
*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
=====================================================================



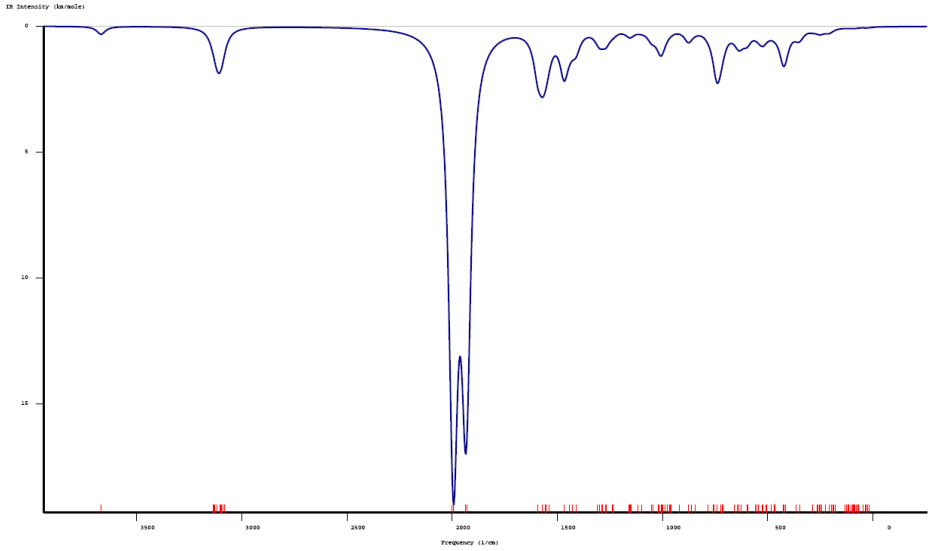
============================================================
SCAN POTENTIAL ENERGY SURFACE ALONG A RANGE OF NORMAL MODES  ***  with IR intensities  ***
============================================================

RANGE OF FREQUENCIES: from  -1000.000 to      0.000


==================
Vibration symmetry:  ***  A  ***
==================

Total number of frequencies of this symmetry:   153
Frequencies, cm^(-1):
     17.041      26.438      33.277      37.135      45.483      67.493      68.886      70.801
     78.201      87.303      88.529      92.791      93.964      97.530     104.064     115.017
    117.821     127.009     132.650     178.572     186.165     189.285     196.560     206.681
    227.062     244.675     249.716     253.365     261.493     263.663     285.352     286.236
```

```
    348.786     365.689     366.209     413.962     415.716     422.869     424.036     426.156
    465.696     467.034     469.624     470.217     482.896     483.445     504.884     507.808
    522.531     524.153     527.154     544.701     550.094     557.549     558.095     594.813
    599.000     626.447     627.419     637.214     638.490     643.115     644.174     660.267
    660.580     714.348     715.966     723.424     723.901     741.371     741.598     755.986
    757.806     783.243     783.953     844.224     844.312     863.520     863.783     877.387
    921.342     921.641     960.281     961.230     965.003     966.710     977.224     986.831
   1000.796    1002.895    1007.297    1007.607    1017.733    1018.826    1045.359    1046.157
   1053.060    1053.928    1097.562    1098.331    1116.936    1117.332    1150.827    1151.527
   1157.882    1158.874    1235.093    1237.613    1269.077    1270.489    1284.350    1288.717
   1299.143    1300.502    1311.724    1311.811    1411.723    1411.861    1427.450    1428.273
   1441.710    1442.296    1466.758    1468.609    1539.792    1541.146    1554.774    1555.876
   1570.688    1571.826    1592.638    1593.486    1928.160    1937.661    1992.541    2000.225
   3082.212    3082.231    3090.937    3091.285    3097.434    3101.303    3102.452    3103.429
   3104.655    3105.112    3116.821    3117.328    3130.234    3131.199    3136.535    3137.367
   3669.446
Number of frequencies in the requested range:     0
```



c) eq-eq-3c

```
*****************************************************************************
*                                                                           *
*   ------------------------------------                                    *
*    Amsterdam Density Functional  (ADF)         2007.01   August 20, 2007   *
*   ------------------------------------                                    *
*                                               Build 200711141748          *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |      A D F    |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
*    Online information and documentation:  http://www.scm.com              *
*    E-mail:  support@scm.com   info@scm.com                                *
*                                                                           *
*    Scientific publications using ADF results must be properly referenced  *
*    See the User Manuals (or the web site) for recommended citations       *
*    The terms and conditions of the End User License Agreement apply to    *
*    the use of ADF, http://www.scm.com/Sales/LicAgreement.html             *
*                                                                           *
*****************************  pentium64_linux  *****************************

ADF 2007.01  RunTime: Jul21-2008 14:55:51
equatorial-OH


============================
A T T A C H E D   F I L E S
============================



================================
M O D E L   P A R A M E T E R S
================================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                         VWN
   Gradient Corrections:        Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                    Restricted
   Fragments:                   Restricted

OTHER ASPECTS
   Relativistic Corrections:    scalar (ZORA,SAPA)                   *** SPECIAL ***
   Core Treatment:              -

   Electric Field:              ---
```

```
   Hyperfine or Zeeman Interaction:   ---

Fragment File(s)
----------------
C:
        file : t21.C
        jobid: ADF 2007.01  RunTime: Jul21-2008 14:55:50
        title: Carbon (TZP)
H:
        file : t21.H
        jobid: ADF 2007.01  RunTime: Jul21-2008 14:55:48
        title: Hydrogen (TZP)
O:
        file : t21.O
        jobid: ADF 2007.01  RunTime: Jul21-2008 14:55:50
        title: Oxygen (TZP)
N:
        file : t21.N
        jobid: ADF 2007.01  RunTime: Jul21-2008 14:55:48
        title: Nitrogen (TZP)
Ru:
        file : t21.Ru
        jobid: ADF 2007.01  RunTime: Jul21-2008 14:55:49
        title: Ruthenium (TZP, all electron)
Cl:
        file : t21.Cl
        jobid: ADF 2007.01  RunTime: Jul21-2008 14:55:48
        title: Chlorine (TZP)


                                  ******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  ******************************************



==========================
Geometry Convergence Tests
==========================

Energy  old :        -13.28127687
        new :        -13.28129072

Convergence tests:
(Energies in hartree, Gradients in hartree/angstr or radian, Lengths in angstrom, Angles in degrees)

      Item               Value         Criterion    Conv.        Ratio
-------------------------------------------------------------------------
change in energy      -0.00001385     0.00100000    YES        3.02500724
gradient max           0.00091858     0.00100000    YES        0.65098898
gradient rms           0.00017813     0.00066667    YES        0.80069931
cart. step max         0.00239815     0.01000000    YES        0.95527167
cart. step rms         0.00076030     0.00666667    YES        0.99891458

prediction dE :       -0.00000930


*********************************************************************************************************
                           Geometry CONVERGED
*********************************************************************************************************


                                        ********************
                                        *  Final Geometry  *
                                        ********************


Coordinates (Cartesian)
=======================

    Atom                   bohr                                  angstrom                 Geometric Variables
                  X          Y          Z          X          Y          Z       (0:frozen, *:LT par.)
-----------------------------------------------------------------------------------------------------------
    1 C       6.297919   -0.661172   -5.694266    3.332715   -0.349877   -3.013276      1        2        3
    2 H       2.194933   -0.511439   -5.210282    1.161508   -0.270642   -2.757163      4        5        6
    3 O      -0.239925    7.188616   -5.082958   -0.126963    3.804052   -2.689786      7        8        9
    4 C       4.047745    0.189410   -4.639367    2.141974    0.100231   -2.455048     10       11       12
    5 C       8.569264    0.317993   -4.760013    4.534659    0.168274   -2.518890     13       14       15
    6 O      -1.230123   -0.111281   -2.692998   -0.650953   -0.058887   -1.425073     16       17       18
    7 C       0.098548    5.666371   -3.526985    0.052149    2.998514   -1.866400     19       20       21
    8 N       3.998163    1.922902   -2.776327    2.115737    1.017556   -1.469169     22       23       24
    9 O       3.390550   -6.003242   -2.138229    1.794202   -3.176779   -1.131502     25       26       27
   10 C       8.512800    2.109978   -2.841200    4.504780    1.116552   -1.503498     28       29       30
   11 O      -4.420933   -7.183936   -2.535749   -2.339457   -3.801575   -1.341860     31       32       33
   12 H      10.263614    2.892637   -2.101268    5.431271    1.530718   -1.111943     34       35       36
   13 C       1.693656   -4.859326   -1.324795    0.896244   -2.571445   -0.701051     37       38       39
   14 C       6.186378    2.929447   -1.855197    3.273690    1.550197   -0.981728     40       41       42
   15 C      -3.179112   -5.673832   -1.520861   -1.682314   -3.002463   -0.804805     43       44       45
   16 Ru      0.605551    3.269703   -0.997698    0.320444    1.730252   -0.527959     46       47       48
   17 H      -5.736672    0.539140   -0.558410   -3.035716    0.285301   -0.295498     49       50       51
   18 Ru     -1.147645   -3.293353    0.099683   -0.607308   -1.742767    0.052750     52       53       54
   19 C       5.847403    4.850842    0.100135    3.094313    2.566955    0.052989     55       56       57
   20 C      -2.031066    4.739824    0.854431   -1.074794    2.508207    0.452145     58       59       60
   21 C       3.319201    5.515607    0.732326    1.756445    2.918734    0.387530     61       62       63
   22 C      -6.032978   -0.143454    1.359926   -3.192514   -0.075912    0.719642     64       65       66
   23 Cl      1.418260   -0.011256    2.305880    0.750511   -0.005957    1.220219     67       68       69
   24 H       9.836122    5.469713    0.858795    5.205051    2.894447    0.454455     70       71       72
   25 H      -9.327312    2.133745    2.058318   -4.935801    1.129129    1.089215     73       74       75
   26 C       7.904672    6.020752    1.320151    4.182972    3.186045    0.698594     76       77       78
   27 O      -3.558716    5.836056    2.006845   -1.883192    3.088308    1.061977     79       80       81
   28 N      -4.345342   -1.852091    2.203283   -2.299456   -0.980085    1.165927     82       83       84
   29 H       2.139194   -8.009416    2.533462    1.132013   -4.238401    1.340650     85       86       87
   30 C      -8.019930    0.743770    2.826783   -4.243964    0.393586    1.495869     88       89       90
   31 C       2.968086    7.421472    2.549454    1.570644    3.927274    1.349113     91       92       93
   32 H       1.066113    8.013539    3.077427    0.564163    4.240582    1.628504     94       95       96
   33 C      -0.964508   -5.456851    3.353013   -0.510395   -2.887641    1.774338     97       98       99
   34 C       7.500586    7.873114    3.142553    3.969139    4.166272    1.662968    100      101      102
   35 C       0.777934   -7.374595    3.943985    0.411665   -3.902468    2.087067    103      104      105
   36 C       5.021651    8.581225    3.743219    2.657343    4.540989    1.980826    106      107      108
   37 H       9.099587    8.759874    4.092043    4.815294    4.635526    2.165416    109      110      111
   38 C      -4.568272   -2.806537    4.593515   -2.417426   -1.485155    2.430784    112      113      114
```

39	C	-8.249395	-0.172420	5.296590	-4.365392	-0.091241	2.802834	115	116	117
40	H	4.683247	10.040232	5.161742	2.478268	5.313062	2.731476	118	119	120
41	C	-2.711374	-4.734210	5.263183	-1.434797	-2.505236	2.785157	121	122	123
42	C	-6.524568	-1.943649	6.174009	-3.452653	-1.028535	3.267145	124	125	126
43	C	0.833737	-8.493692	6.337107	0.441195	-4.494668	3.353453	127	128	129
44	H	2.222052	-9.965126	6.740524	1.175859	-5.273318	3.566932	130	131	132
45	H	-9.767887	0.491510	6.522215	-5.168943	0.260096	3.451408	133	134	135
46	C	-2.636607	-5.865641	7.673871	-1.395233	-3.103963	4.060838	136	137	138
47	H	-6.683862	-2.684657	8.084408	-3.536947	-1.420659	4.278085	139	140	141
48	C	-0.868366	-7.733018	8.217424	-0.459519	-4.092137	4.348473	142	143	144
49	H	-3.956408	-5.276234	9.142636	-2.093641	-2.792063	4.838074	145	146	147
50	H	-0.810014	-8.592360	10.088920	-0.428641	-4.546881	5.338826	148	149	150
51	H	10.374263	-0.315639	-5.528174	5.489823	-0.167029	-2.925384	151	152	153
52	H	6.262264	-2.071899	-7.191736	3.313848	-1.096402	-3.805703	154	155	156
53	H	-2.894959	0.206005	-3.406223	-1.531946	0.109013	-1.802496	157	158	159

Number of elements of the density matrix on this node (used, total): 110446 436645

==========
Numerical Integration : Voronoi Polyhedra (Te Velde) *** (parameters, tests) ***
==========

General Accuracy Parameter : 4.50

Symmetry used in the points section: NOSYM

Summary of the Symmetry Unique Points:

Nr. of used Symmetry Operators	1
Points in the Atomic Spheres	34100
Points in the Atomic Polyhedra	350078
Points in the Outer Region	28232
Total	412410
Sum of Weights	160042.049757

Total nr. of points: 412410
Nr. of blocks: 3222
Block length: 128
Nr. of dummy points: 6

Test of Precision of the Numerical Integration Grid
==========

Integral of the Total Core Density: 0.00000000000000

==========
B O N D I N G E N E R G Y *** (decomposition) ***
==========

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	155.613715490342486	4234.4646	97649.09	408563.75
Delta V^Pauli Coulomb:	-81.126247664590210	-2207.5575	-50907.49	-212996.93
Delta V^Pauli LDA-XC:	-19.212791055266962	-522.8066	-12056.21	-50443.18
Delta V^Pauli GGA-Exchange:	1.115304599827454	30.3490	699.86	2928.23
Delta V^Pauli GGA-Correlation:	-0.312584890754518	-8.5059	-196.15	-820.69
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	56.077396479558246	1525.9436	35189.10	147231.18
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	56.077396479558246	1525.9436	35189.10	147231.18
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-11.937367003857224	-324.8323	-7490.81	-31341.55
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	44.140029475701020	1201.1113	27698.29	115889.63
Orbital Interactions				
A:	-57.416027579238865	-1562.3696	-36029.11	-150745.76
Total Orbital Interactions:	-57.421311759939783	-1562.5134	-36032.42	-150759.63
Alternative Decomposition Orb.Int.				
Kinetic:	-143.020143406212128	-3891.7761	-89746.50	-375499.33
Coulomb:	78.857855445746409	2145.8314	49484.06	207041.27
XC:	6.740976200525938	183.4313	4230.03	17698.43

Total Orbital Interactions:	-57.421311759939783	-1562.5134	-36032.42	-150759.63
Residu (E=Steric+OrbInt+Res):	-0.000017337666824	-0.0005	-0.01	-0.05
Total Bonding Energy:	-13.281299621905587	-361.4026	-8334.14	-34870.05

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.937367003857224	-324.8323	-7490.81	-31341.55
Kinetic Energy:	12.593572084130358	342.6885	7902.59	33064.42
Coulomb (Steric+OrbInt) Energy:	-2.268409556510619	-61.7266	-1423.45	-5955.71
XC Energy:	-11.669095145668091	-317.5322	-7322.47	-30637.20
Total Bonding Energy:	-13.281299621905577	-361.4026	-8334.14	-34870.05

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): -0.0146752026
2. Electrostatic (Fit correction): 0.0000000000

Scaled ZORA energy correction, not included in bonding energy (hartree): -0.0009369310
WARNING: This scaled ZORA energy correction should only be used to compare two calculations in which the only difference in the calculation is the electron configuration. Then the difference in energy of this term should be added to the difference in energy of the two electron configurations. This term should not be used otherwise. In practice it is useful only for core excitation energy calculations.

B O N D - O R D E R A N A L Y S I S

			DIST. [A]	BOND-ORDERS (THRESHOLD = 0.050)				
				MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
C	1 - C	4	1.3900	1.4260	1.4355	1.4936	1.4833	1.5318
C	1 - C	5	1.3991	1.3557	1.3996	1.4581	1.4224	1.5157
C	1 - C	14	2.7823	0.0593	0.0932	0.0964	0.1241	0.0970
C	1 - H	52	1.0889	1.0291	0.9230	0.9703	0.9857	0.9052
H	2 - C	4	1.0909	1.0158	0.8922	0.9331	0.9194	0.8472
O	3 - C	7	1.1657	2.0275	2.1718	2.3450	2.3569	2.3886
O	3 - Ru	16	3.0289	0.2244	0.2595	0.3007	0.4289	0.2968
C	4 - N	8	1.3469	1.3690	1.3913	1.4667	1.4530	1.5137
C	4 - C	10	2.7425	0.0631	0.1082	0.1125	0.1089	0.1152
C	5 - N	8	2.7703	0.0368	0.0929	0.0980	0.0677	0.1025
C	5 - C	10	1.3897	1.4139	1.4691	1.5295	1.4960	1.5875
C	5 - H	51	1.0909	1.0271	0.9239	0.9688	0.9753	0.8987
O	6 - Ru	16	2.2247	0.3080	0.2762	0.3549	0.7718	0.3979
O	6 - Ru	18	2.2408	0.2961	0.2629	0.3384	0.7542	0.3794
O	6 - C	21	4.2364	0.0478	0.1030	0.1247	-0.0085	0.1491
O	6 - C	33	4.2729	0.0431	0.1016	0.1231	-0.0076	0.1471
O	6 - H	53	0.9730	1.1497	0.8768	1.1211	1.1870	1.1470
C	7 - Ru	16	1.8633	1.1076	1.1245	1.2164	1.0484	1.1138
C	7 - C	20	2.6241	0.0859	0.0760	0.0763	0.0397	0.0723
C	7 - C	21	2.8269	0.0685	0.0562	0.0566	0.0850	0.0560
C	7 - Cl	23	4.3637	0.0697	0.1369	0.1568	0.2212	0.1736
N	8 - C	14	1.3646	1.2879	1.3057	1.3688	1.3884	1.3864
N	8 - Ru	16	2.1487	0.2841	0.3386	0.3778	0.4921	0.3671
N	8 - C	20	4.0116	0.0444	0.1212	0.1258	0.1630	0.1267
O	9 - C	13	1.1654	2.0047	2.1733	2.3519	2.3624	2.3991
O	9 - Ru	18	3.0374	0.2275	0.2517	0.2925	0.4215	0.2889
C	10 - H	12	1.0878	1.0181	0.9218	0.9640	0.9775	0.9032
C	10 - C	14	1.4057	1.3668	1.3433	1.3889	1.4062	1.3950
O	11 - C	15	1.1657	2.0281	2.1730	2.3462	2.3578	2.3901
O	11 - Ru	18	3.0305	0.2247	0.2599	0.3018	0.4284	0.2979
C	13 - C	15	2.6164	0.0923	0.0762	0.0766	0.0358	0.0724
C	13 - Ru	18	1.8750	1.0800	1.0935	1.1873	1.0282	1.0889
C	13 - N	28	4.0287	0.0428	0.1184	0.1232	0.1660	0.1238
C	14 - C	19	1.4617	1.1765	1.1025	1.1356	1.1373	1.1201
C	15 - Ru	18	1.8649	1.1013	1.1211	1.2153	1.0506	1.1137
C	15 - Cl	23	4.3587	0.0709	0.1388	0.1590	0.2225	0.1760
C	15 - C	33	2.8352	0.0706	0.0543	0.0547	0.0822	0.0542
Ru	16 - C	20	1.8742	1.1148	1.1053	1.1972	1.0504	1.1009
Ru	16 - C	21	2.0767	0.6650	0.7236	0.7863	0.8396	0.7534
Ru	16 - Cl	23	2.5011	0.5946	0.3252	0.3982	0.5744	0.4266
Ru	16 - O	27	3.0378	0.2266	0.2574	0.2987	0.4333	0.2955
H	17 - C	22	1.0888	1.0139	0.9136	0.9501	0.9394	0.8739
Ru	18 - Cl	23	2.4946	0.6008	0.3315	0.4067	0.5807	0.4357
Ru	18 - N	28	2.1643	0.2814	0.3315	0.3711	0.4872	0.3610
Ru	18 - C	33	2.0698	0.6612	0.7350	0.8005	0.8515	0.7670
C	19 - C	21	1.4232	1.3293	1.3166	1.3474	1.3393	1.3761
C	19 - C	26	1.4090	1.3400	1.3433	1.3922	1.3821	1.4253
C	19 - C	36	2.7936	0.0527	0.0924	0.0958	0.0902	0.0980
C	20 - O	27	1.1670	1.9969	2.1556	2.3342	2.3416	2.3917
C	21 - C	31	1.4058	1.3994	1.4142	1.4506	1.4175	1.5063
C	21 - C	34	2.8424	0.0423	0.0997	0.1025	0.0761	0.1066
C	22 - N	28	1.3469	1.3693	1.3923	1.4685	1.4552	1.5160
C	22 - C	30	1.3887	1.4313	1.4407	1.4981	1.4886	1.5358
C	22 - C	42	2.7322	0.0626	0.1080	0.1123	0.1094	0.1148
H	24 - C	26	1.0905	1.0266	0.9270	0.9636	0.9745	0.9102
H	25 - C	30	1.0886	1.0265	0.9228	0.9703	0.9857	0.9048
C	26 - C	31	2.7923	0.0599	0.1092	0.1134	0.0843	0.1180
C	26 - C	34	1.3916	1.4124	1.4650	1.5247	1.4836	1.5884
N	28 - C	38	1.3671	1.2858	1.3037	1.3682	1.3886	1.3862
N	28 - C	39	2.7817	0.0372	0.0923	0.0976	0.0671	0.1021
H	29 - C	35	1.0904	1.0237	0.9226	0.9611	0.9734	0.9037
C	30 - C	38	2.7821	0.0577	0.0913	0.0945	0.1227	0.0950
C	30 - C	39	1.3993	1.3496	1.3926	1.4510	1.4159	1.5080
C	31 - H	32	1.0905	1.0241	0.9226	0.9612	0.9735	0.9039
C	31 - C	36	1.3988	1.3996	1.4352	1.4904	1.4527	1.5503
C	33 - C	35	1.4064	1.3997	1.4111	1.4477	1.4152	1.5028
C	33 - C	41	1.4221	1.3282	1.3147	1.3460	1.3381	1.3743
C	33 - C	48	2.8425	0.0414	0.0987	0.1015	0.0757	0.1054
C	34 - C	36	1.4008	1.3674	1.4050	1.4618	1.4221	1.5223

C	34 - H	37	1.0902	1.0314	0.9288	0.9724	0.9859	0.9137
C	35 - C	43	1.3983	1.4010	1.4374	1.4925	1.4553	1.5522
C	35 - C	46	2.7925	0.0605	0.1095	0.1137	0.0848	0.1183
C	36 - H	40	1.0916	1.0302	0.9275	0.9690	0.9795	0.9070
C	38 - C	41	1.4600	1.1783	1.1068	1.1401	1.1419	1.1242
C	38 - C	42	1.4070	1.3619	1.3386	1.3838	1.4012	1.3888
C	39 - C	42	1.3882	1.4194	1.4743	1.5350	1.5026	1.5922
C	39 - H	45	1.0908	1.0275	0.9233	0.9686	0.9748	0.8976
C	41 - C	43	2.7929	0.0519	0.0912	0.0945	0.0889	0.0967
C	41 - C	46	1.4098	1.3373	1.3391	1.3881	1.3781	1.4210
C	42 - H	47	1.0876	1.0184	0.9210	0.9633	0.9764	0.9015
C	43 - H	44	1.0916	1.0303	0.9272	0.9688	0.9791	0.9062
C	43 - C	48	1.4012	1.3647	1.4020	1.4586	1.4195	1.5186
C	46 - C	48	1.3910	1.4146	1.4681	1.5280	1.4872	1.5916
C	46 - H	49	1.0905	1.0256	0.9269	0.9634	0.9743	0.9100
C	48 - H	50	1.0902	1.0316	0.9286	0.9723	0.9858	0.9133
Sum :				73.4184	74.0459	78.4523	78.4523	78.4523

Atomic summation :

C	1	3.9566	3.9822	4.1564	4.1539	4.1900
H	2	1.0784	0.9777	1.0280	1.0411	0.9394
O	3	2.2886	2.5065	2.7315	2.7360	2.7786
C	4	3.9805	3.9549	4.1435	4.1050	4.1469
C	5	3.9282	3.9759	4.1492	4.1283	4.1985
O	6	1.9564	1.8657	2.3644	2.6187	2.5741
C	7	3.4174	3.6678	3.9619	3.9036	3.9194
N	8	3.2111	3.4952	3.6991	3.7036	3.7681
O	9	2.2765	2.5017	2.7313	2.7381	2.7818
C	10	3.9640	3.9863	4.1456	4.1396	4.1539
O	11	2.2891	2.5074	2.7329	2.7376	2.7803
H	12	1.0400	0.9799	1.0250	1.0360	0.9592
C	13	3.3808	3.6235	3.9138	3.8596	3.8659
C	14	4.1127	4.0023	4.1546	4.1478	4.1582
C	15	3.4192	3.6649	3.9618	3.9036	3.9206
Ru	16	4.5754	4.6150	5.1563	5.2368	4.9643
H	17	1.0657	0.9847	1.0264	1.0383	0.9453
Ru	18	4.5278	4.5945	5.1429	5.2218	4.9478
C	19	4.0256	4.0196	4.1445	4.1318	4.1914
C	20	3.4031	3.6270	3.9156	3.8543	3.8813
C	21	3.7750	3.9617	4.1268	4.0826	4.2125
C	22	3.9965	3.9717	4.1539	4.1204	4.1646
Cl	23	1.3600	1.1706	1.4015	1.4344	1.5325
H	24	1.0378	0.9872	1.0262	1.0345	0.9681
H	25	1.0451	0.9749	1.0254	1.0379	0.9553
C	26	3.9649	3.9926	4.1499	4.1434	4.2003
O	27	2.2705	2.4940	2.7246	2.7358	2.7859
N	28	3.2063	3.4843	3.6909	3.6970	3.7608
H	29	1.0722	0.9840	1.0258	1.0353	0.9634
C	30	3.9545	3.9825	4.1563	4.1539	4.1885
C	31	4.0038	3.9885	4.1296	4.1214	4.1925
H	32	1.0698	0.9840	1.0258	1.0353	0.9635
C	33	3.7716	3.9600	4.1281	4.0837	4.2114
C	34	3.9579	3.9859	4.1534	4.1460	4.2227
C	35	4.0075	3.9886	4.1299	4.1219	4.1917
C	36	3.9744	3.9854	4.1491	4.1348	4.2110
H	37	1.0435	0.9808	1.0268	1.0369	0.9637
C	38	4.1096	4.0015	4.1549	4.1484	4.1573
C	39	3.9299	3.9751	4.1493	4.1281	4.1962
H	40	1.0401	0.9799	1.0238	1.0350	0.9573
C	41	4.0271	4.0191	4.1450	4.1324	4.1908
C	42	3.9643	3.9860	4.1451	4.1383	4.1504
C	43	3.9746	3.9850	4.1486	4.1339	4.2090
H	44	1.0401	0.9796	1.0236	1.0350	0.9566
H	45	1.0368	0.9756	1.0235	1.0378	0.9469
C	46	3.9647	3.9927	4.1502	4.1436	4.2002
H	47	1.0419	0.9794	1.0247	1.0360	0.9577
C	48	3.9581	3.9857	4.1534	4.1459	4.2215
H	49	1.0380	0.9872	1.0262	1.0345	0.9680
H	50	1.0438	0.9806	1.0268	1.0369	0.9633
H	51	1.0361	0.9762	1.0236	1.0375	0.9481
H	52	1.0449	0.9750	1.0254	1.0377	0.9557
H	53	1.1783	0.9039	1.1516	1.0529	1.1722

(*) Values from:
- Mayer bond-order analysis
- Gophinatan-Jug bond order analysis
- Nalewajski-Mrozek bond order analysis
  a) N-M (1) - bond-orders calculated from two-electron valence indices based on partitioning of tr(Delta_P^2] (3-index set)
  b) N-M (2) - bond-orders calculated from two-electron valence indices based on partitioning of tr(Delta_P^2] (4-index set)
  c) N-M (3) - bond-orders calculated from valence indices based on partitioning of tr(P*Delta_P]

A. Michalak, R.L. DeKock, T. Ziegler, J. Comp. Chem., subm.
and original articles by Nalewajski et al.)

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No memory problems found
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Maximum number of active allocate calls:        7993

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                            A D F   E X I T
NORMAL TERMINATION


********************************** NBO 5.0 **********************************
          N A T U R A L   A T O M I C   O R B I T A L   A N D
        N A T U R A L   B O N D   O R B I T A L   A N A L Y S I S
*****************************************************************************
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         Cite this program as:
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          NBO 5.0.  E. D. Glendening, J. K. Badenhoop, A. E. Reed,
          J. E. Carpenter, J. A. Bohmann, C. M. Morales, and F. Weinhold
          (Theoretical Chemistry Institute, University of Wisconsin,
          Madison, WI, 2001); http://www.chem.wisc.edu/~nbo5

        /3CBOND / : Search for 3-center bonds
        /NLMO   / : Form Natural Localized Molecular Orbitals
        /NRT    / : Natural Resonance Theory Analysis
        /AONBO  / : Write the AO to NBO transformation to LFN 37
        /AONLMO / : Write the AO to NLMO transformation to LFN 39
        /NAOMO  / : Print core and valence MOs in the NAO basis
        /NBONLMO/ : Write the NBO to NLMO transformation to LFN 49
        /NLMOMO / : Write the NLMO to MO transformation to LFN 49
        /STERIC / : Print NBO/NLMO steric analysis
        /CMO    / : Print analysis of canonical MOs
        /FILE   / : Set to nbodata

 Job title: ***equatorial-OH

 Storage needed:     4369259 in NPA,     3495107 in NBO,
                     3496903 in NLMO (    10000000 available)


 Atom distance matrix: (Angstroms)
```

Atom	1	2	3	4	5	6	7	8
1. C	0.0000	1.3900	1.3991	4.8259	2.4091	4.0272	2.7823	6.0880
2. C	1.3900	0.0000	2.3945	3.6213	2.7425	3.4302	2.3567	5.1938
3. C	1.3991	2.3945	0.0000	5.3412	1.3897	4.9039	2.4213	7.1863
4. C	4.8259	3.6213	5.3412	0.0000	4.8476	5.7528	3.6412	6.3362
5. C	2.4091	2.7425	1.3897	4.8476	0.0000	5.2218	1.4057	7.4656
6. C	4.0272	3.4302	4.9039	5.7528	5.2218	0.0000	4.7664	2.6164
7. C	2.7823	2.3567	2.4213	3.6412	1.4057	4.7664	0.0000	6.7320
8. C	6.0880	5.1938	7.1863	6.3362	7.4656	2.6164	6.7320	0.0000
9. C	4.2387	3.6444	3.8004	3.6229	2.5526	5.6394	1.4617	7.3872
10. C	6.2932	4.9596	6.7652	2.6241	6.0740	5.5694	4.6779	5.6848
11. C	4.9733	4.0215	4.8714	2.8269	3.7917	5.6628	2.4596	6.9503
12. C	7.5225	6.2102	8.3819	5.1641	8.1002	4.9964	6.8812	3.6290
13. C	5.1965	4.8614	4.4252	4.8660	3.0390	6.7757	2.5152	8.6579
14. C	8.8482	7.5151	9.6557	6.0454	9.2768	6.3277	7.9995	4.8361
15. C	6.3584	5.4263	6.1544	3.6753	4.9645	6.8477	3.7395	7.9525
16. C	6.6431	5.8181	7.2954	6.9439	7.2062	2.8646	6.4506	2.8352
17. C	6.5321	6.0687	5.8131	5.4003	4.4288	7.7736	3.7844	9.4562
18. C	6.8678	6.2965	7.4017	7.9613	7.4052	3.1273	6.8804	3.6821
19. C	7.0227	6.2978	6.5492	4.8957	5.2231	7.8026	4.2546	9.1376
20. C	7.9994	6.8683	8.6928	6.6834	8.3764	4.6871	7.2971	3.6485
21. C	9.6517	8.3683	10.3730	7.1318	9.9339	6.7907	8.6818	5.3562
22. C	7.8100	6.8587	8.4211	7.3579	8.1724	4.1943	7.2668	3.6327
23. C	9.2707	8.0819	9.9352	7.4064	9.5227	6.0861	8.3634	4.8591
24. C	8.1287	7.5990	8.5431	9.1404	8.4610	4.5105	7.9597	4.9017
25. C	8.9432	8.0768	9.4427	8.6294	9.1425	5.3113	8.2999	4.8752
26. C	9.0874	8.4043	9.5002	9.4427	9.2747	5.4450	8.6130	5.4073
27. H	2.1877	1.0909	3.4099	3.5653	3.8306	3.0970	3.3059	4.4002
28. H	3.3994	3.8301	2.1540	5.6266	1.0878	6.1289	2.1616	8.4408
29. H	6.9532	5.6131	7.8910	4.4005	7.6818	4.8771	6.4714	3.5917
30. H	5.1046	5.0651	4.0893	5.6524	2.7358	7.0553	2.7568	9.1540
31. H	9.3481	7.9822	10.1799	6.0918	9.7901	7.1353	8.4771	5.5895
32. H	6.2386	5.8524	6.7744	7.9890	6.9383	2.6463	6.5945	3.7485
33. H	7.0911	6.0256	7.0391	3.7442	5.9243	7.2070	4.6253	7.9643
34. H	7.3397	7.0046	6.4790	6.4516	5.0932	8.6900	4.6691	10.4585
35. H	8.1118	7.3612	7.6331	5.6907	6.2970	8.7436	5.3460	9.9480
36. H	8.4966	8.1285	8.8278	9.9603	8.8103	5.0590	8.4647	5.6954
37. H	10.6978	9.4001	11.3935	7.9396	10.9025	7.8770	9.6226	6.3966
38. H	10.0749	8.9386	10.6712	8.3765	10.2242	6.7653	9.1036	5.6372
39. H	9.8516	8.9160	10.3355	9.1151	9.9515	6.2984	9.0296	5.6618
40. H	10.0757	9.4312	10.4216	10.4441	10.1602	6.4914	9.5305	6.4576
41. H	2.1666	3.3913	1.0909	6.3805	2.1540	5.6418	3.4114	7.9985
42. H	1.0889	2.1516	2.1785	5.5828	3.4082	4.2023	3.8705	6.1319
43. H	5.0340	3.7314	6.1090	3.2959	6.1275	3.7808	5.0838	3.2710
44. O	5.4156	4.3499	5.9143	1.1657	5.4848	6.7564	4.4229	7.2319
45. O	4.2985	2.9810	5.3046	3.1681	5.2886	3.0383	4.2648	3.1801
46. O	3.7282	3.5513	4.5414	6.4583	5.0910	1.1654	4.9554	3.4962
47. O	6.8470	6.0454	8.0249	7.2275	8.4296	3.5205	7.7639	1.1657
48. O	7.4589	6.1237	7.9081	3.5113	7.1607	6.5472	5.7564	6.3736
49. N	2.3948	1.3469	2.7703	2.8880	2.3913	3.8676	1.3646	5.5702
50. N	7.0416	5.8314	7.8487	5.5276	7.6039	4.0287	6.4865	2.8904
51. Ru	4.4246	3.1127	4.9156	1.8633	4.3402	4.3435	2.9933	5.1465
52. Ru	5.1831	4.1526	6.0585	5.1573	6.0606	1.8750	5.1938	1.8649
53. Cl	4.9708	3.9313	5.3227	4.3637	4.7721	3.2085	3.6928	4.3587

Atom	9	10	11	12	13	14	15	16
1. C	4.2387	6.2932	4.9733	7.5225	5.1965	8.8482	6.3584	6.6431
2. C	3.6444	4.9596	4.0215	6.2102	4.8614	7.5151	5.4263	5.8181
3. C	3.8004	6.7652	4.8714	8.3819	4.4252	9.6557	6.1544	7.2954
4. C	3.6229	2.6241	2.8269	5.1641	4.8660	6.0454	3.6753	6.9439
5. C	2.5526	6.0740	3.7917	8.1002	3.0390	9.2768	4.9645	7.2062
6. C	5.6394	5.5694	5.6628	4.9964	6.7757	6.3277	6.8477	2.8646
7. C	1.4617	4.6779	2.4596	6.8812	2.5152	7.9995	3.7395	6.4506
8. C	7.3872	5.6848	6.9503	3.6290	8.6579	4.8361	7.9525	2.8352
9. C	0.0000	4.1886	1.4232	6.8523	1.4090	7.7882	2.4191	6.7609
10. C	4.1886	0.0000	2.8616	3.3517	5.3070	3.9503	3.1332	5.5841
11. C	1.4232	2.8616	0.0000	5.7940	2.4609	6.6038	1.4058	6.3856
12. C	6.8523	3.3517	5.7940	0.0000	8.0647	1.3887	6.2538	4.0264
13. C	1.4090	5.3070	2.4609	8.0647	0.0000	8.9133	2.7923	7.7508
14. C	7.7882	3.9503	6.6038	1.3887	8.9133	0.0000	6.8057	4.9783
15. C	2.4191	3.1332	1.4058	6.2538	2.7923	6.8057	0.0000	7.1382
16. C	6.7609	5.5841	6.3856	4.0264	7.7508	4.9783	7.1382	0.0000
17. C	2.4321	5.4458	2.8424	8.3771	1.3916	9.0397	2.4307	8.3568
18. C	7.2930	6.7808	7.1572	5.4316	8.1485	6.3624	7.9494	1.4064
19. C	2.7936	4.5164	2.4458	7.5583	2.4099	8.0662	1.3988	8.0785
20. C	7.2424	4.6545	6.4024	2.3483	8.2696	2.7821	6.8095	2.4566
21. C	8.3830	4.8074	7.2367	2.3907	9.3938	1.3993	7.3143	4.8722
22. C	7.3283	5.5414	6.7344	3.6411	8.2646	4.2376	7.2438	1.4221
23. C	8.1315	5.1075	7.1420	2.7322	9.0919	2.4054	7.3125	3.7870
24. C	8.2340	7.7302	8.0923	6.2981	8.9466	7.0211	8.7305	2.4457
25. C	8.2691	6.6800	7.7265	4.8542	9.0546	5.1891	8.0987	2.4613
26. C	8.6847	7.6892	8.3518	6.0636	9.3726	6.5254	8.7994	2.8425
27. H	4.4367	4.7982	4.5183	5.5753	5.7463	6.9100	5.8865	5.4935
28. H	2.8093	6.7625	4.2047	8.9613	2.7525	10.0848	5.1677	7.9471
29. H	6.5502	3.0570	5.5106	1.0888	7.8430	2.1635	6.0981	4.5529
30. H	2.1734	6.2917	3.4493	8.9114	1.0905	9.8297	3.8828	8.2366
31. H	8.2234	4.1491	6.9628	2.1512	9.3560	1.0886	7.0874	6.0157
32. H	7.1987	7.1538	7.2473	6.0344	8.0525	7.0979	8.1775	2.1703
33. H	3.4183	2.6592	2.1700	5.7940	3.8823	6.1591	1.0905	7.2102

34.	H	3.4210	6.4926	3.9325	9.4028	2.1569	10.0256	3.4199	9.2257
35.	H	3.8852	5.0682	3.4275	8.0775	3.4004	8.4212	2.1576	8.7806
36.	H	8.8033	8.6787	8.8066	7.3623	9.4250	8.1103	9.4724	3.4276
37.	H	9.2278	5.5508	8.0260	3.3885	10.1783	2.1674	7.9555	5.8671
38.	H	8.8162	6.0113	7.8732	3.8196	9.6763	3.3959	7.9540	4.1929
39.	H	8.8618	6.9547	8.2002	5.0544	9.6057	5.0934	8.4113	3.4500
40.	H	9.5372	8.6065	9.2209	6.9975	10.1290	7.3303	9.5774	3.9326
41.	H	4.6993	7.8523	5.8682	9.4169	5.1073	10.7055	7.0989	8.0927
42.	H	5.3252	7.0981	6.0108	7.9908	6.2756	9.3513	7.4060	6.9979
43.	H	5.5576	3.3239	4.8481	3.0254	6.9559	4.2796	5.8428	4.7767
44.	O	4.4079	3.5284	3.7150	6.0063	5.5171	6.7897	4.3829	8.0532
45.	O	4.8069	3.2084	4.2364	3.3256	6.1973	4.6526	5.3405	4.2729
46.	O	6.0070	6.5619	6.2821	6.1571	7.0385	7.4907	7.5280	3.7200
47.	O	8.4870	6.6807	8.0579	4.3426	9.7741	5.4110	9.0700	3.7271
48.	O	5.1054	1.1670	3.7055	3.4415	6.0778	3.6087	3.5659	6.1728
49.	N	2.3823	4.0116	2.6816	5.8450	3.6980	7.0446	4.0873	5.7155
50.	N	6.5508	3.7653	5.6795	1.3469	7.7199	2.4035	6.2525	2.6851
51.	Ru	2.9550	1.8742	2.0767	4.1424	4.3061	5.1688	3.1485	5.2265
52.	Ru	5.6812	4.2952	5.2373	3.1475	6.9034	4.4578	6.2107	2.0698
53.	Cl	3.6709	3.2004	3.2030	3.9753	4.7162	5.0180	4.0199	3.1939

Atom		17	18	19	20	21	22	23	24
1.	C	6.5321	6.8678	7.0227	7.9994	9.6517	7.8100	9.2707	8.1287
2.	C	6.0687	6.2965	6.2978	6.8683	8.3683	6.8587	8.0819	7.5990
3.	C	5.8131	7.4017	6.5492	8.6928	10.3730	8.4211	9.9352	8.5431
4.	C	5.4003	7.9613	4.8957	6.6834	7.1318	7.3579	7.4064	9.1404
5.	C	4.4288	7.4052	5.2231	8.3764	9.9339	8.1724	9.5227	8.4610
6.	C	7.7736	3.1273	7.8026	4.6871	6.7907	4.1943	6.0861	4.5105
7.	C	3.7844	6.8804	4.2546	7.2971	8.6818	7.2668	8.3634	7.9597
8.	C	9.4562	3.6821	9.1376	3.6485	5.3562	3.6327	4.8591	4.9017
9.	C	2.4321	7.2930	2.7936	7.2424	8.3830	7.3283	8.1315	8.2340
10.	C	5.4458	6.7808	4.5164	4.6545	4.8074	5.5414	5.1075	7.7302
11.	C	2.8424	7.1572	2.4458	6.4024	7.2367	6.7344	7.1420	8.0923
12.	C	8.3771	5.4316	7.5583	2.3483	2.3907	3.6411	2.7322	6.2981
13.	C	1.3916	8.1485	2.4099	8.2696	9.3938	8.2646	9.0919	8.9466
14.	C	9.0397	6.3624	8.0662	2.7821	1.3993	4.2376	2.4054	7.0211
15.	C	2.4307	7.9494	1.3988	6.8095	7.3143	7.2438	7.3125	8.7305
16.	C	8.3568	1.4064	8.0785	2.4566	4.8722	1.4221	3.7870	2.4457
17.	C	0.0000	8.8284	1.4008	8.5625	9.4282	8.6586	9.2001	9.5035
18.	C	8.8284	0.0000	8.7376	3.7370	6.1529	2.4185	4.9583	1.3983
19.	C	1.4008	8.7376	0.0000	7.8911	8.4529	8.1879	8.3670	9.4042
20.	C	8.5625	3.7370	7.8911	0.0000	2.4240	1.4600	1.4070	4.2521
21.	C	9.4282	6.1529	8.4529	2.4240	0.0000	3.7969	1.3882	6.5419
22.	C	8.6586	2.4185	8.1879	1.4600	3.7969	0.0000	2.5465	2.7929
23.	C	9.2001	4.9583	8.3670	1.4070	1.3882	2.5465	0.0000	5.2138
24.	C	9.5035	1.3983	9.4042	4.2521	6.5419	2.7929	5.2138	0.0000
25.	C	9.3479	2.7925	8.8992	2.5145	4.4137	1.4098	3.0283	2.4098
26.	C	9.7481	2.4308	9.4790	3.7825	5.8010	2.4317	4.4174	1.4012
27.	H	6.8634	6.1007	6.9165	6.4186	7.8417	6.5155	7.6261	7.4633
28.	H	4.0968	8.0591	5.1305	9.1241	10.6738	8.8667	10.2299	9.0081
29.	H	8.2441	5.9244	7.4635	3.3090	3.3926	4.4543	3.8200	6.9464
30.	H	2.1460	8.4759	3.3958	9.0105	10.2967	8.8700	9.9125	9.2573
31.	H	9.4261	7.4100	8.3721	3.8699	2.1797	5.3237	3.4057	8.1035
32.	H	8.8765	1.0904	8.9339	4.6225	7.0398	3.4175	5.9189	2.1434
33.	H	3.4060	8.1574	2.1438	6.5052	6.6667	7.1302	6.8252	8.9048
34.	H	1.0902	9.6071	2.1679	9.4787	10.3457	9.5099	10.0824	10.1934
35.	H	2.1632	9.4664	1.0916	8.3830	8.7205	8.7430	8.6993	10.0363
36.	H	10.0266	2.1571	10.0514	5.3435	7.6252	3.8845	6.2874	1.0916
37.	H	10.0976	7.0945	9.0410	3.4144	1.0908	4.6941	2.1541	7.3547
38.	H	9.7157	5.1528	8.8988	2.1610	2.1518	2.7972	1.0876	5.1118
39.	H	9.7600	3.8830	9.1929	2.7582	4.0740	2.1750	2.7248	3.3953
40.	H	10.4294	3.4198	10.1680	4.6676	6.4639	3.4208	5.0809	2.1682
41.	H	6.4918	8.0539	7.3661	9.6411	11.3993	9.2751	10.9113	9.1455
42.	H	7.6178	7.1429	8.1053	8.4789	10.1811	8.2446	9.7885	8.4293
43.	H	7.6637	5.9159	7.1768	4.6093	5.4109	5.2811	5.5393	7.1883
44.	O	5.9880	9.0829	5.4873	7.7099	7.9565	8.4553	8.3606	10.2816
45.	O	6.9809	5.3139	6.6109	4.4746	5.6279	4.9320	5.5504	6.6108
46.	O	8.1523	3.5773	8.3663	5.7697	7.9335	5.1203	7.1758	4.8664
47.	O	10.5978	4.3973	10.2765	4.4277	5.9203	4.4194	5.4929	5.5008
48.	O	5.9811	7.4289	4.8550	4.8037	4.3933	5.8701	4.9269	8.2556
49.	N	4.8125	6.3053	4.9609	6.4825	7.8412	6.5663	7.5912	7.5131
50.	N	8.1257	4.0913	7.4643	1.3671	2.7817	2.3866	2.3974	4.9647
51.	Ru	4.9038	6.2108	4.4334	5.1564	6.0307	5.6566	6.0208	7.3369
52.	Ru	7.6455	3.1370	7.3390	2.9997	4.9410	2.9550	4.3518	4.4235
53.	Cl	5.2880	4.0061	4.9889	3.6999	5.3558	3.6703	4.7856	4.9794

Atom		25	26	27	28	29	30	31	32
1.	C	8.9432	9.0874	2.1877	3.3994	6.9532	5.1046	9.3481	6.2386
2.	C	8.0768	8.4043	1.0909	3.8301	5.6131	5.0651	7.9822	5.8524
3.	C	9.4427	9.5002	3.4099	2.1540	7.8910	4.0893	10.1799	6.7744
4.	C	8.6294	9.4427	3.5653	5.6266	4.4005	5.6524	6.0918	7.9890
5.	C	9.1425	9.2747	3.8306	1.0878	7.6818	2.7358	9.7901	6.9383
6.	C	5.3113	5.4450	3.0970	6.1289	4.8771	7.0553	7.1353	2.6463
7.	C	8.2999	8.6130	3.3059	2.1616	6.4714	2.7568	8.4771	6.5945
8.	C	4.8752	5.4073	4.4002	8.4408	3.5917	9.1540	5.5895	3.7485
9.	C	8.2691	8.6847	4.4367	2.8093	6.5502	2.1734	8.2234	7.1987
10.	C	6.6800	7.6892	4.7982	6.7625	3.0570	6.2917	4.1491	7.1538
11.	C	7.7265	8.3518	4.5183	4.2047	5.5106	3.4493	6.9628	7.2473
12.	C	4.8542	6.0636	5.5753	8.9613	1.0888	8.9114	2.1512	6.0344
13.	C	9.0546	9.3726	5.7463	2.7525	7.8430	1.0905	9.3560	8.0525
14.	C	5.1891	6.5254	6.9100	10.0848	2.1635	9.8297	1.0886	7.0979
15.	C	8.0987	8.7994	5.8865	5.1677	6.0981	3.8828	7.0874	8.1775
16.	C	2.4613	2.8425	5.4935	7.9471	4.5529	8.2366	6.0157	2.1703
17.	C	9.3479	9.7481	6.8634	4.0968	8.2441	2.1460	9.4261	8.8765
18.	C	2.7925	2.4308	6.1007	8.0591	5.9244	8.4759	7.4100	1.0904
19.	C	8.8992	9.4790	6.9165	5.1305	7.4635	3.3958	8.3721	8.9339
20.	C	2.5145	3.7825	6.4186	9.1241	3.3090	9.0105	3.8699	4.6225
21.	C	4.4137	5.8010	7.8417	10.6738	3.3926	10.2967	2.1797	7.0398
22.	C	1.4098	2.4317	6.5155	8.8667	4.4543	8.8700	5.3237	3.4175
23.	C	3.0283	4.4174	7.6261	10.2299	3.8200	9.9125	3.4057	5.9189
24.	C	2.4098	1.4012	7.4633	9.0081	6.9464	9.2573	8.1035	2.1434
25.	C	0.0000	1.3910	7.8134	9.7385	5.7581	9.6203	6.2678	3.8824
26.	C	1.3910	0.0000	8.2293	9.8048	6.8822	9.8012	7.6106	3.4061
27.	H	7.8134	8.2293	0.0000	4.9176	4.8975	6.0566	7.3438	5.7040
28.	H	9.7385	9.8048	4.9176	0.0000	8.5969	2.0891	10.6058	7.6014
29.	H	5.7581	6.8822	4.8975	8.5969	0.0000	8.6764	2.4980	6.3648
30.	H	9.6203	9.8012	6.0566	2.0891	8.6764	0.0000	10.3129	8.2615
31.	H	6.2678	7.6106	7.3438	10.6058	2.4980	10.3129	0.0000	8.1051
32.	H	3.8824	3.4061	5.7040	7.6014	6.3648	8.2615	8.1051	0.0000
33.	H	7.9811	8.8250	6.3200	6.2082	5.6838	4.9728	6.3420	8.5029
34.	H	10.1026	10.4289	7.8519	4.5564	9.3069	2.4720	10.4181	9.6433
35.	H	9.3604	9.9851	7.9396	6.1480	8.0526	4.2977	8.6701	9.7456
36.	H	3.4001	2.1634	8.0636	9.2895	7.9721	9.6247	9.1915	2.4555
37.	H	5.0921	6.4750	8.8827	11.6105	4.3117	11.1149	2.5278	8.0246

38.	H	2.7327	4.0758	8.5377	10.8716	4.9071	10.4720	4.3159	6.1941
39.	H	1.0905	2.1448	8.6395	10.5220	6.0590	10.2383	6.1243	4.9728
40.	H	2.1563	1.0902	9.2930	10.6249	7.8672	10.5342	8.4018	4.3030
41.	H	10.2390	10.1838	4.3328	2.4848	8.9334	4.5691	11.2468	7.3325
42.	H	9.3855	9.4712	2.5326	4.3176	7.3856	6.1362	9.8473	6.4123
43.	H	6.6873	7.5256	2.8827	7.1403	2.1362	7.6315	4.5814	5.9897
44.	O	9.7417	10.5829	4.2741	6.2090	5.1551	6.2565	6.6754	9.0835
45.	O	6.3184	7.0454	2.2593	6.2943	2.6611	6.8226	5.1081	5.3194
46.	O	6.0941	5.9956	3.3895	5.9489	6.0011	7.1421	8.2925	2.7708
47.	O	5.5288	5.9999	5.1698	9.4271	4.2758	10.2461	6.0797	4.4088
48.	O	6.8975	8.0241	5.9278	7.7880	3.3208	7.1169	3.6273	7.9278
49.	N	7.7392	8.1600	2.0564	3.3740	5.3340	4.0947	7.5021	6.0405
50.	N	3.7026	4.8165	5.2794	8.4414	2.0686	8.4756	3.3771	4.7352
51.	Ru	6.8826	7.6347	3.1113	5.1480	3.6614	5.1166	5.5322	6.3068
52.	Ru	4.3056	4.8984	3.6320	6.9668	3.1830	7.4464	5.2970	3.3033
53.	Cl	4.7192	5.2865	4.0073	5.4507	4.0887	5.3704	5.8000	4.2513

Atom		33	34	35	36	37	38	39	40
1.	C	7.0911	7.3397	8.1118	8.4966	10.6978	10.0749	9.8516	10.0757
2.	C	6.0256	7.0046	7.3612	8.1285	9.4001	8.9386	8.9160	9.4312
3.	C	7.0391	6.4790	7.6331	8.8278	11.3935	10.6712	10.3355	10.4216
4.	C	3.7442	6.4516	5.6907	9.9603	7.9396	8.3765	9.1151	10.4441
5.	C	5.9243	5.0932	6.2970	8.8103	10.9025	10.2242	9.9515	10.1602
6.	C	7.2070	8.6900	8.7436	5.0590	7.8770	6.7653	6.2984	6.4914
7.	C	4.6253	4.6691	5.3460	8.4647	9.6226	9.1036	9.0296	9.5305
8.	C	7.9643	10.4585	9.9480	5.6954	6.3966	5.6372	5.6618	6.4576
9.	C	3.4183	3.4210	3.8852	8.8033	9.2278	8.8162	8.8618	9.5372
10.	C	2.6592	6.4926	5.0682	8.6787	5.5508	6.0113	6.9547	8.6065
11.	C	2.1700	3.9325	3.4275	8.8066	8.0260	7.8732	8.2002	9.2209
12.	C	5.7940	9.4028	8.0775	7.3623	3.3885	3.8196	5.0544	6.9975
13.	C	3.8823	2.1569	3.4004	9.4250	10.1783	9.6763	9.6057	10.1290
14.	C	6.1591	10.0256	8.4212	8.1103	2.1674	3.3959	5.0934	7.3303
15.	C	1.0905	3.4199	2.1576	9.4724	7.9555	7.9540	8.4113	9.5774
16.	C	7.2102	9.2257	8.7806	3.4276	5.8671	4.1929	3.4500	3.9326
17.	C	3.4060	1.0902	2.1632	10.0266	10.0976	9.7157	9.7600	10.4294
18.	C	8.1574	9.6071	9.4664	2.1571	7.0945	5.1528	3.8830	3.4198
19.	C	2.1438	2.1679	1.0916	10.0514	9.0410	8.8988	9.1929	10.1680
20.	C	6.5052	9.4787	8.3830	5.3435	3.4144	2.1610	2.7582	4.6676
21.	C	6.6667	10.3457	8.7205	7.6252	1.0908	2.1518	4.0740	6.4639
22.	C	7.1302	9.5099	8.7430	3.8845	4.6941	2.7972	2.1750	3.4208
23.	C	6.8252	10.0824	8.6993	6.2874	2.1541	1.0876	2.7248	5.0809
24.	C	8.9048	10.1934	10.0363	1.0916	7.3547	5.1118	3.3953	2.1682
25.	C	7.9811	10.1026	9.3604	3.4001	5.0921	2.7327	1.0905	2.1563
26.	C	8.8250	10.4289	9.9851	2.1634	6.4750	4.0758	2.1448	1.0902
27.	H	6.3200	7.8519	7.9396	8.0636	8.8827	8.5377	8.6395	9.2930
28.	H	6.2082	4.5564	6.1480	9.2895	11.6105	10.8716	10.5220	10.6249
29.	H	5.6838	9.3069	8.0526	7.9721	4.3117	4.9071	6.0590	7.8672
30.	H	4.9728	2.4720	4.2977	9.6247	11.1149	10.4720	10.2383	10.5342
31.	H	6.3420	10.4181	8.6701	9.1915	2.5278	4.3159	6.1243	8.4018
32.	H	8.5029	9.6433	9.7456	2.4555	8.0246	6.1941	4.9728	4.3030
33.	H	0.0000	4.3031	2.4557	9.7286	7.2136	7.4759	8.1746	9.5902
34.	H	4.3031	0.0000	2.4982	10.6487	10.9765	10.5309	10.4903	11.0402
35.	H	2.4557	2.4982	0.0000	10.6989	9.1941	9.1607	9.5411	10.6050
36.	H	9.7286	10.6487	10.6989	0.0000	8.4195	6.1286	4.2968	2.4983
37.	H	7.2136	10.9765	9.1941	8.4195	0.0000	2.4843	4.5493	7.0100
38.	H	7.4759	10.5309	9.1607	6.1286	2.4843	0.0000	2.0682	4.5343
39.	H	8.1746	10.4903	9.5411	4.2968	4.5493	2.0682	0.0000	2.4703
40.	H	9.5902	11.0402	10.6050	2.4983	7.0100	4.5343	2.4703	0.0000
41.	H	8.0266	7.0311	8.4321	9.3185	12.4280	11.6165	11.1656	11.0684
42.	H	8.0978	8.4121	9.1932	8.7392	11.2456	10.6012	10.3359	10.4659
43.	H	5.7650	8.7476	7.9825	8.0705	6.3917	6.5828	7.2684	8.5961
44.	O	4.3950	6.9778	6.2012	11.1015	8.7003	9.3529	10.2003	11.5883
45.	O	5.4117	8.0504	7.4784	7.4463	6.6554	6.5352	6.9842	8.1205
46.	O	8.0092	9.0016	9.3524	5.1820	9.0167	7.7954	7.1344	6.9773
47.	O	9.0515	11.6050	11.0851	6.2145	6.8905	6.2198	6.2667	6.9884
48.	O	2.7637	6.9628	5.1729	9.2493	4.9502	5.7801	6.9916	8.8715
49.	N	4.7319	5.7955	6.0190	8.1130	8.8234	8.4219	8.4861	9.1534
50.	N	5.9724	9.1189	8.0549	6.0228	3.8724	3.3780	4.1000	5.7996
51.	Ru	3.3184	5.9915	5.3025	8.1578	6.9376	6.9214	7.4211	8.6245
52.	Ru	6.2973	8.6343	8.1536	5.2909	6.0308	5.1517	5.1195	5.9865
53.	Cl	4.2702	6.2417	5.7932	5.7821	6.3316	5.4529	5.3796	6.2429

Atom		41	42	43	44	45	46	47	48
1.	C	2.1666	1.0889	5.0340	5.4156	4.2985	3.7282	6.8470	7.4589
2.	C	3.3913	2.1516	3.7314	4.3499	2.9810	3.5513	6.0454	6.1237
3.	C	1.0909	2.1785	6.1090	5.9143	5.3046	4.5414	8.0249	7.9081
4.	C	6.3805	5.5828	3.2959	1.1657	3.1681	6.4583	7.2275	3.5113
5.	C	2.1540	3.4082	6.1275	5.4848	5.2886	5.0910	8.4296	7.1607
6.	C	5.6418	4.2023	3.7808	6.7564	3.0383	1.1654	3.5205	6.5472
7.	C	3.4114	3.8705	5.0838	4.4229	4.2648	4.9554	7.7639	5.7564
8.	C	7.9985	6.1319	3.2710	7.2319	3.1801	3.4962	1.1657	6.3736
9.	C	4.6993	5.3252	5.5576	4.4079	4.8069	6.0070	8.4870	5.1054
10.	C	7.8523	7.0981	3.3239	3.5284	3.2084	6.5619	6.6807	1.1670
11.	C	5.8682	6.0108	4.8481	3.7150	4.2364	6.2821	8.0579	3.7055
12.	C	9.4169	7.9908	3.0254	6.0063	3.3256	6.1571	4.3426	3.4415
13.	C	5.1073	6.2756	6.9559	5.5171	6.1973	7.0385	9.7741	6.0778
14.	C	10.7055	9.3513	4.2796	6.7897	4.6526	7.4907	5.4110	3.6087
15.	C	7.0989	7.4060	5.8428	4.3829	5.3405	7.5280	9.0700	3.5659
16.	C	8.0927	6.9979	4.7767	8.0532	4.2729	3.7200	3.7271	6.1728
17.	C	6.4918	7.6178	7.6637	5.9880	6.9809	8.1523	10.5978	5.9811
18.	C	8.0539	7.1429	5.9159	9.0829	5.3139	3.5773	4.3973	7.4289
19.	C	7.3661	8.1053	7.1768	5.4873	6.6109	8.3663	10.2765	4.8550
20.	C	9.6411	8.4789	4.6093	7.7099	4.4746	5.7697	4.4277	4.8037
21.	C	11.3993	10.1811	5.4109	7.9565	5.6279	7.9335	5.9203	4.3933
22.	C	9.2751	8.2446	5.2811	8.4553	4.9320	5.1203	4.4194	5.8701
23.	C	10.9113	9.7885	5.5393	8.3606	5.5504	7.1758	5.4929	4.9269
24.	C	9.1455	8.4293	7.1883	10.2816	6.6108	4.8664	5.5008	8.2556
25.	C	10.2390	9.3855	6.6873	9.7417	6.3184	6.0941	5.5288	6.8975
26.	C	10.1838	9.4712	7.5256	10.5829	7.0454	5.9956	5.9999	8.0241
27.	H	4.3328	2.5326	2.8827	4.2741	2.2593	3.3895	5.1698	5.9278
28.	H	2.4848	4.3176	7.1403	6.2090	6.2943	5.9489	9.4271	7.7880
29.	H	8.9334	7.3856	2.1362	5.1551	2.6611	6.0011	4.2758	3.3208
30.	H	4.5691	6.1362	7.6315	6.2565	6.8226	7.1421	10.2461	7.1169
31.	H	11.2468	9.8473	4.5814	6.6754	5.1081	8.2925	6.0797	3.6273
32.	H	7.3325	6.4123	5.9897	9.0835	5.3194	2.7708	4.4088	7.9278
33.	H	8.0266	8.0978	5.7650	4.3950	5.4117	8.0092	9.0515	2.7637
34.	H	7.0311	8.4121	8.7476	6.9778	8.0504	9.0016	11.6050	6.9628
35.	H	8.4321	9.1932	7.9825	6.2012	7.4784	9.3524	11.0851	5.1729
36.	H	9.3185	8.7392	8.0705	11.1015	7.4463	5.1820	6.2145	9.2493
37.	H	12.4280	11.2456	6.3917	8.7003	6.6554	9.0167	6.8905	4.9502
38.	H	11.6165	10.6012	6.5828	9.3529	6.5352	7.7954	6.2198	5.7801
39.	H	11.1656	10.3359	7.2684	10.2003	6.9842	7.1344	6.2667	6.9916
40.	H	11.0684	10.4659	8.5961	11.5883	8.1205	6.9773	6.9884	8.8715
41.	H	0.0000	2.5246	7.1163	6.8828	6.3223	5.0926	8.7758	8.9921

42.	H	2.5246	0.0000	5.3803	6.0909	4.7396	3.7133	6.7341	8.2593
43.	H	7.1163	5.3803	0.0000	4.0515	0.9730	4.7233	4.0196	4.1479
44.	O	6.8828	6.0909	4.0515	0.0000	4.0983	7.4062	8.0348	4.2038
45.	O	6.3223	4.7396	0.9730	4.0983	0.0000	3.9732	4.1068	4.1963
46.	O	5.0926	3.7133	4.7233	7.4062	3.9732	0.0000	4.1859	7.5885
47.	O	8.7758	6.7341	4.0196	8.0348	4.1068	4.1859	0.0000	7.3114
48.	O	8.9921	8.2593	4.1479	4.2038	4.1963	7.5885	7.3114	0.0000
49.	N	3.8611	3.3710	3.7739	3.7794	2.9690	4.2202	6.5642	5.1659
50.	N	8.8359	7.4993	3.2537	6.5172	3.2062	5.1828	3.7751	4.0910
51.	Ru	6.0058	5.2625	2.7720	3.0289	2.2247	5.1590	6.1918	3.0378
52.	Ru	6.9662	5.5390	2.7796	6.2064	2.2408	3.0374	3.0305	5.0976
53.	Cl	6.2987	5.7463	3.7894	5.2294	2.9941	4.0834	5.5244	4.0664

Atom		49	50	51	52	53
1.	C	2.3948	7.0416	4.4246	5.1831	4.9708
2.	C	1.3469	5.8314	3.1127	4.1526	3.9313
3.	C	2.7703	7.8487	4.9156	6.0585	5.3227
4.	C	2.8880	5.5276	1.8633	5.1573	4.3637
5.	C	2.3913	7.6039	4.3402	6.0606	4.7721
6.	C	3.8676	4.0287	4.3435	1.8750	3.2085
7.	C	1.3646	6.4865	2.9933	5.1938	3.6928
8.	C	5.5702	2.8904	5.1465	1.8649	4.3587
9.	C	2.3823	6.5508	2.9550	5.6812	3.6709
10.	C	4.0116	3.7653	1.8742	4.2952	3.2004
11.	C	2.6816	5.6795	2.0767	5.2373	3.2030
12.	C	5.8450	1.3469	4.1424	3.1475	3.9753
13.	C	3.6980	7.7199	4.3061	6.9034	4.7162
14.	C	7.0446	2.4035	5.1688	4.4578	5.0180
15.	C	4.0873	6.2525	3.1485	6.2107	4.0199
16.	C	5.7155	2.6851	5.2265	2.0698	3.1939
17.	C	4.8125	8.1257	4.9038	7.6455	5.2880
18.	C	6.3053	4.0913	6.2108	3.1370	4.0061
19.	C	4.9609	7.4643	4.4334	7.3390	4.9889
20.	C	6.4825	1.3671	5.1564	2.9997	3.6999
21.	C	7.8412	2.7817	6.0307	4.9410	5.3558
22.	C	6.5663	2.3866	5.6566	2.9550	3.6703
23.	C	7.5912	2.3974	6.0208	4.3518	4.7856
24.	C	7.5131	4.9647	7.3369	4.4235	4.9794
25.	C	7.7392	3.7026	6.8826	4.3056	4.7192
26.	C	8.1600	4.8165	7.6347	4.8984	5.2865
27.	H	2.0564	5.2794	3.1113	3.6320	4.0073
28.	H	3.3740	8.4414	5.1480	6.9668	5.4507
29.	H	5.3340	2.0686	3.6614	3.1830	4.0887
30.	H	4.0947	8.4756	5.1166	7.4464	5.3704
31.	H	7.5021	3.3771	5.5322	5.2970	5.8000
32.	H	6.0405	4.7352	6.3068	3.3033	4.2513
33.	H	4.7319	5.9724	3.3184	6.2973	4.2702
34.	H	5.7955	9.1189	5.9915	8.6343	6.2417
35.	H	6.0190	8.0549	5.3025	8.1536	5.7932
36.	H	8.1130	6.0228	8.1578	5.2909	5.7821
37.	H	8.8234	3.8724	6.9376	6.0308	6.3316
38.	H	8.4219	3.3780	6.9214	5.1517	5.4529
39.	H	8.4861	4.1000	7.4211	5.1195	5.3796
40.	H	9.1534	5.7996	8.6245	5.9865	6.2429
41.	H	3.8611	8.8359	6.0058	6.9662	6.2987
42.	H	3.3710	7.4993	5.2625	5.5390	5.7463
43.	H	3.7739	3.2537	2.7720	2.7796	3.7894
44.	O	3.7794	6.5172	3.0289	6.2064	5.5294
45.	O	2.9690	3.2062	2.2247	2.2408	2.9941
46.	O	4.2202	5.1828	5.1590	3.0374	4.0834
47.	O	6.5642	3.7751	6.1918	3.0305	5.5244
48.	O	5.1659	4.0910	3.0378	5.0976	4.0664
49.	N	0.0000	5.5162	2.1487	4.1654	3.1850
50.	N	5.5162	0.0000	4.1327	2.1643	3.2022
51.	Ru	2.1487	4.1327	0.0000	3.6414	2.5011
52.	Ru	4.1654	2.1643	3.6414	0.0000	2.4946
53.	Cl	3.1850	3.2022	2.5011	2.4946	0.0000

NATURAL POPULATIONS: Natural atomic orbital occupancies

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	C	1	s	Cor(1s)	1.99935	-9.79315
2	C	1	s	Val(2s)	1.01478	-0.23896
3	C	1	s	Ryd(3s)	0.00118	1.18139
4	C	1	s	Ryd(4s)	0.00016	14.75897
5	C	1	s	Ryd(5s)	0.00000	22.85790
6	C	1	s	Ryd(6s)	0.00000	41.45194
7	C	1	px	Val(2p)	1.03347	-0.07204
8	C	1	px	Ryd(3p)	0.00228	1.26524
9	C	1	px	Ryd(4p)	0.00017	3.46327
10	C	1	py	Val(2p)	1.08994	-0.10643
11	C	1	py	Ryd(3p)	0.00230	1.04067
12	C	1	py	Ryd(4p)	0.00019	3.04073
13	C	1	pz	Val(2p)	1.10251	-0.10277
14	C	1	pz	Ryd(3p)	0.00227	1.02966
15	C	1	pz	Ryd(4p)	0.00018	3.20311
16	C	1	dxy	Ryd(3d)	0.00072	2.46271
17	C	1	dxz	Ryd(3d)	0.00079	2.56948
18	C	1	dyz	Ryd(3d)	0.00088	2.88753
19	C	1	dx2y2	Ryd(3d)	0.00080	2.81166
20	C	1	dz2	Ryd(3d)	0.00052	2.06453
21	C	2	s	Cor(1s)	1.99935	-9.82595
22	C	2	s	Val(2s)	0.97261	-0.21647
23	C	2	s	Ryd(3s)	0.00288	1.11652
24	C	2	s	Ryd(4s)	0.00025	11.73971
25	C	2	s	Ryd(5s)	0.00000	25.97867
26	C	2	s	Ryd(6s)	0.00000	41.52754
27	C	2	px	Val(2p)	1.14897	-0.07106
28	C	2	px	Ryd(3p)	0.00385	1.60955
29	C	2	px	Ryd(4p)	0.00048	3.68255
30	C	2	py	Val(2p)	0.91604	-0.09706
31	C	2	py	Ryd(3p)	0.00487	0.97082
32	C	2	py	Ryd(4p)	0.00023	3.25218
33	C	2	pz	Val(2p)	0.91170	-0.09146
34	C	2	pz	Ryd(3p)	0.00399	0.96659
35	C	2	pz	Ryd(4p)	0.00030	3.60965
36	C	2	dxy	Ryd(3d)	0.00080	2.35137
37	C	2	dxz	Ryd(3d)	0.00083	2.45114
38	C	2	dyz	Ryd(3d)	0.00063	3.46182
39	C	2	dx2y2	Ryd(3d)	0.00099	2.90240
40	C	2	dz2	Ryd(3d)	0.00086	2.23580

41	C	3	s	Cor(1s)	1.99938	-9.80271
42	C	3	s	Val(2s)	1.00988	-0.24268
43	C	3	s	Ryd(3s)	0.00116	1.70920
44	C	3	s	Ryd(4s)	0.00012	12.34821
45	C	3	s	Ryd(6s)	0.00000	39.24667
46	C	3	s	Ryd(5s)	0.00000	27.61125
47	C	3	px	Val(2p)	1.13625	-0.07488
48	C	3	px	Ryd(3p)	0.00233	1.41552
49	C	3	px	Ryd(4p)	0.00007	3.99133
50	C	3	py	Val(2p)	0.99791	-0.10807
51	C	3	py	Ryd(3p)	0.00179	0.98195
52	C	3	py	Ryd(4p)	0.00011	2.80249
53	C	3	pz	Val(2p)	1.01083	-0.10350
54	C	3	pz	Ryd(3p)	0.00185	1.03156
55	C	3	pz	Ryd(4p)	0.00010	2.91123
56	C	3	dxy	Ryd(3d)	0.00072	2.30658
57	C	3	dxz	Ryd(3d)	0.00081	2.35557
58	C	3	dyz	Ryd(3d)	0.00080	3.42504
59	C	3	dx2y2	Ryd(3d)	0.00091	2.71197
60	C	3	dz2	Ryd(3d)	0.00061	2.10729
61	C	4	s	Cor(1s)	1.99944	-9.90050
62	C	4	s	Val(2s)	1.16236	-0.34025
63	C	4	s	Ryd(3s)	0.02265	2.62962
64	C	4	s	Ryd(4s)	0.00024	8.27405
65	C	4	s	Ryd(5s)	0.00000	26.91209
66	C	4	s	Ryd(6s)	0.00000	45.36258
67	C	4	px	Val(2p)	0.66763	-0.12573
68	C	4	px	Ryd(3p)	0.00377	1.05717
69	C	4	px	Ryd(4p)	0.00023	2.19409
70	C	4	py	Val(2p)	0.76627	-0.08992
71	C	4	py	Ryd(3p)	0.00748	1.14948
72	C	4	py	Ryd(4p)	0.00051	2.87308
73	C	4	pz	Val(2p)	0.75837	-0.08350
74	C	4	pz	Ryd(3p)	0.00738	1.13726
75	C	4	pz	Ryd(4p)	0.00048	2.84222
76	C	4	dxy	Ryd(3d)	0.00089	2.14067
77	C	4	dxz	Ryd(3d)	0.00104	2.23538
78	C	4	dyz	Ryd(3d)	0.00048	3.99396
79	C	4	dx2y2	Ryd(3d)	0.00073	2.39078
80	C	4	dz2	Ryd(3d)	0.00148	2.50349
81	C	5	s	Cor(1s)	1.99929	-9.79400
82	C	5	s	Val(2s)	1.00412	-0.22870
83	C	5	s	Ryd(3s)	0.00123	1.13486
84	C	5	s	Ryd(4s)	0.00022	11.06117
85	C	5	s	Ryd(6s)	0.00000	39.49287
86	C	5	s	Ryd(5s)	0.00000	29.10941
87	C	5	px	Val(2p)	1.13217	-0.06921
88	C	5	px	Ryd(3p)	0.00284	1.21376
89	C	5	px	Ryd(4p)	0.00015	3.97226
90	C	5	py	Val(2p)	1.04069	-0.10685
91	C	5	py	Ryd(3p)	0.00147	0.99270
92	C	5	py	Ryd(4p)	0.00020	2.80683
93	C	5	pz	Val(2p)	1.03925	-0.10274
94	C	5	pz	Ryd(3p)	0.00142	1.02087
95	C	5	pz	Ryd(4p)	0.00019	2.88875
96	C	5	dxy	Ryd(3d)	0.00072	2.29216
97	C	5	dxz	Ryd(3d)	0.00076	2.40364
98	C	5	dyz	Ryd(3d)	0.00085	3.34679
99	C	5	dx2y2	Ryd(3d)	0.00084	2.74108
100	C	5	dz2	Ryd(3d)	0.00054	2.10632
101	C	6	s	Cor(1s)	1.99945	-9.89704
102	C	6	s	Val(2s)	1.18534	-0.34320
103	C	6	s	Ryd(3s)	0.02108	2.78769
104	C	6	s	Ryd(4s)	0.00027	6.25878
105	C	6	s	Ryd(5s)	0.00000	25.47617
106	C	6	s	Ryd(6s)	0.00000	45.29418
107	C	6	px	Val(2p)	0.76621	-0.07364
108	C	6	px	Ryd(3p)	0.01006	0.93029
109	C	6	px	Ryd(4p)	0.00065	3.14495
110	C	6	py	Val(2p)	0.71166	-0.10181
111	C	6	py	Ryd(3p)	0.00595	0.99343
112	C	6	py	Ryd(4p)	0.00045	3.06560
113	C	6	pz	Val(2p)	0.68925	-0.11606
114	C	6	pz	Ryd(3p)	0.00481	0.94186
115	C	6	pz	Ryd(4p)	0.00029	2.65834
116	C	6	dxy	Ryd(3d)	0.00079	3.25833
117	C	6	dxz	Ryd(3d)	0.00096	2.82321
118	C	6	dyz	Ryd(3d)	0.00054	2.21150
119	C	6	dx2y2	Ryd(3d)	0.00137	2.61957
120	C	6	dz2	Ryd(3d)	0.00080	2.17780
121	C	7	s	Cor(1s)	1.99926	-9.83446
122	C	7	s	Val(2s)	0.90797	-0.17100
123	C	7	s	Ryd(3s)	0.00200	1.23014
124	C	7	s	Ryd(4s)	0.00022	13.85795
125	C	7	s	Ryd(5s)	0.00000	24.15492
126	C	7	s	Ryd(6s)	0.00000	42.86774
127	C	7	px	Val(2p)	0.94241	-0.05580
128	C	7	px	Ryd(3p)	0.00357	1.47681
129	C	7	px	Ryd(4p)	0.00057	4.14631
130	C	7	py	Val(2p)	0.95792	-0.09780
131	C	7	py	Ryd(3p)	0.00573	0.94704
132	C	7	py	Ryd(4p)	0.00016	3.15057
133	C	7	pz	Val(2p)	0.96499	-0.09751
134	C	7	pz	Ryd(3p)	0.00620	0.97952
135	C	7	pz	Ryd(4p)	0.00017	3.16139
136	C	7	dxy	Ryd(3d)	0.00084	2.69521
137	C	7	dxz	Ryd(3d)	0.00087	2.77864
138	C	7	dyz	Ryd(3d)	0.00054	3.50852
139	C	7	dx2y2	Ryd(3d)	0.00096	3.04554
140	C	7	dz2	Ryd(3d)	0.00093	2.22241
141	C	8	s	Cor(1s)	1.99944	-9.90194
142	C	8	s	Val(2s)	1.16555	-0.34278
143	C	8	s	Ryd(3s)	0.02294	1.72900
144	C	8	s	Ryd(4s)	0.00023	5.71245
145	C	8	s	Ryd(5s)	0.00000	27.01122
146	C	8	s	Ryd(6s)	0.00000	45.30702
147	C	8	px	Val(2p)	0.71676	-0.10321
148	C	8	px	Ryd(3p)	0.00639	1.03058
149	C	8	px	Ryd(4p)	0.00043	2.60058
150	C	8	py	Val(2p)	0.76632	-0.09308
151	C	8	py	Ryd(3p)	0.00739	1.01928

152	C	8	py	Ryd(4p)	0.00050	2.85993
153	C	8	pz	Val(2p)	0.71045	-0.10839
154	C	8	pz	Ryd(3p)	0.00460	1.08076
155	C	8	pz	Ryd(4p)	0.00029	2.41705
156	C	8	dxy	Ryd(3d)	0.00063	3.25969
157	C	8	dxz	Ryd(3d)	0.00067	2.52180
158	C	8	dyz	Ryd(3d)	0.00073	2.80837
159	C	8	dx2y2	Ryd(3d)	0.00151	2.37121
160	C	8	dz2	Ryd(3d)	0.00108	2.18780
161	C	9	s	Cor(1s)	1.99918	-9.77454
162	C	9	s	Val(2s)	0.94995	-0.15605
163	C	9	s	Ryd(3s)	0.00166	1.10777
164	C	9	s	Ryd(4s)	0.00016	15.42363
165	C	9	s	Ryd(5s)	0.00000	25.56670
166	C	9	s	Ryd(6s)	0.00000	41.86693
167	C	9	px	Val(2p)	1.09857	-0.06524
168	C	9	px	Ryd(3p)	0.00290	1.29447
169	C	9	px	Ryd(4p)	0.00051	4.07177
170	C	9	py	Val(2p)	1.03541	-0.07777
171	C	9	py	Ryd(3p)	0.00577	0.97792
172	C	9	py	Ryd(4p)	0.00021	3.47821
173	C	9	pz	Val(2p)	1.03847	-0.07701
174	C	9	pz	Ryd(3p)	0.00546	0.91728
175	C	9	pz	Ryd(4p)	0.00019	3.41459
176	C	9	dxy	Ryd(3d)	0.00069	2.51667
177	C	9	dxz	Ryd(3d)	0.00071	2.53405
178	C	9	dyz	Ryd(3d)	0.00067	3.40373
179	C	9	dx2y2	Ryd(3d)	0.00085	2.87329
180	C	9	dz2	Ryd(3d)	0.00058	2.18511
181	C	10	s	Cor(1s)	1.99945	-9.89526
182	C	10	s	Val(2s)	1.19057	-0.33962
183	C	10	s	Ryd(3s)	0.02224	3.17588
184	C	10	s	Ryd(4s)	0.00028	7.08053
185	C	10	s	Ryd(5s)	0.00000	25.24557
186	C	10	s	Ryd(6s)	0.00000	45.55751
187	C	10	px	Val(2p)	0.76030	-0.08345
188	C	10	px	Ryd(3p)	0.00772	1.14257
189	C	10	px	Ryd(4p)	0.00049	3.30981
190	C	10	py	Val(2p)	0.71229	-0.10447
191	C	10	py	Ryd(3p)	0.00588	1.04042
192	C	10	py	Ryd(4p)	0.00042	3.04029
193	C	10	pz	Val(2p)	0.70892	-0.10350
194	C	10	pz	Ryd(3p)	0.00758	1.00624
195	C	10	pz	Ryd(4p)	0.00048	2.66848
196	C	10	dxy	Ryd(3d)	0.00071	2.93048
197	C	10	dxz	Ryd(3d)	0.00063	3.18948
198	C	10	dyz	Ryd(3d)	0.00065	2.45229
199	C	10	dx2y2	Ryd(3d)	0.00133	2.39500
200	C	10	dz2	Ryd(3d)	0.00116	2.18821
201	C	11	s	Cor(1s)	1.99907	-9.78078
202	C	11	s	Val(2s)	1.02733	-0.20600
203	C	11	s	Ryd(3s)	0.00554	2.71038
204	C	11	s	Ryd(4s)	0.00027	14.13423
205	C	11	s	Ryd(5s)	0.00000	26.90260
206	C	11	s	Ryd(6s)	0.00000	40.47168
207	C	11	px	Val(2p)	1.03778	-0.06278
208	C	11	px	Ryd(3p)	0.01027	1.10308
209	C	11	px	Ryd(4p)	0.00034	3.95041
210	C	11	py	Val(2p)	0.97346	-0.08169
211	C	11	py	Ryd(3p)	0.00947	0.97163
212	C	11	py	Ryd(4p)	0.00028	3.56713
213	C	11	pz	Val(2p)	0.96273	-0.07660
214	C	11	pz	Ryd(3p)	0.00935	0.84110
215	C	11	pz	Ryd(4p)	0.00026	3.42003
216	C	11	dxy	Ryd(3d)	0.00051	2.65763
217	C	11	dxz	Ryd(3d)	0.00050	2.53094
218	C	11	dyz	Ryd(3d)	0.00085	3.36570
219	C	11	dx2y2	Ryd(3d)	0.00100	2.83844
220	C	11	dz2	Ryd(3d)	0.00069	2.21317
221	C	12	s	Cor(1s)	1.99935	-9.83875
222	C	12	s	Val(2s)	0.96194	-0.22451
223	C	12	s	Ryd(3s)	0.00275	1.08893
224	C	12	s	Ryd(4s)	0.00025	11.63756
225	C	12	s	Ryd(5s)	0.00000	25.81380
226	C	12	s	Ryd(6s)	0.00000	41.69128
227	C	12	px	Val(2p)	0.94061	-0.09387
228	C	12	px	Ryd(3p)	0.00319	1.05375
229	C	12	px	Ryd(4p)	0.00048	3.49442
230	C	12	py	Val(2p)	0.92644	-0.10964
231	C	12	py	Ryd(3p)	0.00498	0.88655
232	C	12	py	Ryd(4p)	0.00023	2.98382
233	C	12	pz	Val(2p)	1.11682	-0.09295
234	C	12	pz	Ryd(3p)	0.00505	1.25124
235	C	12	pz	Ryd(4p)	0.00026	3.43841
236	C	12	dxy	Ryd(3d)	0.00072	3.27113
237	C	12	dxz	Ryd(3d)	0.00092	2.87485
238	C	12	dyz	Ryd(3d)	0.00070	2.53101
239	C	12	dx2y2	Ryd(3d)	0.00086	2.08829
240	C	12	dz2	Ryd(3d)	0.00090	2.52233
241	C	13	s	Cor(1s)	1.99930	-9.77248
242	C	13	s	Val(2s)	0.99410	-0.20014
243	C	13	s	Ryd(3s)	0.00128	1.14319
244	C	13	s	Ryd(4s)	0.00024	10.59404
245	C	13	s	Ryd(6s)	0.00000	39.00237
246	C	13	s	Ryd(5s)	0.00000	30.11588
247	C	13	px	Val(2p)	1.13286	-0.04209
248	C	13	px	Ryd(3p)	0.00293	1.24941
249	C	13	px	Ryd(4p)	0.00015	3.87466
250	C	13	py	Val(2p)	1.02338	-0.07909
251	C	13	py	Ryd(3p)	0.00175	0.92926
252	C	13	py	Ryd(4p)	0.00018	2.85748
253	C	13	pz	Val(2p)	1.02284	-0.07966
254	C	13	pz	Ryd(3p)	0.00179	0.92811
255	C	13	pz	Ryd(4p)	0.00018	2.87111
256	C	13	dxy	Ryd(3d)	0.00069	2.43440
257	C	13	dxz	Ryd(3d)	0.00065	2.44223
258	C	13	dyz	Ryd(3d)	0.00082	3.48540
259	C	13	dx2y2	Ryd(3d)	0.00083	2.66076
260	C	13	dz2	Ryd(3d)	0.00057	2.10467
261	C	14	s	Cor(1s)	1.99934	-9.79932

262	C 14	s	Val(2s)	1.01382	-0.24534
263	C 14	s	Ryd(3s)	0.00115	1.15768
264	C 14	s	Ryd(4s)	0.00016	14.89671
265	C 14	s	Ryd(5s)	0.00000	22.63493
266	C 14	s	Ryd(6s)	0.00000	41.39231
267	C 14	px	Val(2p)	1.08721	-0.10161
268	C 14	px	Ryd(3p)	0.00262	1.04287
269	C 14	px	Ryd(4p)	0.00017	3.45591
270	C 14	py	Val(2p)	1.08826	-0.11377
271	C 14	py	Ryd(3p)	0.00234	1.02199
272	C 14	py	Ryd(4p)	0.00019	2.97371
273	C 14	pz	Val(2p)	1.05081	-0.08655
274	C 14	pz	Ryd(3p)	0.00193	1.24355
275	C 14	pz	Ryd(4p)	0.00019	3.15521
276	C 14	dxy	Ryd(3d)	0.00082	2.77853
277	C 14	dxz	Ryd(3d)	0.00082	2.72267
278	C 14	dyz	Ryd(3d)	0.00077	2.52390
279	C 14	dx2y2	Ryd(3d)	0.00049	1.97028
280	C 14	dz2	Ryd(3d)	0.00080	2.74433
281	C 15	s	Cor(1s)	1.99930	-9.75945
282	C 15	s	Val(2s)	1.01057	-0.19998
283	C 15	s	Ryd(3s)	0.00164	1.32324
284	C 15	s	Ryd(4s)	0.00016	13.12139
285	C 15	s	Ryd(6s)	0.00000	41.66772
286	C 15	s	Ryd(5s)	0.00000	25.15032
287	C 15	px	Val(2p)	1.14643	-0.03867
288	C 15	px	Ryd(3p)	0.00407	1.57841
289	C 15	px	Ryd(4p)	0.00026	3.80713
290	C 15	py	Val(2p)	1.04889	-0.07215
291	C 15	py	Ryd(3p)	0.00274	1.00420
292	C 15	py	Ryd(4p)	0.00025	3.69914
293	C 15	pz	Val(2p)	1.04128	-0.07433
294	C 15	pz	Ryd(3p)	0.00270	0.87063
295	C 15	pz	Ryd(4p)	0.00024	3.35981
296	C 15	dxy	Ryd(3d)	0.00081	2.41731
297	C 15	dxz	Ryd(3d)	0.00076	2.40194
298	C 15	dyz	Ryd(3d)	0.00087	3.20883
299	C 15	dx2y2	Ryd(3d)	0.00086	2.65723
300	C 15	dz2	Ryd(3d)	0.00049	2.06955
301	C 16	s	Cor(1s)	1.99908	-9.78197
302	C 16	s	Val(2s)	1.02606	-0.21084
303	C 16	s	Ryd(3s)	0.00518	2.58281
304	C 16	s	Ryd(4s)	0.00027	13.75188
305	C 16	s	Ryd(5s)	0.00000	27.02058
306	C 16	s	Ryd(6s)	0.00000	40.30294
307	C 16	px	Val(2p)	0.93340	-0.04980
308	C 16	px	Ryd(3p)	0.00764	0.75240
309	C 16	px	Ryd(4p)	0.00028	3.47924
310	C 16	py	Val(2p)	0.96885	-0.08183
311	C 16	py	Ryd(3p)	0.00901	0.69248
312	C 16	py	Ryd(4p)	0.00028	3.46446
313	C 16	pz	Val(2p)	1.06884	-0.09528
314	C 16	pz	Ryd(3p)	0.01232	0.96286
315	C 16	pz	Ryd(4p)	0.00031	3.86412
316	C 16	dxy	Ryd(3d)	0.00080	3.33644
317	C 16	dxz	Ryd(3d)	0.00108	2.83407
318	C 16	dyz	Ryd(3d)	0.00059	2.49586
319	C 16	dx2y2	Ryd(3d)	0.00050	2.06373
320	C 16	dz2	Ryd(3d)	0.00058	2.48336
321	C 17	s	Cor(1s)	1.99937	-9.76593
322	C 17	s	Val(2s)	1.00270	-0.20925
323	C 17	s	Ryd(3s)	0.00128	1.69032
324	C 17	s	Ryd(4s)	0.00013	10.79046
325	C 17	s	Ryd(6s)	0.00000	39.29143
326	C 17	s	Ryd(5s)	0.00000	28.97771
327	C 17	px	Val(2p)	1.11448	-0.04559
328	C 17	px	Ryd(3p)	0.00240	1.31718
329	C 17	px	Ryd(4p)	0.00010	3.37876
330	C 17	py	Val(2p)	1.04999	-0.07520
331	C 17	py	Ryd(3p)	0.00254	0.91764
332	C 17	py	Ryd(4p)	0.00015	2.81652
333	C 17	pz	Val(2p)	1.05306	-0.07582
334	C 17	pz	Ryd(3p)	0.00252	0.90841
335	C 17	pz	Ryd(4p)	0.00015	2.80837
336	C 17	dxy	Ryd(3d)	0.00074	2.34013
337	C 17	dxz	Ryd(3d)	0.00073	2.30579
338	C 17	dyz	Ryd(3d)	0.00081	3.39679
339	C 17	dx2y2	Ryd(3d)	0.00086	2.81384
340	C 17	dz2	Ryd(3d)	0.00051	2.14161
341	C 18	s	Cor(1s)	1.99930	-9.76141
342	C 18	s	Val(2s)	1.01095	-0.20207
343	C 18	s	Ryd(3s)	0.00162	1.32830
344	C 18	s	Ryd(4s)	0.00016	12.91951
345	C 18	s	Ryd(6s)	0.00000	41.63261
346	C 18	s	Ryd(5s)	0.00000	25.11890
347	C 18	px	Val(2p)	1.09384	-0.07092
348	C 18	px	Ryd(3p)	0.00362	0.97203
349	C 18	px	Ryd(4p)	0.00016	3.34419
350	C 18	py	Val(2p)	1.05037	-0.07591
351	C 18	py	Ryd(3p)	0.00279	0.79188
352	C 18	py	Ryd(4p)	0.00024	3.22036
353	C 18	pz	Val(2p)	1.09166	-0.04826
354	C 18	pz	Ryd(3p)	0.00294	1.23427
355	C 18	pz	Ryd(4p)	0.00032	3.26531
356	C 18	dxy	Ryd(3d)	0.00085	3.01037
357	C 18	dxz	Ryd(3d)	0.00080	2.41811
358	C 18	dyz	Ryd(3d)	0.00084	2.59701
359	C 18	dx2y2	Ryd(3d)	0.00041	1.89126
360	C 18	dz2	Ryd(3d)	0.00090	2.75136
361	C 19	s	Cor(1s)	1.99937	-9.76929
362	C 19	s	Val(2s)	1.00949	-0.21196
363	C 19	s	Ryd(3s)	0.00115	1.69677
364	C 19	s	Ryd(4s)	0.00016	11.38578
365	C 19	s	Ryd(5s)	0.00000	29.11434
366	C 19	s	Ryd(6s)	0.00000	38.46814
367	C 19	px	Val(2p)	1.03432	-0.04040
368	C 19	px	Ryd(3p)	0.00220	1.32010
369	C 19	px	Ryd(4p)	0.00015	3.25015
370	C 19	py	Val(2p)	1.07024	-0.07487
371	C 19	py	Ryd(3p)	0.00236	0.99067
372	C 19	py	Ryd(4p)	0.00012	3.05383

373	C 19	pz	Val(2p)	1.06499	-0.07623
374	C 19	pz	Ryd(3p)	0.00234	0.95997
375	C 19	pz	Ryd(4p)	0.00012	2.93657
376	C 19	dxy	Ryd(3d)	0.00075	2.52879
377	C 19	dxz	Ryd(3d)	0.00074	2.50170
378	C 19	dyz	Ryd(3d)	0.00087	3.02136
379	C 19	dx2y2	Ryd(3d)	0.00087	2.86173
380	C 19	dz2	Ryd(3d)	0.00047	2.13242
381	C 20	s	Cor(1s)	1.99926	-9.83976
382	C 20	s	Val(2s)	0.90906	-0.17641
383	C 20	s	Ryd(3s)	0.00195	1.21972
384	C 20	s	Ryd(4s)	0.00022	13.79434
385	C 20	s	Ryd(5s)	0.00000	24.12429
386	C 20	s	Ryd(6s)	0.00000	42.78640
387	C 20	px	Val(2p)	0.99774	-0.09652
388	C 20	px	Ryd(3p)	0.00516	1.00469
389	C 20	px	Ryd(4p)	0.00032	3.20493
390	C 20	py	Val(2p)	0.95891	-0.10324
391	C 20	py	Ryd(3p)	0.00565	0.91207
392	C 20	py	Ryd(4p)	0.00016	3.12457
393	C 20	pz	Val(2p)	0.90476	-0.06804
394	C 20	pz	Ryd(3p)	0.00468	1.33293
395	C 20	pz	Ryd(4p)	0.00042	3.75112
396	C 20	dxy	Ryd(3d)	0.00063	3.30188
397	C 20	dxz	Ryd(3d)	0.00098	2.84973
398	C 20	dyz	Ryd(3d)	0.00076	2.83731
399	C 20	dx2y2	Ryd(3d)	0.00091	2.05745
400	C 20	dz2	Ryd(3d)	0.00090	3.07355
401	C 21	s	Cor(1s)	1.99938	-9.80762
402	C 21	s	Val(2s)	1.00957	-0.24736
403	C 21	s	Ryd(3s)	0.00112	1.73132
404	C 21	s	Ryd(4s)	0.00013	12.08443
405	C 21	s	Ryd(6s)	0.00000	39.46529
406	C 21	s	Ryd(5s)	0.00000	27.35105
407	C 21	px	Val(2p)	1.07718	-0.10188
408	C 21	px	Ryd(3p)	0.00191	1.13893
409	C 21	px	Ryd(4p)	0.00009	3.17398
410	C 21	py	Val(2p)	0.99729	-0.11374
411	C 21	py	Ryd(3p)	0.00176	0.97702
412	C 21	py	Ryd(4p)	0.00011	2.76829
413	C 21	pz	Val(2p)	1.06868	-0.08572
414	C 21	pz	Ryd(3p)	0.00227	1.32344
415	C 21	pz	Ryd(4p)	0.00008	3.69509
416	C 21	dxy	Ryd(3d)	0.00080	3.09646
417	C 21	dxz	Ryd(3d)	0.00093	2.49436
418	C 21	dyz	Ryd(3d)	0.00072	2.59346
419	C 21	dx2y2	Ryd(3d)	0.00054	1.90414
420	C 21	dz2	Ryd(3d)	0.00086	2.80246
421	C 22	s	Cor(1s)	1.99918	-9.77656
422	C 22	s	Val(2s)	0.94938	-0.15844
423	C 22	s	Ryd(3s)	0.00163	1.06227
424	C 22	s	Ryd(4s)	0.00016	15.31901
425	C 22	s	Ryd(5s)	0.00000	25.55531
426	C 22	s	Ryd(6s)	0.00000	41.78573
427	C 22	px	Val(2p)	1.05551	-0.08012
428	C 22	px	Ryd(3p)	0.00562	0.96223
429	C 22	px	Ryd(4p)	0.00022	3.57101
430	C 22	py	Val(2p)	1.03582	-0.08121
431	C 22	py	Ryd(3p)	0.00587	0.84501
432	C 22	py	Ryd(4p)	0.00020	3.29970
433	C 22	pz	Val(2p)	1.08347	-0.06897
434	C 22	pz	Ryd(3p)	0.00275	1.12221
435	C 22	pz	Ryd(4p)	0.00049	3.68342
436	C 22	dxy	Ryd(3d)	0.00071	3.14910
437	C 22	dxz	Ryd(3d)	0.00074	2.74360
438	C 22	dyz	Ryd(3d)	0.00065	2.73644
439	C 22	dx2y2	Ryd(3d)	0.00046	1.94170
440	C 22	dz2	Ryd(3d)	0.00094	2.84398
441	C 23	s	Cor(1s)	1.99929	-9.79850
442	C 23	s	Val(2s)	1.00462	-0.23361
443	C 23	s	Ryd(3s)	0.00121	1.13719
444	C 23	s	Ryd(4s)	0.00022	10.87075
445	C 23	s	Ryd(6s)	0.00000	39.54202
446	C 23	s	Ryd(5s)	0.00000	29.20437
447	C 23	px	Val(2p)	1.02353	-0.09617
448	C 23	px	Ryd(3p)	0.00172	0.99137
449	C 23	px	Ryd(4p)	0.00016	3.30119
450	C 23	py	Val(2p)	1.03587	-0.11175
451	C 23	py	Ryd(3p)	0.00148	0.98281
452	C 23	py	Ryd(4p)	0.00020	2.79996
453	C 23	pz	Val(2p)	1.14892	-0.08440
454	C 23	pz	Ryd(3p)	0.00249	1.22794
455	C 23	pz	Ryd(4p)	0.00018	3.47787
456	C 23	dxy	Ryd(3d)	0.00077	3.20189
457	C 23	dxz	Ryd(3d)	0.00086	2.76138
458	C 23	dyz	Ryd(3d)	0.00079	2.44264
459	C 23	dx2y2	Ryd(3d)	0.00045	2.01361
460	C 23	dz2	Ryd(3d)	0.00083	2.45900
461	C 24	s	Cor(1s)	1.99937	-9.77140
462	C 24	s	Val(2s)	1.00987	-0.21430
463	C 24	s	Ryd(3s)	0.00115	1.71953
464	C 24	s	Ryd(4s)	0.00016	11.38869
465	C 24	s	Ryd(5s)	0.00000	29.05947
466	C 24	s	Ryd(6s)	0.00000	38.46909
467	C 24	px	Val(2p)	1.06351	-0.07209
468	C 24	px	Ryd(3p)	0.00216	1.05864
469	C 24	px	Ryd(4p)	0.00013	2.85639
470	C 24	py	Val(2p)	1.07036	-0.07668
471	C 24	py	Ryd(3p)	0.00235	0.96127
472	C 24	py	Ryd(4p)	0.00012	2.89104
473	C 24	pz	Val(2p)	1.03291	-0.04894
474	C 24	pz	Ryd(3p)	0.00234	1.19807
475	C 24	pz	Ryd(4p)	0.00014	3.23870
476	C 24	dxy	Ryd(3d)	0.00088	2.86322
477	C 24	dxz	Ryd(3d)	0.00084	2.73131
478	C 24	dyz	Ryd(3d)	0.00075	2.68674
479	C 24	dx2y2	Ryd(3d)	0.00035	1.88466
480	C 24	dz2	Ryd(3d)	0.00089	2.86152
481	C 25	s	Cor(1s)	1.99930	-9.77486
482	C 25	s	Val(2s)	0.99408	-0.20266

483	C 25	s	Ryd(3s)	0.00128	1.13032
484	C 25	s	Ryd(4s)	0.00025	10.52977
485	C 25	s	Ryd(6s)	0.00000	38.93275
486	C 25	s	Ryd(5s)	0.00000	30.21501
487	C 25	px	Val(2p)	1.06966	-0.07823
488	C 25	px	Ryd(3p)	0.00200	1.05554
489	C 25	px	Ryd(4p)	0.00018	2.89064
490	C 25	py	Val(2p)	1.02474	-0.08131
491	C 25	py	Ryd(3p)	0.00175	0.93597
492	C 25	py	Ryd(4p)	0.00018	2.85312
493	C 25	pz	Val(2p)	1.08333	-0.04858
494	C 25	pz	Ryd(3p)	0.00270	1.09272
495	C 25	pz	Ryd(4p)	0.00014	3.79141
496	C 25	dxy	Ryd(3d)	0.00081	3.19919
497	C 25	dxz	Ryd(3d)	0.00082	2.43291
498	C 25	dyz	Ryd(3d)	0.00070	2.70818
499	C 25	dx2y2	Ryd(3d)	0.00045	1.89555
500	C 25	dz2	Ryd(3d)	0.00077	2.88138
501	C 26	s	Cor(1s)	1.99937	-9.76795
502	C 26	s	Val(2s)	1.00272	-0.21132
503	C 26	s	Ryd(3s)	0.00128	1.69344
504	C 26	s	Ryd(4s)	0.00013	10.54289
505	C 26	s	Ryd(6s)	0.00000	39.30640
506	C 26	s	Ryd(5s)	0.00000	28.95545
507	C 26	px	Val(2p)	1.02692	-0.07271
508	C 26	px	Ryd(3p)	0.00258	0.96377
509	C 26	px	Ryd(4p)	0.00014	2.78622
510	C 26	py	Val(2p)	1.04845	-0.07697
511	C 26	py	Ryd(3p)	0.00253	0.92108
512	C 26	py	Ryd(4p)	0.00015	2.81194
513	C 26	pz	Val(2p)	1.14170	-0.05312
514	C 26	pz	Ryd(3p)	0.00234	1.25804
515	C 26	pz	Ryd(4p)	0.00011	3.37310
516	C 26	dxy	Ryd(3d)	0.00078	3.31217
517	C 26	dxz	Ryd(3d)	0.00076	2.70146
518	C 26	dyz	Ryd(3d)	0.00077	2.44123
519	C 26	dx2y2	Ryd(3d)	0.00043	1.94610
520	C 26	dz2	Ryd(3d)	0.00091	2.58774
521	H 27	s	Val(1s)	0.75315	0.04123
522	H 27	s	Ryd(2s)	0.00135	1.59322
523	H 27	s	Ryd(3s)	0.00054	1.85395
524	H 27	px	Ryd(2p)	0.00082	3.06329
525	H 27	py	Ryd(2p)	0.00025	1.51359
526	H 27	pz	Ryd(2p)	0.00016	1.50961
527	H 28	s	Val(1s)	0.77587	0.02446
528	H 28	s	Ryd(3s)	0.00043	1.98041
529	H 28	s	Ryd(2s)	0.00022	1.70044
530	H 28	px	Ryd(2p)	0.00044	3.37030
531	H 28	py	Ryd(2p)	0.00032	1.52414
532	H 28	pz	Ryd(2p)	0.00030	1.52460
533	H 29	s	Val(1s)	0.78958	0.00446
534	H 29	s	Ryd(2s)	0.00146	1.52513
535	H 29	s	Ryd(3s)	0.00052	1.94261
536	H 29	px	Ryd(2p)	0.00025	1.44040
537	H 29	py	Ryd(2p)	0.00038	1.55405
538	H 29	pz	Ryd(2p)	0.00073	3.17327
539	H 30	s	Val(1s)	0.79464	0.03600
540	H 30	s	Ryd(3s)	0.00049	1.98973
541	H 30	s	Ryd(2s)	0.00025	1.61468
542	H 30	px	Ryd(2p)	0.00054	3.77820
543	H 30	py	Ryd(2p)	0.00035	1.38674
544	H 30	pz	Ryd(2p)	0.00034	1.34786
545	H 31	s	Val(1s)	0.76554	0.02359
546	H 31	s	Ryd(2s)	0.00035	1.59988
547	H 31	s	Ryd(3s)	0.00019	2.14183
548	H 31	px	Ryd(2p)	0.00038	2.08268
549	H 31	py	Ryd(2p)	0.00050	2.09584
550	H 31	pz	Ryd(2p)	0.00014	1.61886
551	H 32	s	Val(1s)	0.78249	0.05509
552	H 32	s	Ryd(3s)	0.00109	1.81774
553	H 32	s	Ryd(2s)	0.00053	1.81631
554	H 32	px	Ryd(2p)	0.00051	2.17526
555	H 32	py	Ryd(2p)	0.00029	1.42433
556	H 32	pz	Ryd(2p)	0.00040	2.46388
557	H 33	s	Val(1s)	0.78259	0.05710
558	H 33	s	Ryd(3s)	0.00109	1.82693
559	H 33	s	Ryd(2s)	0.00052	1.81340
560	H 33	px	Ryd(2p)	0.00064	3.44765
561	H 33	py	Ryd(2p)	0.00028	1.39408
562	H 33	pz	Ryd(2p)	0.00028	1.35489
563	H 34	s	Val(1s)	0.78168	0.04764
564	H 34	s	Ryd(3s)	0.00044	2.04171
565	H 34	s	Ryd(2s)	0.00022	1.83489
566	H 34	px	Ryd(2p)	0.00028	2.78997
567	H 34	py	Ryd(2p)	0.00040	1.58254
568	H 34	pz	Ryd(2p)	0.00042	1.64173
569	H 35	s	Val(1s)	0.78184	0.04896
570	H 35	s	Ryd(2s)	0.00036	1.78555
571	H 35	s	Ryd(3s)	0.00015	2.26444
572	H 35	px	Ryd(2p)	0.00007	1.50807
573	H 35	py	Ryd(2p)	0.00046	2.28010
574	H 35	pz	Ryd(2p)	0.00047	2.21451
575	H 36	s	Val(1s)	0.78119	0.04742
576	H 36	s	Ryd(2s)	0.00036	1.77619
577	H 36	s	Ryd(3s)	0.00015	2.26167
578	H 36	px	Ryd(2p)	0.00041	2.19871
579	H 36	py	Ryd(2p)	0.00046	2.29757
580	H 36	pz	Ryd(2p)	0.00011	1.47325
581	H 37	s	Val(1s)	0.77189	0.02091
582	H 37	s	Ryd(2s)	0.00040	1.92013
583	H 37	s	Ryd(3s)	0.00018	2.09957
584	H 37	px	Ryd(2p)	0.00035	2.36668
585	H 37	py	Ryd(2p)	0.00025	1.32869
586	H 37	pz	Ryd(2p)	0.00021	2.07240

587	H 38	s	Val(1s)	0.77468	0.02118
588	H 38	s	Ryd(3s)	0.00043	1.98019
589	H 38	s	Ryd(2s)	0.00022	1.65574
590	H 38	px	Ryd(2p)	0.00021	1.31936
591	H 38	py	Ryd(2p)	0.00030	1.46868
592	H 38	pz	Ryd(2p)	0.00054	3.62506
593	H 39	s	Val(1s)	0.79497	0.03354
594	H 39	s	Ryd(3s)	0.00049	1.99075
595	H 39	s	Ryd(2s)	0.00024	1.57199
596	H 39	px	Ryd(2p)	0.00044	2.27447
597	H 39	py	Ryd(2p)	0.00035	1.40861
598	H 39	pz	Ryd(2p)	0.00045	2.82908
599	H 40	s	Val(1s)	0.78127	0.04566
600	H 40	s	Ryd(3s)	0.00043	2.03459
601	H 40	s	Ryd(2s)	0.00022	1.63022
602	H 40	px	Ryd(2p)	0.00029	1.20639
603	H 40	py	Ryd(2p)	0.00039	1.55771
604	H 40	pz	Ryd(2p)	0.00042	3.24280
605	H 41	s	Val(1s)	0.77341	0.02515
606	H 41	s	Ryd(2s)	0.00040	1.95157
607	H 41	s	Ryd(3s)	0.00018	2.20707
608	H 41	px	Ryd(2p)	0.00033	3.02126
609	H 41	py	Ryd(2p)	0.00025	1.31950
610	H 41	pz	Ryd(2p)	0.00024	1.45240
611	H 42	s	Val(1s)	0.76647	0.03011
612	H 42	s	Ryd(2s)	0.00035	1.62831
613	H 42	s	Ryd(3s)	0.00019	2.18285
614	H 42	px	Ryd(2p)	0.00004	1.41333
615	H 42	py	Ryd(2p)	0.00049	2.13452
616	H 42	pz	Ryd(2p)	0.00047	2.28609
617	H 43	s	Val(1s)	0.51583	0.16839
618	H 43	s	Ryd(3s)	0.00145	1.63220
619	H 43	s	Ryd(2s)	0.00038	1.61722
620	H 43	px	Ryd(2p)	0.00047	3.01099
621	H 43	py	Ryd(2p)	0.00060	2.18485
622	H 43	pz	Ryd(2p)	0.00100	1.89318
623	O 44	s	Cor(1s)	1.99980	-18.58320
624	O 44	s	Val(2s)	1.71237	-0.91346
625	O 44	s	Ryd(3s)	0.00203	1.98450
626	O 44	s	Ryd(4s)	0.00003	10.57181
627	O 44	s	Ryd(5s)	0.00000	65.08831
628	O 44	s	Ryd(6s)	0.00000	100.67315
629	O 44	px	Val(2p)	1.53954	-0.28215
630	O 44	px	Ryd(3p)	0.00216	0.74789
631	O 44	px	Ryd(4p)	0.00002	4.60533
632	O 44	py	Val(2p)	1.57688	-0.30766
633	O 44	py	Ryd(3p)	0.00207	0.79491
634	O 44	py	Ryd(4p)	0.00007	5.35629
635	O 44	pz	Val(2p)	1.57532	-0.30914
636	O 44	pz	Ryd(3p)	0.00191	0.83263
637	O 44	pz	Ryd(4p)	0.00007	5.36618
638	O 44	dxy	Ryd(3d)	0.00319	1.35176
639	O 44	dxz	Ryd(3d)	0.00326	1.34837
640	O 44	dyz	Ryd(3d)	0.00974	1.88767
641	O 44	dx2y2	Ryd(3d)	0.00382	1.40920
642	O 44	dz2	Ryd(3d)	0.00529	1.50009
643	O 45	s	Cor(1s)	1.99990	-18.60336
644	O 45	s	Val(2s)	1.78244	-0.84156
645	O 45	s	Ryd(3s)	0.00327	4.64964
646	O 45	s	Ryd(4s)	0.00006	5.26175
647	O 45	s	Ryd(5s)	0.00000	76.50250
648	O 45	s	Ryd(6s)	0.00000	92.24406
649	O 45	px	Val(2p)	1.63930	-0.23588
650	O 45	px	Ryd(3p)	0.00601	1.91732
651	O 45	px	Ryd(4p)	0.00003	5.01218
652	O 45	py	Val(2p)	1.75598	-0.25954
653	O 45	py	Ryd(3p)	0.00424	2.15953
654	O 45	py	Ryd(4p)	0.00003	4.21390
655	O 45	pz	Val(2p)	1.82723	-0.24367
656	O 45	pz	Ryd(3p)	0.00544	1.19983
657	O 45	pz	Ryd(4p)	0.00002	4.52438
658	O 45	dxy	Ryd(3d)	0.00097	1.92987
659	O 45	dxz	Ryd(3d)	0.00173	2.03190
660	O 45	dyz	Ryd(3d)	0.00045	2.20515
661	O 45	dx2y2	Ryd(3d)	0.00235	2.16929
662	O 45	dz2	Ryd(3d)	0.00076	1.69235
663	O 46	s	Cor(1s)	1.99980	-18.58750
664	O 46	s	Val(2s)	1.71160	-0.91600
665	O 46	s	Ryd(3s)	0.00258	2.38119
666	O 46	s	Ryd(4s)	0.00004	9.18114
667	O 46	s	Ryd(5s)	0.00000	68.23529
668	O 46	s	Ryd(6s)	0.00000	98.26460
669	O 46	px	Val(2p)	1.58351	-0.32340
670	O 46	px	Ryd(3p)	0.00160	0.65791
671	O 46	px	Ryd(4p)	0.00008	5.49801
672	O 46	py	Val(2p)	1.56297	-0.30203
673	O 46	py	Ryd(3p)	0.00218	0.75431
674	O 46	py	Ryd(4p)	0.00004	5.07414
675	O 46	pz	Val(2p)	1.55826	-0.29341
676	O 46	pz	Ryd(3p)	0.00230	0.74366
677	O 46	pz	Ryd(4p)	0.00003	4.80897
678	O 46	dxy	Ryd(3d)	0.00794	1.64920
679	O 46	dxz	Ryd(3d)	0.00587	1.51337
680	O 46	dyz	Ryd(3d)	0.00302	1.33477
681	O 46	dx2y2	Ryd(3d)	0.00576	1.49910
682	O 46	dz2	Ryd(3d)	0.00338	1.34159
683	O 47	s	Cor(1s)	1.99980	-18.58476
684	O 47	s	Val(2s)	1.71241	-0.91540
685	O 47	s	Ryd(3s)	0.00201	1.97681
686	O 47	s	Ryd(4s)	0.00003	10.31312
687	O 47	s	Ryd(5s)	0.00000	64.97825
688	O 47	s	Ryd(6s)	0.00000	100.66455
689	O 47	px	Val(2p)	1.55320	-0.30291
690	O 47	px	Ryd(3p)	0.00183	0.64588
691	O 47	px	Ryd(4p)	0.00005	5.06633
692	O 47	py	Val(2p)	1.57566	-0.31180

693	O	47	py	Ryd(3p)	0.00207	0.60675
694	O	47	py	Ryd(4p)	0.00007	5.29781
695	O	47	pz	Val(2p)	1.56178	-0.29515
696	O	47	pz	Ryd(3p)	0.00222	0.70875
697	O	47	pz	Ryd(4p)	0.00004	4.89533
698	O	47	dxy	Ryd(3d)	0.00722	1.57749
699	O	47	dxz	Ryd(3d)	0.00423	1.40050
700	O	47	dyz	Ryd(3d)	0.00567	1.50969
701	O	47	dx2y2	Ryd(3d)	0.00484	1.45189
702	O	47	dz2	Ryd(3d)	0.00338	1.34894
703	O	48	s	Cor(1s)	1.99980	-18.58676
704	O	48	s	Val(2s)	1.71094	-0.91335
705	O	48	s	Ryd(3s)	0.00262	2.40405
706	O	48	s	Ryd(4s)	0.00004	9.30062
707	O	48	s	Ryd(5s)	0.00000	69.75610
708	O	48	s	Ryd(6s)	0.00000	96.90612
709	O	48	px	Val(2p)	1.59258	-0.31166
710	O	48	px	Ryd(3p)	0.00215	0.95927
711	O	48	px	Ryd(4p)	0.00007	5.37567
712	O	48	py	Val(2p)	1.56307	-0.29882
713	O	48	py	Ryd(3p)	0.00225	0.80613
714	O	48	py	Ryd(4p)	0.00004	5.05541
715	O	48	pz	Val(2p)	1.55755	-0.29933
716	O	48	pz	Ryd(3p)	0.00191	0.82439
717	O	48	pz	Ryd(4p)	0.00004	5.00389
718	O	48	dxy	Ryd(3d)	0.00639	1.57680
719	O	48	dxz	Ryd(3d)	0.00691	1.63970
720	O	48	dyz	Ryd(3d)	0.00427	1.43247
721	O	48	dx2y2	Ryd(3d)	0.00455	1.45158
722	O	48	dz2	Ryd(3d)	0.00386	1.37949
723	N	49	s	Cor(1s)	1.99947	-13.88797
724	N	49	s	Val(2s)	1.32977	-0.52139
725	N	49	s	Ryd(3s)	0.00507	5.06348
726	N	49	s	Ryd(4s)	0.00018	15.26726
727	N	49	s	Ryd(5s)	0.00001	26.89017
728	N	49	s	Ryd(6s)	0.00000	48.87008
729	N	49	px	Val(2p)	1.42916	-0.23392
730	N	49	px	Ryd(3p)	0.01288	1.97926
731	N	49	px	Ryd(4p)	0.00011	5.24065
732	N	49	py	Val(2p)	1.28803	-0.21553
733	N	49	py	Ryd(3p)	0.00734	1.28079
734	N	49	py	Ryd(4p)	0.00008	4.87151
735	N	49	pz	Val(2p)	1.29723	-0.21755
736	N	49	pz	Ryd(3p)	0.00801	1.36436
737	N	49	pz	Ryd(4p)	0.00009	4.92110
738	N	49	dxy	Ryd(3d)	0.00125	2.27502
739	N	49	dxz	Ryd(3d)	0.00105	2.35715
740	N	49	dyz	Ryd(3d)	0.00180	2.92403
741	N	49	dx2y2	Ryd(3d)	0.00135	2.45844
742	N	49	dz2	Ryd(3d)	0.00109	2.03466
743	N	50	s	Cor(1s)	1.99947	-13.89466
744	N	50	s	Val(2s)	1.33290	-0.52900
745	N	50	s	Ryd(3s)	0.00504	5.11161
746	N	50	s	Ryd(4s)	0.00018	15.00017
747	N	50	s	Ryd(5s)	0.00001	26.88676
748	N	50	s	Ryd(6s)	0.00000	49.04265
749	N	50	px	Val(2p)	1.40856	-0.23966
750	N	50	px	Ryd(3p)	0.01102	1.26536
751	N	50	px	Ryd(4p)	0.00009	4.94670
752	N	50	py	Val(2p)	1.28858	-0.22073
753	N	50	py	Ryd(3p)	0.00745	1.23267
754	N	50	py	Ryd(4p)	0.00008	4.85805
755	N	50	pz	Val(2p)	1.31662	-0.22097
756	N	50	pz	Ryd(3p)	0.01022	1.61512
757	N	50	pz	Ryd(4p)	0.00012	5.20699
758	N	50	dxy	Ryd(3d)	0.00188	2.59203
759	N	50	dxz	Ryd(3d)	0.00075	2.29551
760	N	50	dyz	Ryd(3d)	0.00118	2.51924
761	N	50	dx2y2	Ryd(3d)	0.00088	1.86375
762	N	50	dz2	Ryd(3d)	0.00201	2.60222
763	Ru	51	s	Cor(1s)	2.00000	-826.14408
764	Ru	51	s	Cor(2s)	2.00000	-113.66636
765	Ru	51	s	Cor(3s)	1.99999	-21.94853
766	Ru	51	s	Cor(4s)	1.98721	-4.60926
767	Ru	51	s	Val(5s)	0.38637	0.20972
768	Ru	51	s	Ryd(10s)	0.00453	46.59597
769	Ru	51	s	Ryd(8s)	0.00057	30.02883
770	Ru	51	s	Ryd(6s)	0.00036	10.64812
771	Ru	51	s	Ryd(7s)	0.00006	11.06266
772	Ru	51	s	Ryd(11s)	0.00002	75.82428
773	Ru	51	s	Ryd(9s)	0.00001	32.80034
774	Ru	51	s	Ryd(13s)	0.00000	332.21081
775	Ru	51	s	Ryd(15s)	0.00000	594.36871
776	Ru	51	s	Ryd(12s)	0.00000	88.72352
777	Ru	51	s	Ryd(14s)	0.00000	533.54949
778	Ru	51	s	Ryd(16s)	0.00000	2234.49284
779	Ru	51	s	Ryd(17s)	0.00000	9406.01501
780	Ru	51	s	Ryd(18s)	0.00000	37513.56841
781	Ru	51	px	Cor(2p)	2.00000	-91.91771
782	Ru	51	px	Cor(3p)	2.00000	-28.68760
783	Ru	51	px	Cor(4p)	1.99376	-1.84236
784	Ru	51	px	Ryd(5p)	0.00348	4.85735
785	Ru	51	px	Ryd(6p)	0.00087	7.13259
786	Ru	51	px	Ryd(7p)	0.00015	12.63713
787	Ru	51	px	Ryd(8p)	0.00000	50.46413
788	Ru	51	px	Ryd(9p)	0.00000	186.18646
789	Ru	51	py	Cor(2p)	2.00000	-91.91809
790	Ru	51	py	Cor(3p)	2.00000	-28.68812
791	Ru	51	py	Cor(4p)	1.99510	-1.84653
792	Ru	51	py	Ryd(6p)	0.00347	5.35523
793	Ru	51	py	Ryd(5p)	0.00166	5.25990
794	Ru	51	py	Ryd(7p)	0.00025	11.69108
795	Ru	51	py	Ryd(8p)	0.00000	50.42420
796	Ru	51	py	Ryd(9p)	0.00000	186.17289
797	Ru	51	pz	Cor(2p)	2.00000	-91.91778
798	Ru	51	pz	Cor(3p)	2.00000	-28.68776
799	Ru	51	pz	Cor(4p)	1.99225	-1.84418
800	Ru	51	pz	Ryd(5p)	0.00370	3.98747
801	Ru	51	pz	Ryd(6p)	0.00113	6.00346
802	Ru	51	pz	Ryd(7p)	0.00009	12.23767
803	Ru	51	pz	Ryd(8p)	0.00000	50.49099
804	Ru	51	pz	Ryd(9p)	0.00000	186.18175

805	Ru 51	dxy	Cor(3d)	2.00000	-10.09618
806	Ru 51	dxy	Val(4d)	1.39438	-0.21771
807	Ru 51	dxy	Ryd(5d)	0.00595	0.90897
808	Ru 51	dxy	Ryd(6d)	0.00028	5.15931
809	Ru 51	dxy	Ryd(7d)	0.00001	19.25769
810	Ru 51	dxy	Ryd(8d)	0.00000	53.83702
811	Ru 51	dxz	Cor(3d)	2.00000	-10.09584
812	Ru 51	dxz	Val(4d)	1.45132	-0.21822
813	Ru 51	dxz	Ryd(5d)	0.00448	0.80374
814	Ru 51	dxz	Ryd(6d)	0.00035	5.33941
815	Ru 51	dxz	Ryd(7d)	0.00001	18.89545
816	Ru 51	dxz	Ryd(8d)	0.00000	53.84835
817	Ru 51	dyz	Cor(3d)	2.00000	-10.09692
818	Ru 51	dyz	Val(4d)	1.28541	-0.23620
819	Ru 51	dyz	Ryd(5d)	0.00642	0.94701
820	Ru 51	dyz	Ryd(6d)	0.00075	5.81386
821	Ru 51	dyz	Ryd(7d)	0.00002	19.14108
822	Ru 51	dyz	Ryd(8d)	0.00000	53.82800
823	Ru 51	dx2y2	Cor(3d)	2.00000	-10.09520
824	Ru 51	dx2y2	Val(4d)	1.58111	-0.21668
825	Ru 51	dx2y2	Ryd(5d)	0.00593	0.83882
826	Ru 51	dx2y2	Ryd(6d)	0.00028	4.90223
827	Ru 51	dx2y2	Ryd(7d)	0.00001	19.37973
828	Ru 51	dx2y2	Ryd(8d)	0.00000	53.84397
829	Ru 51	dz2	Cor(3d)	2.00000	-10.09482
830	Ru 51	dz2	Val(4d)	1.66119	-0.21444
831	Ru 51	dz2	Ryd(5d)	0.00505	0.64339
832	Ru 51	dz2	Ryd(6d)	0.00039	4.34317
833	Ru 51	dz2	Ryd(7d)	0.00000	19.58367
834	Ru 51	dz2	Ryd(8d)	0.00000	53.84685
835	Ru 52	s	Cor(1s)	2.00000	-825.13894
836	Ru 52	s	Cor(2s)	2.00000	-114.72809
837	Ru 52	s	Cor(3s)	1.99999	-21.89620
838	Ru 52	s	Ryd(7s)	1.98736	-4.61197
839	Ru 52	s	Ryd(10s)	0.38552	0.07249
840	Ru 52	s	Val(5s)	0.00458	-7.20061
841	Ru 52	s	Ryd(8s)	0.00059	-3.86700
842	Ru 52	s	Ryd(11s)	0.00036	2.67799
843	Ru 52	s	Ryd(9s)	0.00006	-3.60145
844	Ru 52	s	Cor(4s)	0.00002	-17.85108
845	Ru 52	s	Ryd(6s)	0.00001	-6.47123
846	Ru 52	s	Ryd(12s)	0.00000	157.03710
847	Ru 52	s	Ryd(16s)	0.00000	3361.57197
848	Ru 52	s	Ryd(14s)	0.00000	776.76568
849	Ru 52	s	Ryd(15s)	0.00000	3154.32207
850	Ru 52	s	Ryd(18s)	0.00000	29463.38953
851	Ru 52	s	Ryd(13s)	0.00000	765.87255
852	Ru 52	s	Ryd(17s)	0.00000	12892.18483
853	Ru 52	px	Cor(2p)	2.00000	-91.94240
854	Ru 52	px	Cor(3p)	2.00000	-28.66704
855	Ru 52	px	Cor(4p)	1.99252	-1.84539
856	Ru 52	px	Ryd(5p)	0.00363	4.37119
857	Ru 52	px	Ryd(6p)	0.00092	6.69643
858	Ru 52	px	Ryd(7p)	0.00013	12.37870
859	Ru 52	px	Ryd(8p)	0.00000	50.26243
860	Ru 52	px	Ryd(9p)	0.00000	186.27379
861	Ru 52	py	Cor(2p)	2.00000	-91.94220
862	Ru 52	py	Cor(3p)	2.00000	-28.66665
863	Ru 52	py	Cor(4p)	1.99510	-1.84714
864	Ru 52	py	Ryd(5p)	0.00338	5.13471
865	Ru 52	py	Ryd(6p)	0.00174	5.74075
866	Ru 52	py	Ryd(7p)	0.00025	11.75663
867	Ru 52	py	Ryd(8p)	0.00000	50.29525
868	Ru 52	py	Ryd(9p)	0.00000	186.26530
869	Ru 52	pz	Cor(2p)	2.00000	-91.94148
870	Ru 52	pz	Cor(3p)	2.00000	-28.66563
871	Ru 52	pz	Cor(4p)	1.99327	-1.84195
872	Ru 52	pz	Ryd(5p)	0.00373	4.12799
873	Ru 52	pz	Ryd(6p)	0.00097	6.33433
874	Ru 52	pz	Ryd(7p)	0.00010	12.64899
875	Ru 52	pz	Ryd(8p)	0.00000	50.39941
876	Ru 52	pz	Ryd(9p)	0.00000	186.28147
877	Ru 52	dxy	Cor(3d)	2.00000	-10.09768
878	Ru 52	dxy	Val(4d)	1.41334	-0.23194
879	Ru 52	dxy	Ryd(5d)	0.00691	0.91656
880	Ru 52	dxy	Ryd(6d)	0.00051	5.54178
881	Ru 52	dxy	Ryd(7d)	0.00001	19.32222
882	Ru 52	dxy	Ryd(8d)	0.00000	53.81640
883	Ru 52	dxz	Cor(3d)	2.00000	-10.09661
884	Ru 52	dxz	Val(4d)	1.49866	-0.22029
885	Ru 52	dxz	Ryd(5d)	0.00566	0.86184
886	Ru 52	dxz	Ryd(6d)	0.00046	5.01869
887	Ru 52	dxz	Ryd(7d)	0.00001	19.25243
888	Ru 52	dxz	Ryd(8d)	0.00000	53.82804
889	Ru 52	dyz	Cor(3d)	2.00000	-10.09742
890	Ru 52	dyz	Val(4d)	1.25271	-0.22436
891	Ru 52	dyz	Ryd(5d)	0.00490	0.94132
892	Ru 52	dyz	Ryd(6d)	0.00052	5.33226
893	Ru 52	dyz	Ryd(7d)	0.00001	19.16229
894	Ru 52	dyz	Ryd(8d)	0.00000	53.82446
895	Ru 52	dx2y2	Cor(3d)	2.00000	-10.09691
896	Ru 52	dx2y2	Val(4d)	1.55595	-0.21839
897	Ru 52	dx2y2	Ryd(5d)	0.00567	0.75902
898	Ru 52	dx2y2	Ryd(6d)	0.00025	4.57478
899	Ru 52	dx2y2	Ryd(7d)	0.00001	19.45858
900	Ru 52	dx2y2	Ryd(8d)	0.00000	53.83360
901	Ru 52	dz2	Cor(3d)	2.00000	-10.09524
902	Ru 52	dz2	Val(4d)	1.65588	-0.21201
903	Ru 52	dz2	Ryd(5d)	0.00467	0.66897
904	Ru 52	dz2	Ryd(6d)	0.00032	4.39148
905	Ru 52	dz2	Ryd(7d)	0.00000	19.44140
906	Ru 52	dz2	Ryd(8d)	0.00000	53.83748
907	Cl 53	s	Cor(1s)	2.00000	-100.50441
908	Cl 53	s	Cor(2s)	1.99995	-9.80790
909	Cl 53	s	Val(3s)	1.90206	-0.89889
910	Cl 53	s	Ryd(5s)	0.00192	12.04731
911	Cl 53	s	Ryd(4s)	0.00016	4.81208
912	Cl 53	s	Ryd(6s)	0.00001	15.86877
913	Cl 53	s	Ryd(7s)	0.00000	50.21575
914	Cl 53	s	Ryd(8s)	0.00000	170.23105
915	Cl 53	px	Cor(2p)	1.99998	-6.94301
916	Cl 53	px	Val(3p)	1.89882	-0.24488
917	Cl 53	px	Ryd(4p)	0.00299	1.32708
918	Cl 53	px	Ryd(5p)	0.00004	5.02368

919	Cl 53	px	Ryd(6p)	0.00000	17.21284
920	Cl 53	py	Cor(2p)	1.99994	-6.94659
921	Cl 53	py	Val(3p)	1.68790	-0.24823
922	Cl 53	py	Ryd(4p)	0.00145	2.28449
923	Cl 53	py	Ryd(5p)	0.00006	5.74518
924	Cl 53	py	Ryd(6p)	0.00000	17.05099
925	Cl 53	pz	Cor(2p)	1.99996	-6.94452
926	Cl 53	pz	Val(3p)	1.81455	-0.24597
927	Cl 53	pz	Ryd(4p)	0.00250	2.25386
928	Cl 53	pz	Ryd(5p)	0.00004	5.32336
929	Cl 53	pz	Ryd(6p)	0.00000	17.18362
930	Cl 53	dxy	Ryd(3d)	0.00158	0.97467
931	Cl 53	dxz	Ryd(3d)	0.00168	1.01477
932	Cl 53	dyz	Ryd(3d)	0.00221	1.00089
933	Cl 53	dx2y2	Ryd(3d)	0.00132	0.88396
934	Cl 53	dz2	Ryd(3d)	0.00167	0.84869

4 low occupancy (<1.9990e) core orbitals found on Ru 51
4 low occupancy (<1.9990e) core orbitals found on Ru 52

Population inversion found on atom C 3
Population inversion found on atom C 5
Population inversion found on atom C 13
Population inversion found on atom C 15
Population inversion found on atom C 17
Population inversion found on atom C 18
Population inversion found on atom C 21
Population inversion found on atom C 23
Population inversion found on atom C 25
Population inversion found on atom C 26
Population inversion found on atom H 28
Population inversion found on atom H 30
Population inversion found on atom H 32
Population inversion found on atom H 33
Population inversion found on atom H 34
Population inversion found on atom H 38
Population inversion found on atom H 39
Population inversion found on atom H 40
Population inversion found on atom H 43
Population inversion found on atom Ru 51
Population inversion found on atom Ru 52
Population inversion found on atom Cl 53

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C 1	-0.25251	1.99935	4.24071	0.01245	6.25251
C 2	0.03038	1.99935	3.94932	0.02096	5.96962
C 3	-0.16564	1.99938	4.15487	0.01138	6.16564
C 4	0.59856	1.99944	3.35464	0.04736	5.40144
C 5	-0.22696	1.99929	4.21624	0.01143	6.22696
C 6	0.60006	1.99945	3.35246	0.04802	5.39994
C 7	0.20466	1.99926	3.77329	0.02279	5.79534
C 8	0.59410	1.99944	3.35908	0.04738	5.40590
C 9	-0.14193	1.99918	4.12239	0.02036	6.14193
C 10	0.57888	1.99945	3.37209	0.04958	5.42112
C 11	-0.03969	1.99907	4.00129	0.03932	6.03969
C 12	0.03356	1.99935	3.94581	0.02128	5.96644
C 13	-0.18455	1.99930	4.17318	0.01207	6.18455
C 14	-0.25190	1.99934	4.24010	0.01246	6.25190
C 15	-0.26232	1.99930	4.24717	0.01585	6.26232
C 16	-0.03507	1.99908	3.99715	0.03884	6.03507
C 17	-0.23255	1.99937	4.22024	0.01295	6.23255
C 18	-0.26177	1.99930	4.24682	0.01565	6.26177
C 19	-0.19071	1.99937	4.17904	0.01230	6.19071
C 20	0.20755	1.99926	3.77047	0.02273	5.79245
C 21	-0.16341	1.99938	4.15272	0.01132	6.16341
C 22	-0.14382	1.99918	4.12419	0.02044	6.14382
C 23	-0.22359	1.99929	4.21294	0.01136	6.22359
C 24	-0.18825	1.99937	4.17665	0.01224	6.18825
C 25	-0.18315	1.99930	4.17181	0.01204	6.18315
C 26	-0.23208	1.99937	4.21979	0.01292	6.23208
H 27	0.24373	0.00000	0.75315	0.00313	0.75627
H 28	0.22243	0.00000	0.77587	0.00171	0.77757
H 29	0.20708	0.00000	0.78958	0.00334	0.79292
H 30	0.20340	0.00000	0.79464	0.00197	0.79660
H 31	0.23289	0.00000	0.76554	0.00157	0.76711
H 32	0.21470	0.00000	0.78249	0.00281	0.78530
H 33	0.21460	0.00000	0.78259	0.00281	0.78540
H 34	0.21657	0.00000	0.78168	0.00175	0.78343
H 35	0.21666	0.00000	0.78184	0.00151	0.78334
H 36	0.21732	0.00000	0.78119	0.00150	0.78268
H 37	0.22673	0.00000	0.77189	0.00138	0.77327
H 38	0.22363	0.00000	0.77468	0.00169	0.77637
H 39	0.20306	0.00000	0.79497	0.00197	0.79694
H 40	0.21698	0.00000	0.78127	0.00175	0.78302
H 41	0.22519	0.00000	0.77341	0.00141	0.77481
H 42	0.23199	0.00000	0.76647	0.00154	0.76801
H 43	0.48027	0.00000	0.51583	0.00389	0.51973
O 44	-0.43757	1.99980	6.40410	0.03367	8.43757
O 45	-1.03018	1.99990	7.00495	0.02533	9.03018
O 46	-0.45095	1.99980	6.41633	0.03483	8.45095
O 47	-0.43653	1.99980	6.40305	0.03368	8.43653
O 48	-0.45904	1.99980	6.42414	0.03511	8.45904
N 49	-0.38396	1.99947	5.34420	0.04029	7.38396
N 50	-0.38704	1.99947	5.34666	0.04090	7.38704
Ru 51	0.22166	35.96829	7.75978	0.05027	43.77834
Ru 52	0.21934	33.98089	7.38112	2.41865	43.78066
Cl 53	-0.32079	9.99982	7.30333	0.01764	17.32079
* Total *	0.00000	145.92925	182.72917	3.34158	332.00000

	Natural Population
Core	145.92925 (98.6008% of 148)
Valence	182.72917 (99.3093% of 184)
Natural Minimal Basis	328.65842 (98.9935% of 332)
Natural Rydberg Basis	3.34158 (1.0065% of 332)

Atom No	Natural Electron Configuration

```
     C  1      [core]2s( 1.01)2p( 3.23)3p( 0.01)
     C  2      [core]2s( 0.97)2p( 2.98)3p( 0.01)
     C  3      [core]2s( 1.01)2p( 3.14)3p( 0.01)
     C  4      [core]2s( 1.16)2p( 2.19)3s( 0.02)3p( 0.02)
     C  5      [core]2s( 1.00)2p( 3.21)3p( 0.01)
     C  6      [core]2s( 1.19)2p( 2.17)3s( 0.02)3p( 0.02)
     C  7      [core]2s( 0.91)2p( 2.87)3p( 0.02)
     C  8      [core]2s( 1.17)2p( 2.19)3s( 0.02)3p( 0.02)
     C  9      [core]2s( 0.95)2p( 3.17)3p( 0.01)
     C 10      [core]2s( 1.19)2p( 2.18)3s( 0.02)3p( 0.02)
     C 11      [core]2s( 1.03)2p( 2.97)3s( 0.01)3p( 0.03)
     C 12      [core]2s( 0.96)2p( 2.98)3p( 0.01)
     C 13      [core]2s( 0.99)2p( 3.18)3p( 0.01)
     C 14      [core]2s( 1.01)2p( 3.23)3p( 0.01)
     C 15      [core]2s( 1.01)2p( 3.24)3p( 0.01)
     C 16      [core]2s( 1.03)2p( 2.97)3s( 0.01)3p( 0.03)
     C 17      [core]2s( 1.00)2p( 3.22)3p( 0.01)
     C 18      [core]2s( 1.01)2p( 3.24)3p( 0.01)
     C 19      [core]2s( 1.01)2p( 3.17)3p( 0.01)
     C 20      [core]2s( 0.91)2p( 2.86)3p( 0.02)
     C 21      [core]2s( 1.01)2p( 3.14)3p( 0.01)
     C 22      [core]2s( 0.95)2p( 3.17)3p( 0.01)
     C 23      [core]2s( 1.00)2p( 3.21)3p( 0.01)
     C 24      [core]2s( 1.01)2p( 3.17)3p( 0.01)
     C 25      [core]2s( 0.99)2p( 3.18)3p( 0.01)
     C 26      [core]2s( 1.00)2p( 3.22)3p( 0.01)
     H 27            1s( 0.75)
     H 28            1s( 0.78)
     H 29            1s( 0.79)
     H 30            1s( 0.79)
     H 31            1s( 0.77)
     H 32            1s( 0.78)
     H 33            1s( 0.78)
     H 34            1s( 0.78)
     H 35            1s( 0.78)
     H 36            1s( 0.78)
     H 37            1s( 0.77)
     H 38            1s( 0.77)
     H 39            1s( 0.79)
     H 40            1s( 0.78)
     H 41            1s( 0.77)
     H 42            1s( 0.77)
     H 43            1s( 0.52)
     O 44      [core]2s( 1.71)2p( 4.69)3p( 0.01)3d( 0.03)
     O 45      [core]2s( 1.78)2p( 5.22)3p( 0.02)3d( 0.01)
     O 46      [core]2s( 1.71)2p( 4.70)3p( 0.01)3d( 0.03)
     O 47      [core]2s( 1.71)2p( 4.69)3p( 0.01)3d( 0.03)
     O 48      [core]2s( 1.71)2p( 4.71)3p( 0.01)3d( 0.03)
     N 49      [core]2s( 1.33)2p( 4.01)3s( 0.01)3p( 0.03)3d( 0.01)
     N 50      [core]2s( 1.33)2p( 4.01)3s( 0.01)3p( 0.03)3d( 0.01)
    Ru 51      [core]5s( 0.39)4d( 7.37)5p( 0.01)5d( 0.03)6p( 0.01)
    Ru 52      [core]4d( 7.38)5p( 0.01)5d( 0.03)7s( 1.99)
    Cl 53      [core]3s( 1.90)3p( 5.40)3d( 0.01)4p( 0.01)
*** sorry: cannot construct NLMOMO matrix.
***        AOMO matrix not available
```

NATURAL BOND ORBITAL ANALYSIS:

Cycle	Occ. Thresh.	Occupancies Lewis	Occupancies Non-Lewis	Lewis Structure CR	BD	3C	LP	Low occ (L)	High occ (NL)	Dev
1(1)	1.90	319.10127	12.89873	74	70	11	11	21	23	0.47
2(2)	1.90	319.89449	12.10551	74	70	14	8	20	22	0.41
3(3)	1.90	319.89449	12.10551	74	70	14	8	20	22	0.41
4(1)	1.80	318.49424	13.50576	74	66	11	15	19	22	1.08
5(2)	1.80	318.85773	13.14227	74	68	12	12	16	21	1.06
6(3)	1.80	319.18186	12.81814	74	70	11	11	13	20	0.44
7(4)	1.80	319.20260	12.79740	74	70	11	11	13	20	0.47
8(5)	1.80	319.20260	12.79740	74	70	11	11	13	20	0.47
9(6)	1.80	319.25159	12.74841	74	68	14	10	12	21	0.47
10(7)	1.80	319.25159	12.74841	74	68	14	10	12	21	0.47
11(8)	1.80	319.25159	12.74841	74	68	14	10	12	21	0.47
12(9)	1.80	319.25159	12.74841	74	68	14	10	12	21	0.47
13(1)	1.70	319.74547	12.25453	74	67	9	16	11	27	0.47
14(2)	1.70	319.41535	12.58465	74	67	10	15	11	28	0.45
15(3)	1.70	320.30411	11.69589	74	67	10	15	10	25	0.45
16(4)	1.70	319.73427	12.26573	74	67	9	16	11	28	0.47
17(5)	1.70	319.19574	12.80426	74	67	10	15	11	29	0.47
18(6)	1.70	319.15628	12.84372	74	67	10	15	11	29	0.45
19(7)	1.70	320.04503	11.95497	74	67	10	15	10	26	0.45
20(8)	1.70	319.69481	12.30519	74	67	9	16	11	28	0.47
21(9)	1.70	319.15628	12.84372	74	67	10	15	11	29	0.45
22(1)	1.60	322.06906	9.93094	74	72	0	20	1	26	0.47
23(2)	1.60	321.53946	10.46054	74	71	0	21	2	26	0.44
24(3)	1.60	321.59640	10.40360	74	71	0	21	2	26	0.43
25(4)	1.60	321.53946	10.46054	74	71	0	21	2	26	0.44
26(5)	1.60	321.59640	10.40360	74	71	0	21	2	26	0.43
27(6)	1.60	321.53946	10.46054	74	71	0	21	2	26	0.44
28(7)	1.60	321.59640	10.40360	74	71	0	21	2	26	0.43
29(8)	1.60	321.53946	10.46054	74	71	0	21	2	26	0.44
30(9)	1.60	321.59640	10.40360	74	71	0	21	2	26	0.43
31(1)	1.50	318.99399	13.00601	74	65	0	27	0	26	1.09
32(2)	1.50	318.99399	13.00601	74	65	0	27	0	26	1.09
33(1)	1.60	322.06906	9.93094	74	72	0	20	1	26	0.47

Strongly delocalized structure accepted

```
         4 low occupancy (<1.9990e) core orbitals found on Ru51
         4 low occupancy (<1.9990e) core orbitals found on Ru52
```

Core	147.91566 (99.943% of 148)
Valence Lewis	174.15340 (94.649% of 184)
Total Lewis	322.06906 (97.009% of 332)
Valence non-Lewis	9.31359 (2.805% of 332)
Rydberg non-Lewis	0.61735 (0.186% of 332)
Total non-Lewis	9.93094 (2.991% of 332)

```
   (Occupancy)   Bond orbital/ Coefficients/ Hybrids
-------------------------------------------------------------------------------
 1. (1.98282) BD ( 1) C  1- C  2
              ( 50.18%)   0.7084* C  1 s( 34.70%)p 1.88( 65.21%)d 0.00(  0.09%)
                                        0.0000  0.5890 -0.0011  0.0051 -0.0002
                                        0.0001 -0.7039  0.0245  0.0019  0.2495
                                        0.0042 -0.0027  0.3063  0.0027 -0.0048
                                       -0.0151 -0.0185  0.0091  0.0152 -0.0068
              ( 49.82%)   0.7058* C  2 s( 37.50%)p 1.66( 62.40%)d 0.00(  0.09%)
                                       -0.0001  0.6124  0.0048  0.0039 -0.0001
                                        0.0001  0.6705  0.0114  0.0009 -0.2592
                                        0.0162 -0.0030 -0.3266  0.0147 -0.0057
                                       -0.0138 -0.0172  0.0053  0.0180 -0.0087
 2. (1.63590) BD ( 2) C  1- C  2
              ( 54.15%)   0.7358* C  1 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                        0.0000 -0.0004  0.0013 -0.0006  0.0000
                                       -0.0001  0.0388  0.0004  0.0010 -0.7285
                                       -0.0127 -0.0066  0.6834  0.0132  0.0067
                                        0.0063 -0.0048 -0.0013  0.0080  0.0146
              ( 45.85%)   0.6772* C  2 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                        0.0000 -0.0029  0.0002 -0.0010  0.0001
                                        0.0000  0.0524 -0.0015 -0.0001 -0.7297
                                       -0.0095 -0.0033  0.6812  0.0114  0.0052
                                       -0.0151  0.0144  0.0013  0.0011 -0.0013
 3. (1.98475) BD ( 1) C  1- C  3
              ( 49.97%)   0.7069* C  1 s( 35.25%)p 1.83( 64.66%)d 0.00(  0.09%)
                                        0.0000  0.5936  0.0088  0.0036 -0.0002
                                        0.0001  0.7075 -0.0239  0.0016  0.2800
                                        0.0069 -0.0036  0.2585  0.0080 -0.0039
                                        0.0171  0.0161  0.0094  0.0149 -0.0088
              ( 50.03%)   0.7073* C  3 s( 35.11%)p 1.85( 64.80%)d 0.00(  0.09%)
                                        0.0000  0.5925  0.0056  0.0038  0.0001
                                        0.0000 -0.6758  0.0014  0.0048 -0.3129
                                        0.0172 -0.0001 -0.3044  0.0182 -0.0005
                                        0.0155  0.0148  0.0072  0.0169 -0.0100
 4. (1.97639) BD ( 1) C  1- H 42
              ( 61.61%)   0.7850* C  1 s( 30.00%)p 2.33( 69.94%)d 0.00(  0.07%)
                                        0.0004 -0.5476  0.0049  0.0080 -0.0003
                                        0.0002  0.0099 -0.0023 -0.0035  0.5726
                                        0.0037 -0.0050  0.6093  0.0073 -0.0031
                                       -0.0011 -0.0010 -0.0225  0.0106 -0.0077
              ( 38.39%)   0.6196* H 42 s( 99.95%)p 0.00(  0.05%)
                                       -0.9997 -0.0019  0.0003 -0.0009 -0.0160
                                       -0.0155
 5. (1.97198) BD ( 1) C  2- H 27
              ( 62.56%)   0.7909* C  2 s( 30.88%)p 2.24( 69.06%)d 0.00(  0.06%)
                                        0.0004 -0.5553  0.0188  0.0066 -0.0002
                                        0.0002  0.7389  0.0130 -0.0110  0.2874
                                        0.0017 -0.0036  0.2486  0.0058  0.0029
                                       -0.0123 -0.0098 -0.0034 -0.0147  0.0098
              ( 37.44%)   0.6119* H 27 s( 99.89%)p 0.00(  0.11%)
                                       -0.9994 -0.0009 -0.0027 -0.0315 -0.0107
                                       -0.0054
 6. (1.98610) BD ( 1) C  2- N 49
              ( 39.90%)   0.6316* C  2 s( 31.64%)p 2.16( 68.27%)d 0.00(  0.09%)
                                        0.0000  0.5620  0.0244  0.0034 -0.0002
                                        0.0003 -0.0007  0.0148 -0.0024  0.5622
                                       -0.0167  0.0053  0.6047 -0.0180  0.0043
                                        0.0015  0.0018  0.0264 -0.0115  0.0084
              ( 60.10%)   0.7753* N 49 s( 35.46%)p 1.81( 64.37%)d 0.00(  0.17%)
                                       -0.0001  0.5949  0.0280 -0.0010  0.0004
                                        0.0000 -0.0024 -0.0157 -0.0027 -0.5492
                                       -0.0129 -0.0017 -0.5843 -0.0155 -0.0018
                                       -0.0073 -0.0086  0.0361 -0.0118  0.0108
 7. (1.98395) BD ( 1) C  3- C  5
              ( 49.71%)   0.7051* C  3 s( 35.51%)p 1.81( 64.40%)d 0.00(  0.09%)
                                        0.0000  0.5958  0.0058  0.0039  0.0001
                                       -0.0001  0.0041 -0.0199  0.0023  0.5453
                                       -0.0124 -0.0038  0.5881 -0.0122 -0.0040
                                       -0.0019 -0.0023  0.0269 -0.0109  0.0086
              ( 50.29%)   0.7091* C  5 s( 35.94%)p 1.78( 63.97%)d 0.00(  0.09%)
                                        0.0000  0.5993  0.0130  0.0032  0.0001
                                       -0.0001  0.0386 -0.0207  0.0048 -0.5478
                                        0.0065  0.0004 -0.5811  0.0080  0.0003
                                        0.0012  0.0008  0.0271 -0.0104  0.0079
 8. (1.66321) BD ( 2) C  3- C  5
              ( 47.95%)   0.6925* C  3 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                        0.0000 -0.0009  0.0009 -0.0002  0.0000
                                        0.0000  0.0321  0.0004  0.0003 -0.7323
                                       -0.0099 -0.0071  0.6797  0.0085  0.0060
                                        0.0079 -0.0065 -0.0012  0.0083  0.0153
              ( 52.05%)   0.7215* C  5 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                        0.0000 -0.0019  0.0009 -0.0002 -0.0001
                                       -0.0001  0.0336  0.0009  0.0007 -0.7269
                                       -0.0074 -0.0069  0.6856  0.0076  0.0066
                                        0.0075 -0.0077  0.0010 -0.0080 -0.0126
 9. (1.97843) BD ( 1) C  3- H 41
              ( 61.35%)   0.7832* C  3 s( 29.33%)p 2.41( 70.59%)d 0.00(  0.08%)
                                       -0.0003  0.5415 -0.0088 -0.0070 -0.0001
                                        0.0001  0.7353  0.0118 -0.0017 -0.2590
                                       -0.0035  0.0000 -0.3131 -0.0049  0.0000
                                       -0.0130 -0.0160  0.0044  0.0161 -0.0081
              ( 38.65%)   0.6217* H 41 s( 99.96%)p 0.00(  0.04%)
                                        0.9998  0.0022  0.0002 -0.0166  0.0062
                                        0.0069
10. (1.99744) BD ( 1) C  4- O 44
              ( 25.05%)   0.5005* C  4 s(  0.15%)p99.99( 99.61%)d 1.54(  0.23%)
                                        0.0000 -0.0380 -0.0087 -0.0006  0.0003
                                        0.0002  0.7221 -0.0075 -0.0076  0.5234
                                       -0.0065 -0.0091  0.4477 -0.0051 -0.0026
                                        0.0192 -0.0281 -0.0044 -0.0243 -0.0238
              ( 74.95%)   0.8658* O 44 s(  0.23%)p99.99( 99.39%)d 1.71(  0.39%)
                                        0.0000 -0.0475  0.0020  0.0001  0.0000
                                        0.0000  0.7032  0.0002  0.0009  0.6072
                                       -0.0014  0.0003  0.3614  0.0018  0.0008
                                       -0.0247  0.0334  0.0131  0.0334  0.0293
11. (1.99744) BD ( 2) C  4- O 44
              ( 25.68%)   0.5068* C  4 s(  0.00%)p 1.00( 99.77%)d 0.00(  0.22%)
                                        0.0000 -0.0059 -0.0009 -0.0006  0.0001
                                        0.0000 -0.6809  0.0046  0.0083  0.4395
                                       -0.0023 -0.0055  0.5837 -0.0060 -0.0074
                                       -0.0259  0.0178  0.0042 -0.0091 -0.0338
              ( 74.32%)   0.8621* O 44 s(  0.00%)p 1.00( 99.61%)d 0.00(  0.39%)
                                        0.0000 -0.0044  0.0003  0.0000  0.0000
                                        0.0000 -0.6818  0.0007 -0.0008  0.4461
                                       -0.0006  0.0004  0.5764  0.0002  0.0008
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```
                                    0.0335 -0.0253 -0.0052  0.0135  0.0441
12. (1.99514) BD ( 3) C  4- O 44
            ( 31.92%)   0.5649* C  4 s( 39.05%)p 1.56( 60.89%)d 0.00(  0.06%)
                                    0.0000  0.6101  0.1354 -0.0010 -0.0005
                                   -0.0005 -0.0699  0.0073 -0.0040  0.5817
                                   -0.0264  0.0181 -0.5131  0.0288 -0.0195
                                   -0.0036  0.0024 -0.0208 -0.0115  0.0037
            ( 68.08%)   0.8251* O 44 s( 42.47%)p 1.34( 56.76%)d 0.02(  0.77%)
                                    0.0001  0.6512 -0.0237 -0.0025  0.0001
                                    0.0000  0.1628 -0.0049 -0.0009 -0.4722
                                    0.0214  0.0045  0.5632 -0.0218 -0.0046
                                   -0.0178  0.0184 -0.0734 -0.0320  0.0244
13. (1.91955) BD ( 1) C  4-Ru 51
            ( 66.40%)   0.8149* C  4 s( 62.06%)p 0.61( 37.93%)d 0.00(  0.01%)
                                    0.0001  0.7871 -0.0334  0.0003  0.0001
                                    0.0003  0.0851 -0.0001 -0.0007 -0.4299
                                   -0.0295 -0.0056  0.4310  0.0241  0.0045
                                   -0.0017 -0.0006 -0.0085 -0.0049  0.0011
            ( 33.60%)   0.5796*Ru 51 s( 35.74%)p 0.00(  0.09%)d 1.80( 64.17%)
                                    0.0000  0.0000 -0.0001 -0.0009  0.5974
                                    0.0220 -0.0084 -0.0018  0.0004  0.0001
                                   -0.0009  0.0003 -0.0002  0.0000 -0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0003 -0.0181 -0.0111 -0.0009  0.0001
                                    0.0000  0.0000  0.0000 -0.0007 -0.0045
                                    0.0058 -0.0128 -0.0003  0.0000  0.0000
                                    0.0000  0.0007 -0.0080 -0.0142  0.0015
                                    0.0005  0.0000  0.0000 -0.1203 -0.0023
                                   -0.0003  0.0001  0.0000  0.0000  0.1945
                                    0.0122 -0.0052  0.0010  0.0000  0.0000
                                   -0.6690 -0.0320  0.0033 -0.0023 -0.0001
                                    0.0000 -0.2836 -0.0128  0.0039 -0.0011
                                    0.0000  0.0000  0.2447  0.0116  0.0007
                                    0.0009  0.0000
14. (1.97942) BD ( 1) C  5- C  7
            ( 49.70%)   0.7050* C  5 s( 34.43%)p 1.90( 65.48%)d 0.00(  0.09%)
                                    0.0000  0.5867 -0.0070  0.0069  0.0002
                                   -0.0002 -0.6994  0.0067  0.0042  0.2606
                                   -0.0082 -0.0001  0.3122 -0.0096 -0.0002
                                   -0.0130 -0.0159  0.0065  0.0193 -0.0099
            ( 50.30%)   0.7092* C  7 s( 35.53%)p 1.81( 64.41%)d 0.00(  0.07%)
                                   -0.0002  0.5961  0.0000 -0.0024  0.0001
                                    0.0000  0.7089 -0.0063  0.0023 -0.2388
                                    0.0119  0.0000 -0.2901  0.0140 -0.0001
                                   -0.0127 -0.0152  0.0044  0.0140 -0.0068
15. (1.97434) BD ( 1) C  5- H 28
            ( 61.15%)   0.7820* C  5 s( 29.59%)p 2.38( 70.34%)d 0.00(  0.07%)
                                   -0.0004  0.5439 -0.0033 -0.0092 -0.0002
                                    0.0002  0.7121  0.0040 -0.0036  0.3203
                                    0.0025 -0.0058  0.3062  0.0025 -0.0061
                                    0.0149  0.0139  0.0071  0.0124 -0.0075
            ( 38.85%)   0.6233* H 28 s( 99.94%)p 0.00(  0.06%)
                                    0.9997  0.0021  0.0002 -0.0215 -0.0084
                                   -0.0077
16. (1.99654) BD ( 1) C  6- O 46
            ( 25.33%)   0.5033* C  6 s(  0.90%)p99.99( 98.87%)d 0.25(  0.23%)
                                    0.0000  0.0933  0.0183  0.0003 -0.0001
                                    0.0000  0.5398 -0.0146 -0.0039  0.0006
                                   -0.0043 -0.0024  0.8347 -0.0090 -0.0135
                                   -0.0128  0.0221 -0.0230  0.0183 -0.0277
            ( 74.67%)   0.8641* O 46 s(  0.87%)p99.99( 98.72%)d 0.47(  0.41%)
                                    0.0000  0.0931 -0.0032 -0.0004  0.0000
                                    0.0000  0.3742  0.0009  0.0013  0.1119
                                   -0.0045 -0.0003  0.9136 -0.0024  0.0005
                                    0.0030 -0.0386  0.0330 -0.0213  0.0321
17. (1.99612) BD ( 2) C  6- O 46
            ( 25.12%)   0.5012* C  6 s(  0.13%)p99.99( 99.64%)d 1.85(  0.23%)
                                    0.0000  0.0344  0.0087  0.0010 -0.0003
                                    0.0000  0.4567 -0.0071 -0.0061  0.8352
                                   -0.0045 -0.0126 -0.3001 -0.0040  0.0040
                                    0.0193 -0.0183 -0.0069  0.0382  0.0107
            ( 74.88%)   0.8653* O 46 s(  0.10%)p99.99( 99.50%)d 4.07(  0.40%)
                                    0.0000  0.0312 -0.0015 -0.0001  0.0000
                                    0.0000  0.4079  0.0011  0.0007  0.8673
                                   -0.0013  0.0004 -0.2766 -0.0035 -0.0002
                                   -0.0306  0.0223  0.0122 -0.0474 -0.0121
18. (1.99465) BD ( 3) C  6- O 46
            ( 31.30%)   0.5594* C  6 s( 37.49%)p 1.67( 62.45%)d 0.00(  0.06%)
                                   -0.0001  0.5970  0.1361 -0.0023 -0.0007
                                   -0.0006  0.5109 -0.0246  0.0240 -0.4489
                                    0.0169 -0.0156 -0.3998  0.0192 -0.0087
                                   -0.0162 -0.0139  0.0120  0.0016 -0.0039
            ( 68.70%)   0.8289* O 46 s( 42.62%)p 1.33( 56.61%)d 0.02(  0.76%)
                                    0.0001  0.6524 -0.0251 -0.0028  0.0001
                                    0.0000 -0.6540  0.0223  0.0044  0.3347
                                   -0.0157 -0.0033  0.1596 -0.0097 -0.0023
                                   -0.0604 -0.0390  0.0242  0.0308 -0.0303
19. (1.92504) BD ( 1) C  6-Ru 52
            ( 68.20%)   0.8258* C  6 s( 62.92%)p 0.59( 37.08%)d 0.00(  0.01%)
                                    0.0001  0.7923 -0.0385  0.0017  0.0002
                                    0.0003 -0.4763 -0.0313 -0.0064  0.3070
                                    0.0175  0.0042  0.2197  0.0105  0.0017
                                   -0.0055 -0.0042  0.0028  0.0038 -0.0027
            ( 31.80%)   0.5639*Ru 52 s( 36.90%)p 0.00(  0.06%)d 1.71( 63.03%)
                                    0.0000  0.0000  0.0000 -0.0009  0.6070
                                    0.0232 -0.0047 -0.0026 -0.0001  0.0009
                                    0.0000  0.0002  0.0000  0.0000  0.0000
                                    0.0000 -0.0001  0.0001  0.0000  0.0000
                                   -0.0005 -0.0037  0.0129 -0.0061 -0.0005
                                    0.0000  0.0000  0.0000  0.0006  0.0032
                                    0.0002  0.0139  0.0000  0.0000  0.0000
                                    0.0000  0.0003 -0.0096 -0.0115  0.0016
                                    0.0003  0.0000  0.0000 -0.4639 -0.0164
                                    0.0045 -0.0016 -0.0001  0.0000 -0.4796
                                   -0.0153  0.0019 -0.0012 -0.0001  0.0000
                                    0.2184  0.0249 -0.0019  0.0001  0.0001
                                    0.0000  0.3402  0.0229  0.0009  0.0007
                                    0.0001  0.0000 -0.1413 -0.0068 -0.0007
                                   -0.0003 -0.0001
20. (1.97250) BD ( 1) C  7- C  9
            ( 50.89%)   0.7134* C  7 s( 34.57%)p 1.89( 65.38%)d 0.00(  0.05%)
                                   -0.0003  0.5878 -0.0133  0.0015 -0.0004
                                    0.0000 -0.0681  0.0074  0.0033  0.5583
                                   -0.0131 -0.0011  0.5805 -0.0136 -0.0015
                                   -0.0038 -0.0039  0.0179 -0.0093  0.0055
            ( 49.11%)   0.7008* C  9 s( 30.47%)p 2.28( 69.46%)d 0.00(  0.07%)
```

```
                                    -0.0002  0.5519 -0.0084  0.0013 -0.0002
                                     0.0003  0.1337  0.0023  0.0023 -0.5819
                                     0.0104 -0.0004 -0.5813  0.0108 -0.0005
                                    -0.0044 -0.0043  0.0223 -0.0106  0.0066
 21. (1.98200) BD ( 1) C  7- N 49
             ( 40.71%)   0.6380* C  7 s( 29.91%)p 2.34( 70.02%)d 0.00(  0.07%)
                                    -0.0001  0.5465  0.0198 -0.0007  0.0005
                                     0.0002 -0.7001 -0.0120 -0.0016 -0.3352
                                    -0.0007 -0.0002 -0.3123  0.0008 -0.0003
                                     0.0151  0.0141  0.0079  0.0128 -0.0079
             ( 59.29%)   0.7700* N 49 s( 33.99%)p 1.94( 65.84%)d 0.01(  0.17%)
                                    -0.0001  0.5828  0.0142 -0.0003  0.0007
                                    -0.0002  0.6872  0.0088  0.0005  0.3190
                                     0.0105  0.0018  0.2900  0.0120  0.0017
                                     0.0192  0.0156  0.0102  0.0272 -0.0166
 22. (1.72309) BD ( 2) C  7- N 49
             ( 34.09%)   0.5838* C  7 s(  0.00%)p 1.00( 99.92%)d 0.00(  0.08%)
                                     0.0000 -0.0035 -0.0011 -0.0003  0.0000
                                     0.0000 -0.0382 -0.0025  0.0000  0.7189
                                     0.0285 -0.0021 -0.6923 -0.0283  0.0016
                                    -0.0137  0.0138 -0.0009  0.0117  0.0174
             ( 65.91%)   0.8119* N 49 s(  0.00%)p 1.00( 99.91%)d 0.00(  0.09%)
                                     0.0000 -0.0011  0.0004 -0.0006  0.0001
                                     0.0000 -0.0477 -0.0045  0.0005  0.7267
                                     0.0239 -0.0012 -0.6838 -0.0238  0.0012
                                     0.0212 -0.0189 -0.0026  0.0017  0.0086
 23. (1.99736) BD ( 1) C  8- O 47
             ( 25.09%)   0.5009* C  8 s(  0.15%)p99.99( 99.61%)d 1.53(  0.23%)
                                     0.0000 -0.0382 -0.0081 -0.0009  0.0003
                                     0.0002  0.3206 -0.0025 -0.0018 -0.6404
                                     0.0067  0.0103  0.6950 -0.0086 -0.0067
                                     0.0081 -0.0254 -0.0074 -0.0299 -0.0261
             ( 74.91%)   0.8655* O 47 s(  0.21%)p99.99( 99.40%)d 1.87(  0.39%)
                                     0.0000 -0.0456  0.0019  0.0000 -0.0001
                                     0.0000  0.2548  0.0015  0.0006 -0.7199
                                     0.0014 -0.0004  0.6409  0.0010  0.0010
                                    -0.0158  0.0286  0.0060  0.0404  0.0340
 24. (1.99750) BD ( 2) C  8- O 47
             ( 25.68%)   0.5068* C  8 s(  0.01%)p 1.00( 99.77%)d 0.00(  0.22%)
                                     0.0000  0.0072  0.0036 -0.0007  0.0001
                                     0.0000  0.7647 -0.0057 -0.0099 -0.2569
                                     0.0003  0.0023 -0.5889  0.0054  0.0068
                                    -0.0178 -0.0013  0.0245 -0.0282  0.0222
             ( 74.32%)   0.8621* O 47 s(  0.01%)p99.99( 99.60%)d29.53(  0.39%)
                                     0.0000  0.0115 -0.0005  0.0000  0.0000
                                     0.0000  0.7803 -0.0006  0.0009 -0.2368
                                    -0.0002 -0.0003 -0.5753  0.0003 -0.0007
                                     0.0257  0.0019 -0.0310  0.0378 -0.0289
 25. (1.99516) BD ( 3) C  8- O 47
             ( 31.92%)   0.5650* C  8 s( 39.04%)p 1.56( 60.90%)d 0.00(  0.06%)
                                    -0.0001  0.6097  0.1362 -0.0011 -0.0005
                                    -0.0005 -0.4299  0.0223 -0.0155 -0.5770
                                     0.0264 -0.0180 -0.2983  0.0199 -0.0124
                                     0.0170  0.0090  0.0127 -0.0051 -0.0067
             ( 68.08%)   0.8251* O 47 s( 42.48%)p 1.34( 56.75%)d 0.02(  0.77%)
                                     0.0001  0.6513 -0.0236 -0.0025  0.0001
                                     0.0000  0.4295 -0.0173 -0.0036  0.4688
                                    -0.0212 -0.0045  0.4028 -0.0143 -0.0029
                                     0.0573  0.0415  0.0491 -0.0093 -0.0134
 26. (1.91979) BD ( 1) C  8-Ru 52
             ( 66.59%)   0.8160* C  8 s( 62.09%)p 0.61( 37.90%)d 0.00(  0.01%)
                                     0.0001  0.7873 -0.0332  0.0003  0.0001
                                     0.0003  0.3475  0.0211  0.0043  0.4258
                                     0.0295  0.0057  0.2747  0.0114  0.0016
                                     0.0065  0.0025  0.0054 -0.0018 -0.0041
             ( 33.41%)   0.5780*Ru 52 s( 35.82%)p 0.00(  0.09%)d 1.79( 64.09%)
                                     0.0000  0.0000 -0.0001 -0.0009  0.5980
                                     0.0230 -0.0082 -0.0024  0.0004  0.0002
                                    -0.0008  0.0004 -0.0001 -0.0001  0.0000
                                     0.0000 -0.0001  0.0001  0.0000  0.0000
                                     0.0005  0.0003 -0.0084  0.0016  0.0004
                                     0.0000  0.0000  0.0000  0.0007  0.0042
                                    -0.0053  0.0130  0.0003  0.0000  0.0000
                                     0.0000  0.0006 -0.0186 -0.0161  0.0000
                                     0.0003  0.0000  0.0000  0.5358  0.0240
                                    -0.0034  0.0021  0.0001  0.0000  0.4049
                                     0.0236 -0.0041  0.0016  0.0001  0.0000
                                     0.4144  0.0184 -0.0014  0.0009  0.0001
                                     0.0000 -0.0764 -0.0042  0.0048 -0.0005
                                     0.0000  0.0000 -0.1033 -0.0077 -0.0009
                                     0.0000  0.0000
 27. (1.97155) BD ( 1) C  9- C 11
             ( 53.54%)   0.7317* C  9 s( 34.84%)p 1.87( 65.09%)d 0.00(  0.06%)
                                    -0.0001  0.5903  0.0028 -0.0024  0.0000
                                    -0.0002 -0.7593  0.0003  0.0071  0.1990
                                    -0.0038  0.0006  0.1862 -0.0046 -0.0001
                                    -0.0084 -0.0079  0.0048  0.0187 -0.0109
             ( 46.46%)   0.6816* C 11 s( 35.14%)p 1.84( 64.76%)d 0.00(  0.10%)
                                    -0.0001  0.5927  0.0126  0.0013  0.0004
                                     0.0004  0.7403  0.0169  0.0049 -0.2290
                                    -0.0071 -0.0010 -0.2159 -0.0077 -0.0021
                                    -0.0096 -0.0091  0.0057  0.0244 -0.0150
 28. (1.97418) BD ( 1) C  9- C 13
             ( 50.89%)   0.7134* C  9 s( 34.63%)p 1.89( 65.30%)d 0.00(  0.07%)
                                    -0.0003  0.5885  0.0065 -0.0001  0.0003
                                     0.0001  0.6363 -0.0003  0.0025  0.3502
                                    -0.0087  0.0011  0.3540 -0.0069  0.0013
                                     0.0145  0.0149  0.0088  0.0107 -0.0058
             ( 49.11%)   0.7008* C 13 s( 35.26%)p 1.83( 64.66%)d 0.00(  0.08%)
                                     0.0000  0.5937 -0.0062  0.0078  0.0002
                                    -0.0002 -0.6052  0.0050  0.0028 -0.3608
                                     0.0109  0.0014 -0.3872  0.0102  0.0011
                                     0.0158  0.0168  0.0114  0.0108 -0.0058
 29. (1.62982) BD ( 2) C  9- C 13
             ( 52.43%)   0.7241* C  9 s(  0.00%)p 1.00( 99.99%)d 0.00(  0.01%)
                                     0.0000 -0.0035 -0.0009  0.0000  0.0000
                                     0.0000  0.0086 -0.0026  0.0000  0.7059
                                     0.0074  0.0025 -0.7081 -0.0079 -0.0024
                                     0.0055 -0.0052 -0.0004 -0.0029 -0.0054
             ( 47.57%)   0.6897* C 13 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.02%)
                                     0.0000 -0.0022 -0.0013  0.0002  0.0000
                                     0.0001  0.0281  0.0006  0.0001  0.7073
                                     0.0029  0.0057 -0.7061 -0.0033 -0.0058
                                    -0.0108  0.0106 -0.0007  0.0014  0.0039
 30. (1.99651) BD ( 1) C 10- O 48
             ( 25.26%)   0.5026* C 10 s(  0.38%)p99.99( 99.39%)d 0.60(  0.23%)
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                                    0.0000  0.0606  0.0123  0.0005 -0.0001
                                    0.0000  0.4815  0.0025 -0.0084 -0.1110
                                   -0.0062  0.0033  0.8655  0.0198 -0.0113
                                    0.0163 -0.0160  0.0188 -0.0140  0.0351
            ( 74.74%)   0.8645* O 48 s(  0.33%)p99.99( 99.26%)d 1.21(  0.40%)
                                    0.0000  0.0578 -0.0021 -0.0002  0.0000
                                    0.0000  0.5713 -0.0022  0.0000 -0.1759
                                    0.0041  0.0001  0.7970 -0.0018  0.0012
                                   -0.0269  0.0141 -0.0170  0.0199 -0.0493
31. (1.99560) BD ( 2) C 10- O 48
            ( 25.09%)   0.5009* C 10 s(  0.70%)p99.99( 99.07%)d 0.33(  0.23%)
                                    0.0000 -0.0816 -0.0189 -0.0010  0.0004
                                    0.0001  0.5579  0.0002 -0.0045  0.7990
                                    0.0041 -0.0139 -0.2018 -0.0072  0.0010
                                   -0.0142  0.0175  0.0159 -0.0387 -0.0067
            ( 74.91%)   0.8655* O 48 s(  0.72%)p99.99( 98.88%)d 0.56(  0.40%)
                                    0.0000 -0.0846  0.0035  0.0004  0.0000
                                    0.0000  0.4271  0.0052  0.0008  0.8921
                                   -0.0023  0.0002 -0.1030 -0.0006 -0.0007
                                    0.0285 -0.0165 -0.0286  0.0449  0.0097
32. (1.99463) BD ( 3) C 10- O 48
            ( 31.24%)   0.5589* C 10 s( 37.37%)p 1.67( 62.57%)d 0.00(  0.06%)
                                   -0.0001  0.5953  0.1388 -0.0020 -0.0008
                                   -0.0007 -0.5205 -0.0290 -0.0203  0.5058
                                    0.0175  0.0135  0.3109  0.0139  0.0172
                                   -0.0182 -0.0111  0.0115  0.0002 -0.0062
            ( 68.76%)   0.8292* O 48 s( 42.68%)p 1.33( 56.56%)d 0.02(  0.76%)
                                    0.0001  0.6528 -0.0252 -0.0027  0.0001
                                    0.0000  0.5255 -0.0186 -0.0041 -0.2442
                                    0.0150  0.0032 -0.4785  0.0155  0.0030
                                   -0.0470 -0.0592  0.0376  0.0222 -0.0018
33. (1.92613) BD ( 1) C 10-Ru 51
            ( 68.44%)   0.8273* C 10 s( 63.04%)p 0.59( 36.95%)d 0.00(  0.01%)
                                    0.0001  0.7931 -0.0385  0.0016  0.0002
                                    0.0003  0.4185 -0.0230  0.0046 -0.2943
                                    0.0168 -0.0038 -0.3260  0.0237 -0.0052
                                   -0.0048 -0.0059  0.0037  0.0024  0.0000
            ( 31.56%)   0.5618*Ru 51 s( 37.53%)p 0.00(  0.07%)d 1.66( 62.39%)
                                    0.0000  0.0000  0.0000 -0.0009  0.6122
                                    0.0224 -0.0047 -0.0016 -0.0001  0.0008
                                   -0.0001  0.0002 -0.0001  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0004 -0.0082 -0.0173  0.0041  0.0006
                                    0.0000  0.0000  0.0000 -0.0006 -0.0044
                                   -0.0012 -0.0138  0.0000  0.0000  0.0000
                                    0.0000 -0.0003 -0.0080  0.0064 -0.0045
                                   -0.0003  0.0000  0.0000 -0.3840 -0.0243
                                    0.0036 -0.0008 -0.0001  0.0000 -0.5124
                                   -0.0197 -0.0002 -0.0013 -0.0001  0.0000
                                    0.2859  0.0033 -0.0033  0.0012  0.0000
                                    0.0000  0.3499  0.0208 -0.0007  0.0006
                                    0.0001  0.0000 -0.0908  0.0024  0.0023
                                   -0.0002  0.0000
34. (1.97955) BD ( 1) C 11- C 15
            ( 48.03%)   0.6930* C 11 s( 37.24%)p 1.68( 62.67%)d 0.00(  0.09%)
                                   -0.0001  0.6092  0.0352 -0.0021  0.0003
                                    0.0000 -0.1577 -0.0174 -0.0047  0.5609
                                    0.0153  0.0048  0.5352  0.0130  0.0038
                                   -0.0009 -0.0009  0.0272 -0.0123  0.0060
            ( 51.97%)   0.7209* C 15 s( 36.81%)p 1.71( 63.10%)d 0.00(  0.09%)
                                    0.0001  0.6066  0.0082  0.0016  0.0000
                                   -0.0004  0.0809  0.0148 -0.0024 -0.5707
                                    0.0093  0.0037 -0.5461  0.0101  0.0034
                                   -0.0063 -0.0057  0.0264 -0.0116  0.0050
35. (1.60134) BD ( 2) C 11- C 15
            ( 45.95%)   0.6778* C 11 s(  0.01%)p 1.00( 99.94%)d 0.00(  0.05%)
                                    0.0000  0.0064 -0.0030  0.0005  0.0000
                                    0.0000 -0.0107  0.0050 -0.0006 -0.6946
                                   -0.0246  0.0051  0.7176  0.0336 -0.0058
                                   -0.0083  0.0090  0.0010  0.0096  0.0169
            ( 54.05%)   0.7352* C 15 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                   -0.0001 -0.0042  0.0001  0.0003  0.0000
                                    0.0000 -0.0142  0.0005  0.0003 -0.6945
                                    0.0012 -0.0040  0.7191 -0.0026  0.0048
                                   -0.0090  0.0091 -0.0006 -0.0059 -0.0093
36. (1.85393) BD ( 1) C 11-Ru 51
            ( 59.60%)   0.7720* C 11 s( 27.65%)p 2.62( 72.34%)d 0.00(  0.01%)
                                    0.0001 -0.5249  0.0325 -0.0025  0.0006
                                    0.0002  0.6509 -0.0371  0.0030  0.3835
                                   -0.0394  0.0012  0.3860 -0.0292 -0.0005
                                   -0.0053 -0.0031 -0.0036  0.0005  0.0015
            ( 40.40%)   0.6356*Ru 51 s( 26.47%)p 0.00(  0.06%)d 2.78( 73.47%)
                                    0.0000  0.0000  0.0001 -0.0007 -0.5143
                                   -0.0116  0.0086 -0.0010 -0.0008  0.0013
                                   -0.0016  0.0004 -0.0001  0.0000 -0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0007  0.0137 -0.0053  0.0029 -0.0003
                                    0.0000  0.0000  0.0000  0.0008  0.0068
                                   -0.0099  0.0097 -0.0002  0.0000  0.0000
                                    0.0000  0.0010  0.0027 -0.0089  0.0018
                                   -0.0001  0.0000 -0.0001 -0.6055  0.0009
                                    0.0003 -0.0013  0.0000  0.0000 -0.3728
                                   -0.0033 -0.0001 -0.0010  0.0000  0.0000
                                   -0.4386  0.0132 -0.0017 -0.0007  0.0000
                                    0.0000  0.0922  0.0051 -0.0062  0.0000
                                    0.0000  0.0000  0.1673 -0.0060 -0.0001
                                    0.0002  0.0000
37. (1.98338) BD ( 1) C 12- C 14
            ( 50.00%)   0.7071* C 12 s( 37.81%)p 1.64( 62.10%)d 0.00(  0.09%)
                                   -0.0001  0.6149  0.0023  0.0039 -0.0001
                                    0.0000 -0.6016  0.0075 -0.0056  0.2665
                                   -0.0153  0.0023  0.4330  0.0169 -0.0014
                                   -0.0120 -0.0226  0.0093  0.0119  0.0010
            ( 50.00%)   0.7071* C 14 s( 34.64%)p 1.88( 65.26%)d 0.00(  0.09%)
                                    0.0000  0.5886 -0.0006  0.0050 -0.0002
                                    0.0002  0.6003 -0.0088 -0.0051 -0.2623
                                   -0.0041  0.0024 -0.4721  0.0234 -0.0005
                                   -0.0159 -0.0214  0.0091  0.0123 -0.0023
38. (1.64997) BD ( 2) C 12- C 14
            ( 46.66%)   0.6831* C 12 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                    0.0000 -0.0008  0.0009 -0.0012  0.0001
                                   -0.0001  0.5750  0.0124  0.0047  0.7422
                                    0.0112  0.0032  0.3433  0.0044  0.0020
                                   -0.0079  0.0057  0.0118 -0.0072  0.0096
            ( 53.34%)   0.7304* C 14 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                    0.0000 -0.0006  0.0018 -0.0008  0.0000
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                                    -0.0001  0.5853  0.0107  0.0052  0.7388
                                     0.0117  0.0065  0.3330  0.0057  0.0037
                                     0.0045  0.0040 -0.0049  0.0169 -0.0005
39. (1.97414) BD ( 1) C 12- H 29
              ( 60.71%)   0.7792* C 12 s( 29.83%)p 2.35( 70.11%)d 0.00(  0.06%)
                                     0.0004 -0.5458  0.0172  0.0070 -0.0002
                                     0.0002 -0.1153 -0.0012  0.0073 -0.2735
                                     0.0001  0.0040  0.7828  0.0131 -0.0084
                                    -0.0024  0.0065  0.0123  0.0020 -0.0199
              ( 39.29%)   0.6268* H 29 s( 99.91%)p 0.00(  0.09%)
                                    -0.9995 -0.0027 -0.0025  0.0052  0.0126
                                    -0.0270
40. (1.98629) BD ( 1) C 12- N 50
              ( 40.16%)   0.6337* C 12 s( 32.38%)p 2.09( 67.54%)d 0.00(  0.09%)
                                     0.0000  0.5685  0.0233  0.0037 -0.0002
                                     0.0003  0.5408 -0.0235  0.0047 -0.5493
                                     0.0163 -0.0055  0.2833  0.0054 -0.0002
                                    -0.0223  0.0117 -0.0131 -0.0011 -0.0077
              ( 59.84%)   0.7735* N 50 s( 35.27%)p 1.83( 64.56%)d 0.00(  0.18%)
                                     0.0000  0.5932  0.0293 -0.0008  0.0004
                                    -0.0001 -0.5177 -0.0057 -0.0002  0.5439
                                     0.0128  0.0016 -0.2846 -0.0228 -0.0035
                                    -0.0359  0.0085 -0.0107  0.0042 -0.0160
41. (1.98340) BD ( 1) C 13- C 17
              ( 50.37%)   0.7097* C 13 s( 36.14%)p 1.76( 63.78%)d 0.00(  0.09%)
                                     0.0000  0.6010  0.0125  0.0032  0.0001
                                     0.0000 -0.1028 -0.0183  0.0042  0.5623
                                    -0.0095  0.0006  0.5572 -0.0097  0.0006
                                    -0.0065 -0.0061  0.0257 -0.0099  0.0053
              ( 49.63%)   0.7045* C 17 s( 35.55%)p 1.81( 64.36%)d 0.00(  0.09%)
                                     0.0000  0.5962  0.0063  0.0038  0.0001
                                    -0.0001  0.1484 -0.0233  0.0017 -0.5636
                                     0.0126  0.0038 -0.5506  0.0117  0.0039
                                    -0.0046 -0.0042  0.0267 -0.0114  0.0062
42. (1.97486) BD ( 1) C 13- H 30
              ( 60.25%)   0.7762* C 13 s( 28.56%)p 2.50( 71.36%)d 0.00(  0.07%)
                                    -0.0003  0.5343 -0.0035 -0.0101 -0.0002
                                     0.0001  0.7882  0.0036 -0.0050 -0.2290
                                    -0.0028  0.0050 -0.1997 -0.0041  0.0050
                                    -0.0123 -0.0103  0.0033  0.0182 -0.0111
              ( 39.75%)   0.6305* H 30 s( 99.94%)p 0.00(  0.06%)
                                     0.9997  0.0023  0.0003 -0.0235  0.0043
                                     0.0021
43. (1.98417) BD ( 1) C 14- C 21
              ( 50.06%)   0.7076* C 14 s( 35.25%)p 1.83( 64.66%)d 0.00(  0.09%)
                                     0.0000  0.5936  0.0083  0.0036 -0.0002
                                     0.0001 -0.1012  0.0181 -0.0045 -0.2591
                                    -0.0075  0.0035  0.7540 -0.0169 -0.0005
                                    -0.0005 -0.0032 -0.0183 -0.0030  0.0238
              ( 49.94%)   0.7067* C 21 s( 34.98%)p 1.86( 64.93%)d 0.00(  0.09%)
                                     0.0000  0.5914  0.0054  0.0039  0.0001
                                     0.0000  0.0443  0.0154 -0.0027  0.2956
                                    -0.0168  0.0002 -0.7479  0.0100  0.0039
                                     0.0008 -0.0057 -0.0161 -0.0022  0.0244
44. (1.97619) BD ( 1) C 14- H 31
              ( 61.65%)   0.7852* C 14 s( 30.05%)p 2.33( 69.88%)d 0.00(  0.07%)
                                     0.0004 -0.5481  0.0050  0.0080 -0.0003
                                     0.0002  0.5344  0.0075 -0.0009 -0.5634
                                    -0.0036  0.0050  0.3094  0.0025 -0.0047
                                     0.0190 -0.0111  0.0120  0.0014  0.0070
              ( 38.35%)   0.6193* H 31 s( 99.95%)p 0.00(  0.05%)
                                    -0.9997 -0.0018  0.0004 -0.0136  0.0161
                                    -0.0077
45. (1.97849) BD ( 1) C 15- C 19
              ( 49.89%)   0.7063* C 15 s( 35.02%)p 1.85( 64.88%)d 0.00(  0.10%)
                                    -0.0001  0.5917  0.0075  0.0045  0.0002
                                     0.0000  0.6167  0.0080  0.0001  0.3644
                                    -0.0147  0.0050  0.3676 -0.0146  0.0052
                                     0.0178  0.0182  0.0113  0.0126 -0.0072
              ( 50.11%)   0.7079* C 19 s( 36.01%)p 1.77( 63.91%)d 0.00(  0.08%)
                                     0.0000  0.6001  0.0017  0.0056 -0.0001
                                     0.0001 -0.6322  0.0255  0.0032 -0.3363
                                    -0.0033  0.0034 -0.3543 -0.0026  0.0031
                                     0.0165  0.0173  0.0113  0.0095 -0.0049
46. (1.97496) BD ( 1) C 15- H 33
              ( 60.93%)   0.7806* C 15 s( 28.12%)p 2.55( 71.81%)d 0.00(  0.07%)
                                     0.0004 -0.5300  0.0149  0.0061  0.0001
                                    -0.0003  0.7818  0.0105 -0.0076 -0.2411
                                    -0.0039 -0.0007 -0.2205 -0.0028  0.0002
                                     0.0120  0.0105 -0.0029 -0.0177  0.0106
              ( 39.07%)   0.6250* H 33 s( 99.92%)p 0.00(  0.08%)
                                    -0.9996 -0.0013 -0.0025 -0.0259  0.0077
                                     0.0083
47. (1.97959) BD ( 1) C 16- C 18
              ( 48.03%)   0.6931* C 16 s( 37.20%)p 1.69( 62.70%)d 0.00(  0.09%)
                                     0.0001 -0.6090 -0.0344  0.0021 -0.0002
                                     0.0000 -0.5386 -0.0193 -0.0054  0.5660
                                     0.0158  0.0048 -0.1260  0.0088  0.0024
                                     0.0240 -0.0091  0.0127  0.0035  0.0096
              ( 51.97%)   0.7209* C 18 s( 36.77%)p 1.72( 63.14%)d 0.00(  0.09%)
                                    -0.0001 -0.6063 -0.0081 -0.0016  0.0000
                                     0.0004  0.5122 -0.0016 -0.0040 -0.5735
                                     0.0089  0.0039  0.1992 -0.0181  0.0003
                                     0.0261 -0.0057  0.0076  0.0018  0.0125
48. (1.97140) BD ( 1) C 16- C 22
              ( 46.41%)   0.6813* C 16 s( 35.00%)p 1.85( 64.90%)d 0.00(  0.10%)
                                    -0.0001  0.5915  0.0126  0.0014  0.0005
                                     0.0004 -0.5379 -0.0145 -0.0041  0.2456
                                     0.0078  0.0011  0.5467  0.0109  0.0032
                                    -0.0103 -0.0258  0.0067  0.0083  0.0119
              ( 53.59%)   0.7320* C 22 s( 34.87%)p 1.87( 65.07%)d 0.00(  0.06%)
                                    -0.0001  0.5905  0.0028 -0.0024  0.0000
                                    -0.0002  0.5253 -0.0040 -0.0035 -0.2142
                                     0.0037 -0.0004 -0.5734 -0.0020  0.0062
                                    -0.0088 -0.0198  0.0058  0.0070  0.0085
49. (1.85838) BD ( 1) C 16-Ru 52
              ( 59.72%)   0.7728* C 16 s( 27.83%)p 2.59( 72.16%)d 0.00(  0.01%)
                                     0.0001 -0.5265  0.0324 -0.0024  0.0006
                                     0.0002  0.0237 -0.0060 -0.0018 -0.3735
                                     0.0375 -0.0010  0.7602 -0.0477  0.0024
                                     0.0008 -0.0009  0.0065  0.0024 -0.0026
              ( 40.28%)   0.6347*Ru 52 s( 27.00%)p 0.00(  0.05%)d 2.70( 72.94%)
                                     0.0000  0.0000  0.0001 -0.0007 -0.5194
                                    -0.0130  0.0091 -0.0005 -0.0009  0.0011
                                    -0.0015  0.0005 -0.0001  0.0000  0.0000
                                     0.0000 -0.0001  0.0001  0.0000  0.0000
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                                    0.0004 -0.0044 -0.0046  0.0002  0.0000
                                    0.0000  0.0000  0.0000 -0.0006 -0.0062
                                    0.0091 -0.0100  0.0002  0.0000  0.0000
                                    0.0000  0.0012  0.0134 -0.0086  0.0038
                                   -0.0003  0.0000  0.0000  0.0615 -0.0116
                                    0.0024 -0.0001  0.0000  0.0000 -0.0838
                                   -0.0079  0.0021 -0.0003  0.0000  0.0001
                                    0.7381 -0.0062  0.0005  0.0016  0.0000
                                    0.0000  0.3002 -0.0017 -0.0032  0.0006
                                    0.0000  0.0000 -0.2888  0.0042 -0.0040
                                   -0.0010  0.0000
50. (1.98463) BD ( 1) C 17- C 19
              ( 50.20%)   0.7085* C 17 s( 35.29%)p 1.83( 64.62%)d 0.00(  0.09%)
                                    0.0000  0.5940  0.0051  0.0041  0.0001
                                   -0.0001 -0.7414  0.0083  0.0042  0.2350
                                   -0.0179  0.0020  0.2017 -0.0174  0.0021
                                   -0.0119 -0.0097  0.0041  0.0217 -0.0129
              ( 49.80%)   0.7057* C 19 s( 35.33%)p 1.83( 64.58%)d 0.00(  0.09%)
                                    0.0000  0.5943  0.0078  0.0033  0.0000
                                    0.0001  0.7608 -0.0222 -0.0015 -0.1971
                                   -0.0098  0.0026 -0.1655 -0.0103  0.0027
                                   -0.0136 -0.0115  0.0042  0.0208 -0.0126
51. (1.64105) BD ( 2) C 17- C 19
              ( 51.73%)   0.7193* C 17 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                                    0.0000  0.0000 -0.0010  0.0001  0.0000
                                    0.0000  0.0291  0.0002  0.0001  0.7022
                                    0.0122  0.0065 -0.7110 -0.0120 -0.0064
                                   -0.0104  0.0106 -0.0005  0.0011  0.0034
              ( 48.27%)   0.6947* C 19 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                    0.0000 -0.0003 -0.0007  0.0001  0.0000
                                    0.0000  0.0266  0.0006  0.0003  0.7004
                                    0.0104  0.0056 -0.7128 -0.0107 -0.0062
                                    0.0078 -0.0084  0.0005  0.0063  0.0102
52. (1.97742) BD ( 1) C 17- H 34
              ( 60.90%)   0.7804* C 17 s( 29.11%)p 2.43( 70.81%)d 0.00(  0.08%)
                                   -0.0004  0.5394 -0.0090 -0.0073 -0.0001
                                    0.0001  0.6525  0.0079 -0.0038  0.3644
                                    0.0045 -0.0007  0.3865  0.0042 -0.0010
                                    0.0166  0.0174  0.0083  0.0098 -0.0050
              ( 39.10%)   0.6253* H 34 s( 99.96%)p 0.00(  0.04%)
                                    0.9998  0.0022  0.0005 -0.0146 -0.0083
                                   -0.0093
53. (1.97863) BD ( 1) C 18- C 24
              ( 49.88%)   0.7063* C 18 s( 35.03%)p 1.85( 64.87%)d 0.00(  0.10%)
                                   -0.0001  0.5918  0.0077  0.0045  0.0002
                                    0.0000  0.0242 -0.0163  0.0043 -0.3525
                                    0.0149 -0.0049  0.7234 -0.0003  0.0025
                                   -0.0013 -0.0008 -0.0205 -0.0043  0.0234
              ( 50.12%)   0.7079* C 24 s( 36.03%)p 1.77( 63.89%)d 0.00(  0.08%)
                                    0.0000  0.6002  0.0018  0.0056 -0.0001
                                    0.0001 -0.0060 -0.0143  0.0012  0.3240
                                    0.0039 -0.0033 -0.7302  0.0210  0.0043
                                   -0.0019  0.0017 -0.0194 -0.0044  0.0203
54. (1.65806) BD ( 2) C 18- C 24
              ( 51.14%)   0.7151* C 18 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                    0.0000  0.0001  0.0000  0.0001  0.0000
                                    0.0000  0.6509  0.0046  0.0057  0.6906
                                    0.0069  0.0063  0.3146  0.0018  0.0030
                                   -0.0052  0.0081  0.0110 -0.0039  0.0084
              ( 48.86%)   0.6990* C 24 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                    0.0000  0.0020  0.0005 -0.0001  0.0000
                                    0.0000  0.6496  0.0079  0.0058  0.6960
                                    0.0088  0.0061  0.3051  0.0037  0.0026
                                    0.0027 -0.0095 -0.0046 -0.0117 -0.0062
55. (1.97499) BD ( 1) C 18- H 32
              ( 60.93%)   0.7806* C 18 s( 28.15%)p 2.55( 71.78%)d 0.00(  0.07%)
                                   -0.0004  0.5304 -0.0149 -0.0061 -0.0001
                                    0.0003  0.5588  0.0073 -0.0037 -0.2625
                                   -0.0040 -0.0006 -0.5800 -0.0078  0.0066
                                   -0.0088 -0.0206  0.0097  0.0077  0.0057
              ( 39.07%)   0.6250* H 32 s( 99.92%)p 0.00(  0.08%)
                                    0.9996  0.0012  0.0025 -0.0196  0.0085
                                    0.0187
56. (1.97665) BD ( 1) C 19- H 35
              ( 60.88%)   0.7803* C 19 s( 28.61%)p 2.49( 71.31%)d 0.00(  0.08%)
                                   -0.0004  0.5348 -0.0064 -0.0085  0.0001
                                   -0.0001 -0.1361 -0.0001  0.0029  0.5971
                                    0.0083 -0.0018  0.5813  0.0077 -0.0016
                                   -0.0059 -0.0058  0.0232 -0.0125  0.0063
              ( 39.12%)   0.6255* H 35 s( 99.96%)p 0.00(  0.04%)
                                    0.9998  0.0021  0.0000  0.0034 -0.0130
                                   -0.0132
57. (1.97250) BD ( 1) C 20- C 22
              ( 50.93%)   0.7137* C 20 s( 34.65%)p 1.88( 65.30%)d 0.00(  0.05%)
                                   -0.0003  0.5885 -0.0130  0.0016 -0.0004
                                    0.0000  0.5395 -0.0151 -0.0027 -0.5573
                                    0.0130  0.0011  0.2257 -0.0004  0.0021
                                   -0.0174  0.0060 -0.0055 -0.0007 -0.0098
              ( 49.07%)   0.7005* C 22 s( 30.47%)p 2.28( 69.46%)d 0.00(  0.07%)
                                   -0.0002  0.5519 -0.0082  0.0013 -0.0002
                                    0.0003 -0.5678  0.0083 -0.0016  0.5855
                                   -0.0102  0.0006 -0.1708  0.0074  0.0018
                                   -0.0216  0.0073 -0.0074 -0.0006 -0.0110
58. (1.97966) BD ( 1) C 20- C 23
              ( 50.27%)   0.7090* C 20 s( 35.44%)p 1.82( 64.50%)d 0.00(  0.07%)
                                   -0.0002  0.5953 -0.0001 -0.0024  0.0001
                                    0.0000 -0.5887  0.0155 -0.0013  0.2537
                                   -0.0120  0.0001  0.4833  0.0012  0.0020
                                   -0.0103 -0.0190  0.0094  0.0100 -0.0006
              ( 49.73%)   0.7052* C 23 s( 34.40%)p 1.90( 65.50%)d 0.00(  0.09%)
                                    0.0000  0.5865 -0.0072  0.0068  0.0002
                                   -0.0002  0.6007 -0.0114 -0.0022 -0.2720
                                    0.0080  0.0002 -0.4690  0.0011  0.0037
                                   -0.0124 -0.0236  0.0089  0.0113  0.0032
59. (1.98126) BD ( 1) C 20- N 50
              ( 40.69%)   0.6379* C 20 s( 29.92%)p 2.34( 70.01%)d 0.00(  0.07%)
                                    0.0001 -0.5466 -0.0197  0.0008 -0.0004
                                   -0.0002 -0.0565 -0.0065 -0.0006 -0.3186
                                   -0.0004  0.0001  0.7716  0.0098  0.0013
                                   -0.0001  0.0029  0.0163  0.0031 -0.0207
              ( 59.31%)   0.7701* N 50 s( 33.94%)p 1.94( 65.88%)d 0.01(  0.18%)
                                    0.0001 -0.5824 -0.0135  0.0005 -0.0007
                                    0.0002  0.0647 -0.0066 -0.0015  0.3034
                                    0.0105  0.0019 -0.7498 -0.0143 -0.0012
                                    0.0003  0.0153  0.0204  0.0003 -0.0332
60. (1.71962) BD ( 2) C 20- N 50
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            ( 34.10%)   0.5839* C 20 s(  0.00%)p 1.00( 99.92%)d 0.00(  0.08%)
                                       0.0000  0.0036  0.0010  0.0002 -0.0001
                                       0.0000  0.5978  0.0243 -0.0015  0.7221
                                       0.0289 -0.0023  0.3445  0.0153 -0.0007
                                       0.0054 -0.0155 -0.0133 -0.0130 -0.0145
            ( 65.90%)   0.8118* N 50 s(  0.00%)p 1.00( 99.91%)d 0.00(  0.09%)
                                       0.0000  0.0014  0.0000  0.0007 -0.0001
                                       0.0000  0.5824  0.0193 -0.0009  0.7341
                                       0.0243 -0.0013  0.3460  0.0146 -0.0010
                                      -0.0127  0.0054  0.0179 -0.0159  0.0135
61. (1.98409) BD ( 1) C 21- C 23
            ( 49.75%)   0.7053* C 21 s( 35.54%)p 1.81( 64.36%)d 0.00(  0.09%)
                                       0.0000  0.5961  0.0058  0.0039  0.0001
                                      -0.0001  0.5200 -0.0014 -0.0047 -0.5375
                                       0.0118  0.0038  0.2891 -0.0236  0.0001
                                      -0.0246  0.0098 -0.0111  0.0003 -0.0101
            ( 50.25%)   0.7089* C 23 s( 35.95%)p 1.78( 63.96%)d 0.00(  0.09%)
                                       0.0000  0.5994  0.0131  0.0032  0.0001
                                      -0.0001 -0.5311  0.0167 -0.0021  0.5440
                                      -0.0066 -0.0002 -0.2472 -0.0144  0.0043
                                      -0.0233  0.0110 -0.0139 -0.0009 -0.0072
62. (1.66342) BD ( 2) C 21- C 23
            ( 48.05%)   0.6932* C 21 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                       0.0000 -0.0017  0.0009 -0.0002  0.0000
                                      -0.0001  0.5864  0.0074  0.0052  0.7410
                                       0.0099  0.0071  0.3262  0.0041  0.0028
                                       0.0051  0.0036 -0.0064  0.0184 -0.0015
            ( 51.95%)   0.7207* C 23 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                       0.0000 -0.0022  0.0010 -0.0002 -0.0001
                                      -0.0001  0.5934  0.0061  0.0056  0.7327
                                       0.0072  0.0069  0.3323  0.0039  0.0035
                                       0.0024 -0.0104 -0.0076 -0.0102 -0.0087
63. (1.97829) BD ( 1) C 21- H 37
            ( 61.42%)   0.7837* C 21 s( 29.42%)p 2.40( 70.50%)d 0.00(  0.08%)
                                       0.0003 -0.5423  0.0086  0.0070  0.0001
                                      -0.0001  0.6184  0.0100 -0.0007 -0.2710
                                      -0.0036  0.0001 -0.4990 -0.0081  0.0015
                                       0.0105  0.0211 -0.0097 -0.0108 -0.0005
            ( 38.58%)   0.6211* H 37 s( 99.96%)p 0.00(  0.04%)
                                      -0.9998 -0.0021 -0.0002 -0.0138  0.0065
                                       0.0116
64. (1.97412) BD ( 1) C 22- C 25
            ( 50.92%)   0.7136* C 22 s( 34.61%)p 1.89( 65.32%)d 0.00(  0.07%)
                                      -0.0003  0.5883  0.0063 -0.0002  0.0003
                                       0.0000  0.0040 -0.0057  0.0001 -0.3357
                                       0.0088 -0.0010  0.7351 -0.0040  0.0027
                                      -0.0008 -0.0009 -0.0163 -0.0033  0.0194
            ( 49.08%)   0.7006* C 25 s( 35.21%)p 1.84( 64.71%)d 0.00(  0.08%)
                                       0.0000  0.5933 -0.0063  0.0078  0.0002
                                      -0.0002 -0.0447  0.0063 -0.0003  0.3525
                                      -0.0108 -0.0013 -0.7215  0.0094  0.0030
                                      -0.0024  0.0002 -0.0188 -0.0040  0.0208
65. (1.97410) BD ( 1) C 23- H 38
            ( 61.21%)   0.7824* C 23 s( 29.60%)p 2.38( 70.33%)d 0.00(  0.07%)
                                      -0.0004  0.5440 -0.0033 -0.0092 -0.0002
                                       0.0002 -0.0598  0.0002 -0.0037 -0.3034
                                      -0.0027  0.0057  0.7794  0.0048 -0.0061
                                       0.0005 -0.0028 -0.0158 -0.0029  0.0202
            ( 38.79%)   0.6228* H 38 s( 99.94%)p 0.00(  0.06%)
                                       0.9997  0.0021  0.0001  0.0031  0.0078
                                      -0.0230
66. (1.98460) BD ( 1) C 24- C 26
            ( 49.80%)   0.7057* C 24 s( 35.31%)p 1.83( 64.60%)d 0.00(  0.09%)
                                       0.0000  0.5941  0.0077  0.0033  0.0000
                                       0.0001 -0.5059  0.0016  0.0031  0.2134
                                       0.0093 -0.0026  0.5864 -0.0244 -0.0001
                                      -0.0107 -0.0238  0.0106  0.0087  0.0072
            ( 50.20%)   0.7085* C 26 s( 35.27%)p 1.83( 64.64%)d 0.00(  0.09%)
                                       0.0000  0.5938  0.0050  0.0041  0.0001
                                      -0.0001  0.5282 -0.0189 -0.0003 -0.2507
                                       0.0180 -0.0019 -0.5513 -0.0014  0.0047
                                      -0.0098 -0.0235  0.0092  0.0083  0.0091
67. (1.97665) BD ( 1) C 24- H 36
            ( 60.91%)   0.7805* C 24 s( 28.62%)p 2.49( 71.30%)d 0.00(  0.08%)
                                      -0.0004  0.5349 -0.0065 -0.0085  0.0001
                                      -0.0001  0.5664  0.0068 -0.0028 -0.6034
                                      -0.0084  0.0018  0.1670  0.0037  0.0018
                                      -0.0230  0.0069 -0.0064 -0.0015 -0.0134
            ( 39.09%)   0.6252* H 36 s( 99.96%)p 0.00(  0.04%)
                                       0.9998  0.0021  0.0000 -0.0131  0.0132
                                      -0.0035
68. (1.98339) BD ( 1) C 25- C 26
            ( 50.38%)   0.7098* C 25 s( 36.16%)p 1.76( 63.75%)d 0.00(  0.09%)
                                       0.0000  0.6012  0.0125  0.0033  0.0001
                                       0.0000  0.5311  0.0003 -0.0015 -0.5665
                                       0.0091 -0.0005  0.1842 -0.0208  0.0040
                                      -0.0256  0.0049 -0.0071 -0.0005 -0.0116
            ( 49.62%)   0.7044* C 26 s( 35.56%)p 1.81( 64.35%)d 0.00(  0.09%)
                                       0.0000  0.5963  0.0064  0.0037  0.0001
                                      -0.0001 -0.5466  0.0211  0.0025  0.5691
                                      -0.0131 -0.0037 -0.1413 -0.0148  0.0034
                                      -0.0255  0.0071 -0.0092 -0.0017 -0.0115
69. (1.69282) BD ( 2) C 25- C 26
            ( 48.91%)   0.6994* C 25 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                       0.0000 -0.0015  0.0016 -0.0001  0.0000
                                      -0.0001  0.6454  0.0102  0.0060  0.7014
                                       0.0115  0.0071  0.3014  0.0048  0.0031
                                       0.0015  0.0023 -0.0047  0.0150 -0.0007
            ( 51.09%)   0.7148* C 26 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                       0.0000 -0.0012  0.0012 -0.0001  0.0000
                                       0.0000  0.6481  0.0109  0.0056  0.6986
                                       0.0111  0.0060  0.3020  0.0051  0.0027
                                       0.0017 -0.0086 -0.0036 -0.0121 -0.0050
70. (1.97485) BD ( 1) C 25- H 39
            ( 60.23%)   0.7761* C 25 s( 28.58%)p 2.50( 71.34%)d 0.00(  0.07%)
                                       0.0003 -0.5345  0.0034  0.0102  0.0002
                                      -0.0001  0.5462  0.0052 -0.0067 -0.2483
                                      -0.0031  0.0051 -0.5944 -0.0009  0.0020
                                       0.0093  0.0210 -0.0097 -0.0077 -0.0062
            ( 39.77%)   0.6306* H 39 s( 99.94%)p 0.00(  0.06%)
                                      -0.9997 -0.0022 -0.0002 -0.0129  0.0045
                                       0.0198
71. (1.97737) BD ( 1) C 26- H 40
            ( 60.92%)   0.7805* C 26 s( 29.12%)p 2.43( 70.80%)d 0.00(  0.08%)
                                      -0.0004  0.5395 -0.0090 -0.0073 -0.0001
                                       0.0001  0.0243 -0.0001  0.0010 -0.3518
```

```
                                    -0.0043  0.0006  0.7639  0.0091 -0.0038
                                     0.0008  0.0014 -0.0180 -0.0043  0.0206
            ( 39.08%)   0.6251* H 40 s( 99.96%)p 0.00(  0.04%)
                                     0.9998  0.0022  0.0005 -0.0011  0.0081
                                    -0.0174
72. (1.99064) BD ( 1) H 43- O 45
            ( 25.67%)   0.5067* H 43 s( 99.99%)p 0.00(  0.01%)
                                    -0.9999 -0.0036 -0.0005 -0.0006 -0.0013
                                    -0.0093
            ( 74.33%)   0.8621* O 45 s( 22.37%)p 3.46( 77.38%)d 0.01(  0.25%)
                                     0.0000 -0.4725  0.0212  0.0037 -0.0002
                                     0.0000  0.7970  0.0362  0.0010 -0.1547
                                    -0.0063  0.0000  0.3355  0.0268  0.0011
                                     0.0154 -0.0243  0.0057 -0.0349  0.0195
73. (1.99935) CR ( 1) C  1          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000 -0.0002
                                     0.0000  0.0000 -0.0002  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
74. (1.99935) CR ( 1) C  2          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0003  0.0000  0.0000  0.0000
                                     0.0000 -0.0002  0.0000  0.0000 -0.0001
                                     0.0000  0.0000 -0.0002  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
75. (1.99938) CR ( 1) C  3          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0001  0.0000  0.0000  0.0000
                                     0.0000  0.0003  0.0000  0.0000 -0.0001
                                     0.0000  0.0000 -0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
76. (1.99944) CR ( 1) C  4          s(100.00%)
                                     1.0000 -0.0001  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0001
                                     0.0000  0.0000 -0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
77. (1.99929) CR ( 1) C  5          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0003  0.0000  0.0000  0.0002
                                     0.0000  0.0000  0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
78. (1.99945) CR ( 1) C  6          s(100.00%)
                                     1.0000 -0.0001  0.0000  0.0000  0.0000
                                     0.0000  0.0001  0.0000  0.0000 -0.0001
                                     0.0000  0.0000 -0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
79. (1.99926) CR ( 1) C  7          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0003  0.0000  0.0000  0.0000
                                     0.0000  0.0001  0.0000  0.0000  0.0001
                                     0.0000  0.0000  0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
80. (1.99944) CR ( 1) C  8          s(100.00%)
                                     1.0000 -0.0001  0.0000  0.0000  0.0000
                                     0.0000 -0.0001  0.0000  0.0000 -0.0001
                                     0.0000  0.0000 -0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
81. (1.99918) CR ( 1) C  9          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0003  0.0000  0.0000  0.0000
                                     0.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
82. (1.99946) CR ( 1) C 10          s(100.00%)
                                     1.0000 -0.0001  0.0000  0.0000  0.0000
                                     0.0000 -0.0001  0.0000  0.0000  0.0001
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
83. (1.99907) CR ( 1) C 11          s(100.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
84. (1.99935) CR ( 1) C 12          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0003  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0001
                                     0.0000  0.0000 -0.0003  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
85. (1.99930) CR ( 1) C 13          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0003  0.0000  0.0000  0.0000
                                     0.0000  0.0000 -0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
86. (1.99935) CR ( 1) C 14          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000 -0.0002  0.0000  0.0000  0.0002
                                     0.0000  0.0000 -0.0002  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
87. (1.99930) CR ( 1) C 15          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000 -0.0002  0.0000  0.0000  0.0001
                                     0.0000  0.0000  0.0002  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
88. (1.99908) CR ( 1) C 16          s(100.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
89. (1.99937) CR ( 1) C 17          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0003  0.0000  0.0000  0.0002
                                     0.0000  0.0000  0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
90. (1.99930) CR ( 1) C 18          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000  0.0003  0.0000  0.0000 -0.0002
                                     0.0000  0.0000 -0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
91. (1.99937) CR ( 1) C 19          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0002  0.0000  0.0000  0.0000
                                     0.0000 -0.0001  0.0000  0.0000  0.0002
                                     0.0000  0.0000  0.0003  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
92. (1.99926) CR ( 1) C 20          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0003  0.0000  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000 -0.0001
                                     0.0000  0.0000  0.0001  0.0000  0.0000
                                     0.0000  0.0000  0.0000  0.0000  0.0000
93. (1.99938) CR ( 1) C 21          s(100.00%)p 0.00(  0.00%)
                                     1.0000  0.0001  0.0000  0.0000  0.0000
```

```
                                0.0000 -0.0002  0.0000  0.0000  0.0001
                                0.0000  0.0000  0.0002  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
 94. (1.99918) CR ( 1) C 22     s(100.00%)p 0.00(  0.00%)
                                1.0000  0.0003  0.0000  0.0000  0.0000
                                0.0000 -0.0001  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0001  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
 95. (1.99929) CR ( 1) C 23     s(100.00%)p 0.00(  0.00%)
                                1.0000  0.0002  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000 -0.0002
                                0.0000  0.0000  0.0003  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
 96. (1.99937) CR ( 1) C 24     s(100.00%)p 0.00(  0.00%)
                                1.0000  0.0002  0.0000  0.0000  0.0000
                                0.0000  0.0002  0.0000  0.0000 -0.0003
                                0.0000  0.0000  0.0001  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
 97. (1.99930) CR ( 1) C 25     s(100.00%)p 0.00(  0.00%)
                                1.0000  0.0002  0.0000  0.0000  0.0000
                                0.0000 -0.0002  0.0000  0.0000  0.0001
                                0.0000  0.0000  0.0002  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
 98. (1.99937) CR ( 1) C 26     s(100.00%)p 0.00(  0.00%)
                                1.0000  0.0002  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000 -0.0001
                                0.0000  0.0000  0.0003  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
 99. (1.99979) CR ( 1) O 44     s(100.00%)p 0.00(  0.00%)
                                1.0000  0.0002  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0002
                                0.0000  0.0000 -0.0002  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
100. (1.99990) CR ( 1) O 45     s(100.00%)
                                1.0000 -0.0001  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000 -0.0001  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
101. (1.99980) CR ( 1) O 46     s(100.00%)p 0.00(  0.00%)
                                1.0000  0.0002  0.0000  0.0000  0.0000
                                0.0000  0.0002  0.0000  0.0000 -0.0001
                                0.0000  0.0000 -0.0001  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
102. (1.99979) CR ( 1) O 47     s(100.00%)p 0.00(  0.00%)
                                1.0000  0.0002  0.0000  0.0000  0.0000
                                0.0000 -0.0002  0.0000  0.0000 -0.0002
                                0.0000  0.0000 -0.0001  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
103. (1.99980) CR ( 1) O 48     s(100.00%)p 0.00(  0.00%)
                                1.0000  0.0002  0.0000  0.0000  0.0000
                                0.0000 -0.0002  0.0000  0.0000  0.0001
                                0.0000  0.0000  0.0002  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
104. (1.99947) CR ( 1) N 49     s(100.00%)p 0.00(  0.00%)
                                1.0000 -0.0003  0.0000  0.0000  0.0000
                                0.0000  0.0006  0.0000  0.0000 -0.0002
                                0.0000  0.0000 -0.0002  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
105. (1.99947) CR ( 1) N 50     s(100.00%)p 0.00(  0.00%)
                                1.0000 -0.0003  0.0000  0.0000  0.0000
                                0.0000 -0.0004  0.0000  0.0000  0.0002
                                0.0000  0.0000  0.0004  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
106. (2.00000) CR ( 1)Ru 51     s(100.00%)
                                1.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
107. (2.00000) CR ( 2)Ru 51     s(100.00%)
                                0.0000  1.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
108. (1.99999) CR ( 3)Ru 51     s(100.00%)
                                0.0000  0.0000  1.0000  0.0000  0.0001
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000 -0.0001  0.0000  0.0000  0.0000
                                0.0000  0.0000 -0.0001  0.0000  0.0000
                                0.0000  0.0000
109. (1.98720) CR ( 4)Ru 51     s(100.00%)p 0.00(  0.00%)d 0.00(  0.00%)
                                0.0000  0.0000  0.0000  1.0000  0.0007
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
```

```
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000 -0.0009  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0002
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0006  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0013  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0012  0.0000  0.0000
                                    0.0000  0.0000
110. (2.00000) CR ( 5)Ru 51          s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  1.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
111. (2.00000) CR ( 6)Ru 51          s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  1.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
112. (1.99366) CR ( 7)Ru 51          s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -1.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000 -0.0016  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.0007  0.0000  0.0000  0.0000
                                    0.0000  0.0000 -0.0003  0.0000  0.0000
                                    0.0000  0.0000
113. (2.00000) CR ( 8)Ru 51          s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  1.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
114. (2.00000) CR ( 9)Ru 51          s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  1.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
115. (1.99491) CR (10)Ru 51          s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0012
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  1.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000 -0.0007  0.0000
                                    0.0000  0.0000  0.0000  0.0000 -0.0002
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0006  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.0022  0.0000  0.0000  0.0000
                                    0.0000  0.0000 -0.0011  0.0000  0.0000
                                    0.0000  0.0000
116. (2.00000) CR (11)Ru 51          s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  1.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
```

```
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
117. (2.00000) CR (12)Ru 51     s(  0.00%)p 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                1.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
118. (1.99208) CR (13)Ru 51     s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0003
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  1.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0001  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0001
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0018  0.0000  0.0000  0.0000  0.0000
                                0.0000 -0.0007  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0004  0.0000  0.0000
                                0.0000  0.0000
119. (2.00000) CR (14)Ru 51     s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  1.0000 -0.0001  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
120. (2.00000) CR (15)Ru 51     s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  1.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
121. (2.00000) CR (16)Ru 51     s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  1.0000
                               -0.0001  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
122. (2.00000) CR (17)Ru 51     s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                1.0000 -0.0001  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
123. (2.00000) CR (18)Ru 51     s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
```

```
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  1.0000 -0.0001  0.0000  0.0000
                                    0.0000  0.0000
124. (2.00000) CR ( 1)Ru 52         s(100.00%)
                                    1.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
125. (2.00000) CR ( 2)Ru 52         s(100.00%)
                                    0.0000  1.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
126. (1.99999) CR ( 3)Ru 52         s(100.00%)p 0.00(  0.00%)d 0.00(  0.00%)
                                    0.0000  0.0000  1.0000  0.0000  0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.0001  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
127. (1.98735) CR ( 4)Ru 52         s(100.00%)p 0.00(  0.00%)d 0.00(  0.00%)
                                    0.0000  0.0000  0.0000  1.0000  0.0007
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0001  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0003
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0013  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0016  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0010  0.0000  0.0000
                                    0.0000  0.0000
128. (2.00000) CR ( 5)Ru 52         s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  1.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
129. (2.00000) CR ( 6)Ru 52         s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  1.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
130. (1.99242) CR ( 7)Ru 52         s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0002
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    1.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000 -0.0017  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0005
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.0006  0.0000  0.0000  0.0000
                                    0.0000  0.0000 -0.0004  0.0000  0.0000
                                    0.0000  0.0000
131. (2.00000) CR ( 8)Ru 52         s(  0.00%)p 1.00(100.00%)
```

```
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  1.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
132. (2.00000) CR ( 9)Ru 52     s(  0.00%)p 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  1.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
133. (1.99491) CR (10)Ru 52     s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0011
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000 -1.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000 -0.0008  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0001
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0003  0.0000  0.0000  0.0000  0.0000
                                0.0000 -0.0022  0.0000  0.0000  0.0000
                                0.0000  0.0000 -0.0015  0.0000  0.0000
                                0.0000  0.0000
134. (2.00000) CR (11)Ru 52     s(  0.00%)p 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  1.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
135. (2.00000) CR (12)Ru 52     s(  0.00%)p 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                1.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
136. (1.99309) CR (13)Ru 52     s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0001
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  1.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000 -0.0002  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0004
                                0.0000  0.0000  0.0000  0.0000  0.0000
                               -0.0017  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0004  0.0000  0.0000  0.0000
                                0.0000  0.0000 -0.0001  0.0000  0.0000
                                0.0000  0.0000
137. (2.00000) CR (14)Ru 52     s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  1.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000
138. (2.00000) CR (15)Ru 52     s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0000  0.0000  0.0000  0.0000
```

```
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  1.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
139. (2.00000) CR (16)Ru 52         s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  1.0000
                                   -0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
140. (2.00000) CR (17)Ru 52         s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    1.0000 -0.0001  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
141. (2.00000) CR (18)Ru 52         s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  1.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000
142. (2.00000) CR ( 1)Cl 53         s(100.00%)
                                    1.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000
143. (1.99995) CR ( 2)Cl 53         s(100.00%)
                                    0.0000  1.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000
144. (1.99998) CR ( 3)Cl 53         s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000 -0.0001  0.0000  0.0000
                                    0.0000  0.0000  0.0000  1.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000
145. (1.99994) CR ( 4)Cl 53         s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  1.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000
146. (1.99996) CR ( 5)Cl 53         s(  0.00%)p 1.00(100.00%)
                                    0.0000  0.0000  0.0002  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000 -1.0000 -0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000
147. (1.05144) LP ( 1) C 22         s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
                                    0.0000  0.0012  0.0005  0.0000  0.0000
                                    0.0000  0.6332  0.0053  0.0024  0.7056
                                    0.0086  0.0021  0.3178  0.0058  0.0012
                                   -0.0004  0.0002 -0.0005  0.0016 -0.0001
148. (1.97801) LP ( 1) O 44         s( 57.22%)p 0.75( 42.65%)d 0.00(  0.13%)
                                   -0.0004  0.7563  0.0148  0.0014  0.0000
                                    0.0000 -0.1007 -0.0018 -0.0005  0.4504
                                    0.0052  0.0024 -0.4620 -0.0057 -0.0025
                                    0.0062 -0.0069  0.0308  0.0144 -0.0090
149. (1.97470) LP ( 1) O 45         s( 30.37%)p 2.29( 69.58%)d 0.00(  0.05%)
                                    0.0000  0.5510 -0.0015  0.0024  0.0000
                                    0.0000  0.5411 -0.0063  0.0005 -0.2006
                                   -0.0024 -0.0002 -0.6022  0.0043  0.0002
                                    0.0086  0.0167 -0.0043 -0.0094  0.0067
150. (1.80445) LP ( 2) O 45         s( 46.94%)p 1.13( 53.04%)d 0.00(  0.02%)
                                    0.0001  0.6850  0.0130  0.0000 -0.0002
                                    0.0000  0.0976 -0.0010  0.0015 -0.0214
                                    0.0026 -0.0004  0.7214 -0.0070 -0.0003
                                    0.0044 -0.0104  0.0000 -0.0056 -0.0007
151. (1.75552) LP ( 3) O 45         s(  0.29%)p99.99( 99.66%)d 0.17(  0.05%)
                                    0.0000  0.0537  0.0023  0.0000  0.0000
```

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                                    0.0000  0.2425 -0.0072 -0.0005  0.9666
                                   -0.0203 -0.0010 -0.0549  0.0045  0.0002
                                   -0.0139  0.0041  0.0114 -0.0109 -0.0039
152. (1.97792) LP ( 1) O 46         s( 56.34%)p 0.77( 43.52%)d 0.00(  0.14%)
                                   -0.0004  0.7504  0.0163  0.0016  0.0000
                                    0.0000  0.5085  0.0058  0.0029 -0.3433
                                   -0.0047 -0.0018 -0.2422 -0.0035 -0.0014
                                    0.0258  0.0185 -0.0122 -0.0111  0.0113
153. (1.97818) LP ( 1) O 47         s( 57.21%)p 0.75( 42.65%)d 0.00(  0.13%)
                                   -0.0004  0.7563  0.0147  0.0014  0.0000
                                    0.0000 -0.3689 -0.0044 -0.0020 -0.4466
                                   -0.0050 -0.0024 -0.3016 -0.0041 -0.0016
                                   -0.0247 -0.0164 -0.0196  0.0050  0.0066
154. (1.97768) LP ( 1) O 48         s( 56.20%)p 0.78( 43.66%)d 0.00(  0.14%)
                                   -0.0004  0.7495  0.0165  0.0016  0.0000
                                    0.0000 -0.4566 -0.0061 -0.0026  0.3292
                                    0.0043  0.0018  0.3459  0.0034  0.0021
                                    0.0221  0.0240 -0.0170 -0.0077  0.0030
155. (1.65970) LP ( 1) N 49         s( 30.57%)p 2.27( 69.43%)d 0.00(  0.01%)
                                    0.0007  0.5520 -0.0313  0.0006 -0.0007
                                    0.0002 -0.7224  0.0445  0.0002  0.2567
                                   -0.0208 -0.0009  0.3220 -0.0225 -0.0006
                                    0.0024  0.0046 -0.0003 -0.0046  0.0022
156. (1.67087) LP ( 1) N 50         s( 30.82%)p 2.24( 69.18%)d 0.00(  0.01%)
                                    0.0007  0.5542 -0.0313  0.0007 -0.0007
                                    0.0002  0.6201 -0.0411 -0.0005 -0.2654
                                    0.0219  0.0008 -0.4836  0.0288 -0.0002
                                    0.0020  0.0068 -0.0023 -0.0037  0.0000
157. (1.76340) LP ( 1)Ru 51         s(  0.00%)p 0.00(  0.00%)d 1.00( 99.99%)
                                    0.0000  0.0000  0.0000  0.0005  0.0012
                                    0.0034 -0.0005 -0.0011  0.0002 -0.0002
                                    0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0007  0.0025 -0.0001  0.0004  0.0001
                                    0.0000  0.0000  0.0000  0.0004 -0.0018
                                   -0.0011 -0.0001  0.0000  0.0000  0.0000
                                    0.0000  0.0014 -0.0036 -0.0040 -0.0017
                                   -0.0001  0.0000  0.0000  0.3724  0.0010
                                    0.0026  0.0000  0.0000  0.0000 -0.2380
                                    0.0067 -0.0018  0.0004  0.0000  0.0000
                                   -0.5085  0.0051 -0.0026  0.0004  0.0000
                                    0.0000  0.2981  0.0006  0.0006 -0.0001
                                    0.0000  0.0000 -0.6759  0.0143 -0.0036
                                    0.0002  0.0001
158. (1.71227) LP ( 2)Ru 51         s(  0.00%)p 1.00(  0.02%)d99.99( 99.97%)
                                    0.0000  0.0000  0.0001 -0.0016  0.0045
                                   -0.0034  0.0024  0.0019 -0.0003  0.0015
                                    0.0001 -0.0001  0.0001  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0006  0.0061 -0.0047 -0.0016  0.0000
                                    0.0000  0.0000  0.0000  0.0022  0.0024
                                   -0.0109 -0.0039 -0.0002  0.0000  0.0000
                                    0.0000  0.0006  0.0029 -0.0037 -0.0009
                                    0.0000  0.0000  0.0000 -0.0301  0.0019
                                   -0.0005  0.0007  0.0000  0.0000  0.4880
                                   -0.0124  0.0025  0.0004  0.0000  0.0000
                                   -0.1063  0.0021 -0.0001  0.0001  0.0000
                                    0.0001  0.8268 -0.0005  0.0030 -0.0008
                                    0.0000  0.0000  0.2558 -0.0104  0.0020
                                   -0.0003  0.0000
159. (1.66503) LP ( 3)Ru 51         s(  0.01%)p 0.00(  0.01%)d 1.00( 99.98%)
                                    0.0000  0.0000 -0.0001  0.0003  0.0079
                                   -0.0003 -0.0001  0.0007  0.0014  0.0001
                                    0.0005 -0.0001  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0013  0.0031 -0.0048 -0.0020 -0.0002
                                    0.0000  0.0000  0.0000 -0.0013 -0.0032
                                    0.0062  0.0023  0.0001  0.0000  0.0000
                                    0.0000  0.0000  0.0011 -0.0007 -0.0005
                                    0.0000  0.0000 -0.0001 -0.5754  0.0042
                                    0.0001  0.0013  0.0000  0.0000  0.5147
                                   -0.0091 -0.0002 -0.0002  0.0000  0.0000
                                    0.0864 -0.0008  0.0001  0.0004  0.0000
                                    0.0000 -0.1226  0.0008  0.0000  0.0003
                                    0.0000  0.0000 -0.6172  0.0139  0.0010
                                    0.0004  0.0000
160. (1.77295) LP ( 1)Ru 52         s(  0.01%)p 0.00(  0.01%)d 1.00( 99.99%)
                                    0.0000  0.0000  0.0000 -0.0001  0.0087
                                    0.0000  0.0003  0.0020 -0.0005 -0.0002
                                   -0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0014  0.0037  0.0028  0.0016  0.0001
                                    0.0000  0.0000  0.0000  0.0008 -0.0011
                                   -0.0016 -0.0006  0.0000  0.0000  0.0000
                                    0.0000 -0.0004 -0.0040  0.0018  0.0003
                                    0.0000  0.0000  0.0000 -0.6190  0.0027
                                   -0.0037  0.0004  0.0000  0.0000  0.7407
                                   -0.0091  0.0037 -0.0005 -0.0001  0.0000
                                    0.0150  0.0012  0.0004  0.0003  0.0000
                                    0.0000  0.0710 -0.0066  0.0005  0.0001
                                    0.0000  0.0000 -0.2504  0.0009 -0.0003
                                   -0.0001  0.0000
161. (1.71317) LP ( 2)Ru 52         s(  0.01%)p 1.00(  0.03%)d99.99( 99.97%)
                                    0.0000  0.0000 -0.0001  0.0019  0.0020
                                    0.0057 -0.0026 -0.0016  0.0002 -0.0018
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0004  0.0014  0.0008  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0022  0.0019
                                   -0.0107 -0.0040 -0.0002  0.0000  0.0000
                                    0.0000 -0.0001 -0.0090  0.0052  0.0016
                                    0.0001  0.0000  0.0000  0.0437  0.0035
                                    0.0004 -0.0004  0.0000  0.0000 -0.1997
                                    0.0130 -0.0022 -0.0002  0.0000 -0.0001
                                   -0.1623  0.0008 -0.0010  0.0007  0.0000
                                   -0.0001 -0.4709  0.0029 -0.0023  0.0007
                                    0.0000  0.0000 -0.8423  0.0122 -0.0035
                                    0.0001  0.0000
162. (1.66584) LP ( 3)Ru 52         s(  0.00%)p 1.00(  0.01%)d99.99( 99.99%)
                                    0.0000  0.0000 -0.0001  0.0003  0.0057
                                   -0.0007 -0.0002  0.0006  0.0014  0.0003
                                    0.0004 -0.0001  0.0000  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0008  0.0004  0.0018  0.0006  0.0001
                                    0.0000  0.0000  0.0000  0.0015  0.0034
                                   -0.0068 -0.0025 -0.0001  0.0000  0.0000
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                                    0.0000  0.0011  0.0036 -0.0039 -0.0017
                                   -0.0002  0.0000  0.0000 -0.3279  0.0034
                                   -0.0002  0.0003  0.0000  0.0000 -0.0975
                                    0.0045  0.0004  0.0000  0.0000  0.0000
                                    0.4567 -0.0024 -0.0003 -0.0013  0.0000
                                   -0.0001 -0.7487  0.0134  0.0004  0.0007
                                    0.0000  0.0000  0.3368 -0.0083 -0.0005
                                    0.0000  0.0000
163. (1.99093) LP ( 1)Cl 53          s( 71.85%)p 0.39( 28.15%)d 0.00(  0.01%)
                                    0.0000  0.0000  0.8476  0.0106  0.0015
                                   -0.0001  0.0002  0.0000  0.0001  0.2873
                                   -0.0017  0.0002 -0.0003  0.0000 -0.0020
                                    0.0000  0.0000  0.0000  0.0001  0.4460
                                   -0.0026  0.0003 -0.0004  0.0001 -0.0057
                                   -0.0001 -0.0028 -0.0048
164. (1.97091) LP ( 2)Cl 53          s(  0.01%)p 1.00( 99.97%)d 0.00(  0.02%)
                                    0.0000  0.0000  0.0098  0.0002  0.0002
                                    0.0000  0.0000  0.0000  0.0000 -0.8204
                                   -0.0004  0.0020  0.0002  0.0000  0.2563
                                   -0.0030 -0.0011 -0.0002  0.0000  0.5109
                                   -0.0001 -0.0012 -0.0002 -0.0013  0.0061
                                   -0.0023  0.0064 -0.0109
165. (1.67716) LP ( 3)Cl 53          s( 24.71%)p 3.04( 75.21%)d 0.00(  0.08%)
                                    0.0000  0.0000  0.4968 -0.0188 -0.0027
                                    0.0001 -0.0003  0.0000  0.0001 -0.3392
                                   -0.0022  0.0017 -0.0002  0.0000  0.3373
                                   -0.0012  0.0015  0.0001  0.0001 -0.7233
                                   -0.0054  0.0014 -0.0004  0.0013  0.0185
                                   -0.0151 -0.0091  0.0105
166. (1.66947) LP ( 4)Cl 53          s(  3.47%)p27.82( 96.40%)d 0.04(  0.13%)
                                    0.0000  0.0000  0.1860 -0.0072 -0.0010
                                    0.0001 -0.0001  0.0000  0.0001 -0.3590
                                   -0.0029 -0.0016 -0.0002  0.0000 -0.9051
                                    0.0033 -0.0039 -0.0002  0.0000 -0.1261
                                   -0.0009  0.0018 -0.0001  0.0207  0.0120
                                    0.0270  0.0012 -0.0049
167. (0.89449) LP*( 1) C 16          s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                    0.0000  0.0037 -0.0007  0.0000 -0.0001
                                    0.0000  0.6463  0.0275 -0.0047  0.6904
                                    0.0264 -0.0053  0.3217  0.0187 -0.0034
                                   -0.0053  0.0107  0.0088  0.0043  0.0094
168. (0.00291) RY*( 1) C  1          s( 20.48%)p 3.46( 70.86%)d 0.42(  8.67%)
                                    0.0000  0.0015  0.4502 -0.0460 -0.0005
                                   -0.0011  0.0099  0.2778 -0.0568  0.0107
                                   -0.5272  0.0313  0.0114 -0.5890  0.0438
                                   -0.0134  0.0068  0.1896 -0.1883  0.1225
169. (0.00212) RY*( 2) C  1          s(  0.14%)p99.99( 93.85%)d44.38(  6.02%)
                                    0.0000 -0.0021  0.0365 -0.0046 -0.0009
                                    0.0003  0.0022  0.0230 -0.0226 -0.0109
                                    0.7278  0.1081  0.0108 -0.6188 -0.1137
                                   -0.0431  0.0523 -0.0210  0.1296  0.1958
170. (0.00109) RY*( 3) C  1          s(  5.09%)p18.42( 93.73%)d 0.23(  1.18%)
                                    0.0000  0.0001  0.2199 -0.0497  0.0045
                                   -0.0029 -0.0320 -0.9125  0.2634  0.0015
                                   -0.1057  0.0637  0.0033 -0.1343  0.0297
                                   -0.0133  0.0126  0.0711 -0.0362  0.0716
171. (0.00059) RY*( 4) C  1          s( 70.67%)p 0.35( 24.94%)d 0.06(  4.39%)
                                    0.0000 -0.0062  0.8404 -0.0176  0.0022
                                    0.0025 -0.0001  0.0970  0.0166 -0.0101
                                    0.2922 -0.1043 -0.0125  0.3650 -0.1000
                                   -0.0709 -0.1267  0.0103  0.0759 -0.1301
172. (0.00034) RY*( 5) C  1          s(  0.04%)p15.43(  0.65%)d99.99( 99.31%)
                                    0.0000  0.0005  0.0116  0.0165  0.0038
                                    0.0007  0.0006 -0.0031 -0.0519 -0.0066
                                   -0.0392 -0.0109  0.0043  0.0442 -0.0110
                                   -0.7413  0.6577  0.0270  0.0468 -0.0901
173. (0.00012) RY*( 6) C  1          s( 21.24%)p 2.57( 54.56%)d 1.14( 24.20%)
                                    0.0000  0.0092  0.1489  0.4254  0.0799
                                   -0.0527 -0.0056 -0.0629 -0.2920 -0.0072
                                   -0.0492  0.4784 -0.0067 -0.0476  0.4719
                                    0.0757  0.0438 -0.4081  0.1971 -0.1703
174. (0.00010) RY*( 7) C  1          s(  0.82%)p65.49( 53.79%)d55.27( 45.39%)
175. (0.00006) RY*( 8) C  1          s(  3.57%)p11.96( 42.73%)d15.04( 53.70%)
176. (0.00004) RY*( 9) C  1          s( 13.71%)p 2.79( 38.30%)d 3.50( 47.99%)
177. (0.00001) RY*(10) C  1          s(  7.46%)p 2.36( 17.56%)d10.06( 74.98%)
178. (0.00002) RY*(11) C  1          s(  1.57%)p59.39( 93.41%)d 3.19(  5.02%)
179. (0.00001) RY*(12) C  1          s( 56.85%)p 0.05(  2.74%)d 0.71( 40.41%)
180. (0.00001) RY*(13) C  1          s(  1.08%)p11.52( 12.48%)d79.77( 86.43%)
181. (0.00000) RY*(14) C  1          s( 98.60%)p 0.01(  0.53%)d 0.01(  0.87%)
182. (0.00000) RY*(15) C  1          s( 98.74%)p 0.00(  0.11%)d 0.01(  1.15%)
183. (0.00601) RY*( 1) C  2          s(  7.44%)p11.46( 85.20%)d 0.99(  7.36%)
                                    0.0000  0.0024  0.2720 -0.0190  0.0016
                                   -0.0023  0.0240 -0.6080 -0.1241 -0.0089
                                   -0.5615  0.0470 -0.0146 -0.3782  0.0747
                                    0.1737  0.1709 -0.0446  0.0706 -0.0853
184. (0.00498) RY*( 2) C  2          s(  1.58%)p58.25( 92.15%)d 3.96(  6.27%)
                                    0.0000 -0.0026  0.1230 -0.0263 -0.0016
                                   -0.0014  0.0036 -0.1414 -0.0202 -0.0105
                                    0.6692  0.0959  0.0098 -0.6604 -0.0882
                                    0.0366  0.0358 -0.0186  0.1356  0.2032
185. (0.00230) RY*( 3) C  2          s( 31.42%)p 2.18( 68.38%)d 0.01(  0.19%)
                                    0.0000 -0.0108  0.5596 -0.0306  0.0077
                                   -0.0026 -0.0143  0.6948 -0.0898 -0.0260
                                   -0.2341  0.1499 -0.0241 -0.2884  0.1764
                                    0.0055 -0.0219  0.0310 -0.0014 -0.0218
186. (0.00127) RY*( 4) C  2          s( 54.49%)p 0.70( 38.14%)d 0.14(  7.37%)
                                    0.0000 -0.0014  0.7106 -0.1998 -0.0029
                                   -0.0018 -0.0157 -0.2514  0.0661  0.0039
                                    0.3362 -0.1054 -0.0001  0.4317 -0.0553
                                   -0.0157  0.0540  0.0406 -0.0857 -0.2481
187. (0.00058) RY*( 5) C  2          s(  3.79%)p 3.17( 12.00%)d22.22( 84.21%)
                                    0.0000 -0.0024  0.1876 -0.0517 -0.0042
                                    0.0013 -0.0042 -0.0245  0.1894 -0.0040
                                   -0.1259 -0.0594  0.0071  0.2078 -0.1446
                                    0.3416 -0.3492 -0.0814  0.4251  0.6450
188. (0.00036) RY*( 6) C  2          s(  5.27%)p10.63( 56.00%)d 7.35( 38.73%)
                                    0.0000  0.0088  0.0096  0.2281  0.0221
                                   -0.0039  0.0020 -0.0253 -0.5813 -0.0090
                                    0.1521  0.2254 -0.0100  0.2558  0.2862
                                    0.3660  0.2866  0.0918 -0.2221  0.3369
189. (0.00015) RY*( 7) C  2          s( 27.95%)p 0.24(  6.79%)d 2.33( 65.26%)
                                    0.0000  0.0008  0.1982  0.4901 -0.0056
                                   -0.0061 -0.0232 -0.1893 -0.1393 -0.0072
                                   -0.0508 -0.0646 -0.0120 -0.0184  0.0694
                                   -0.6208 -0.3807  0.1099 -0.1821  0.2774
190. (0.00012) RY*( 8) C  2          s( 37.52%)p 1.14( 42.71%)d 0.53( 19.77%)
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                                    0.0000 -0.0006  0.0539  0.6086  0.0209
                                   -0.0379  0.0026 -0.0286  0.4622  0.0080
                                    0.1051  0.2624  0.0090  0.0763  0.3560
                                    0.1403  0.0907 -0.2752  0.2230 -0.2106
191. (0.00009) RY*( 9) C  2          s(  3.46%)p 5.83( 20.19%)d22.04( 76.35%)
192. (0.00009) RY*(10) C  2          s(  6.54%)p 4.11( 26.87%)d10.18( 66.58%)
193. (0.00005) RY*(11) C  2          s( 12.06%)p 5.85( 70.55%)d 1.44( 17.39%)
194. (0.00002) RY*(12) C  2          s(  7.10%)p10.88( 77.25%)d 2.20( 15.65%)
195. (0.00002) RY*(13) C  2          s(  2.60%)p 1.46(  3.80%)d36.06( 93.60%)
196. (0.00000) RY*(14) C  2          s( 99.01%)p 0.00(  0.11%)d 0.01(  0.88%)
197. (0.00000) RY*(15) C  2          s( 99.74%)p 0.00(  0.15%)d 0.00(  0.10%)
198. (0.00252) RY*( 1) C  3          s( 13.86%)p 5.49( 76.06%)d 0.73( 10.09%)
                                    0.0000  0.0023  0.3676 -0.0583 -0.0002
                                   -0.0026 -0.0200  0.7490 -0.0529  0.0060
                                   -0.2850  0.0131  0.0067 -0.3385  0.0189
                                   -0.1742 -0.1952 -0.0492  0.1513 -0.0844
199. (0.00153) RY*( 2) C  3          s(  0.36%)p99.99( 99.18%)d 1.26(  0.45%)
                                    0.0000 -0.0012  0.0599  0.0042 -0.0015
                                    0.0006 -0.0118 -0.5131  0.0677 -0.0188
                                   -0.6060  0.0821 -0.0215 -0.5824  0.0994
                                    0.0214  0.0465 -0.0174  0.0395  0.0086
200. (0.00098) RY*( 3) C  3          s(  0.01%)p 1.00( 92.43%)d 0.08(  7.56%)
                                    0.0000  0.0003  0.0097 -0.0007 -0.0007
                                   -0.0012  0.0006  0.0411 -0.0036  0.0074
                                   -0.6703 -0.1364 -0.0063  0.6649  0.1119
                                   -0.1896  0.1773  0.0154 -0.0355 -0.0820
201. (0.00079) RY*( 4) C  3          s( 85.03%)p 0.14( 11.99%)d 0.04(  2.98%)
                                    0.0000 -0.0047  0.9180 -0.0866 -0.0013
                                    0.0054  0.0203 -0.2544  0.0380 -0.0038
                                    0.1610  0.0135 -0.0055  0.1650  0.0015
                                    0.1049  0.1084  0.0784 -0.0298  0.0020
202. (0.00052) RY*( 5) C  3          s(  0.01%)p50.06(  0.72%)d99.99( 99.26%)
                                    0.0000 -0.0003  0.0108 -0.0053 -0.0010
                                   -0.0002  0.0001  0.0072 -0.0441  0.0081
                                    0.0481 -0.0437 -0.0068 -0.0120 -0.0279
                                   -0.3043  0.3280 -0.0384  0.4725  0.7535
203. (0.00010) RY*( 6) C  3          s(  2.81%)p 2.21(  6.23%)d32.32( 90.96%)
204. (0.00005) RY*( 7) C  3          s( 19.59%)p 1.74( 34.06%)d 2.37( 46.35%)
205. (0.00003) RY*( 8) C  3          s(  1.55%)p54.73( 84.61%)d 8.96( 13.85%)
206. (0.00002) RY*( 9) C  3          s(  1.64%)p10.33( 16.93%)d49.67( 81.43%)
207. (0.00001) RY*(10) C  3          s( 65.68%)p 0.07(  4.43%)d 0.46( 29.89%)
208. (0.00001) RY*(11) C  3          s(  9.16%)p 7.70( 70.57%)d 2.21( 20.27%)
209. (0.00002) RY*(12) C  3          s(  2.99%)p 1.58(  4.72%)d30.92( 92.30%)
210. (0.00000) RY*(13) C  3          s(  0.01%)p 1.00( 97.98%)d 0.02(  2.02%)
211. (0.00000) RY*(14) C  3          s( 99.56%)p 0.00(  0.07%)d 0.00(  0.37%)
212. (0.00000) RY*(15) C  3          s( 97.80%)p 0.00(  0.26%)d 0.02(  1.95%)
213. (0.01427) RY*( 1) C  4          s( 56.28%)p 0.78( 43.62%)d 0.00(  0.10%)
                                    0.0000 -0.0800  0.7457  0.0153  0.0055
                                    0.0045  0.0130  0.0993 -0.0124 -0.0730
                                   -0.4715  0.0535  0.0726  0.4325 -0.0572
                                   -0.0058  0.0023 -0.0263 -0.0089  0.0130
214. (0.00422) RY*( 2) C  4          s( 14.11%)p 5.37( 75.76%)d 0.72( 10.13%)
                                    0.0000 -0.0022  0.3746 -0.0281 -0.0045
                                    0.0024  0.0089 -0.6921 -0.1060 -0.0356
                                    0.5030  0.0042  0.0237  0.0604  0.0940
                                   -0.1494  0.1060 -0.0363 -0.1130 -0.2316
215. (0.00410) RY*( 3) C  4          s( 25.38%)p 2.89( 73.43%)d 0.05(  1.19%)
                                    0.0000  0.0033  0.5011 -0.0520 -0.0007
                                    0.0035  0.0129  0.3796  0.0868 -0.0460
                                    0.2070 -0.0947  0.0360 -0.7261  0.0096
                                   -0.0013 -0.0122 -0.0673 -0.0744 -0.0413
216. (0.00317) RY*( 4) C  4          s(  0.46%)p99.99( 51.31%)d99.99( 48.23%)
                                    0.0000  0.0007  0.0266  0.0617 -0.0088
                                   -0.0046  0.0135 -0.4249 -0.0560  0.0173
                                   -0.4075 -0.0979  0.0116 -0.3913 -0.0077
                                   -0.2118  0.3294  0.0542  0.3657  0.4385
217. (0.00198) RY*( 5) C  4          s(  0.50%)p59.78( 30.08%)d99.99( 69.42%)
                                    0.0000 -0.0030  0.0044  0.0700 -0.0088
                                   -0.0044 -0.0448 -0.3776 -0.0682 -0.0075
                                   -0.2925 -0.1017 -0.0071 -0.2303  0.0497
                                    0.4914 -0.6091 -0.1763 -0.2238  0.0210
218. (0.00160) RY*( 6) C  4          s(  2.44%)p11.13( 27.11%)d28.91( 70.45%)
                                    0.0000  0.0029  0.1557  0.0075 -0.0065
                                   -0.0043 -0.0112  0.0728  0.0070  0.0149
                                    0.4564  0.0062  0.0447  0.2105  0.1038
                                    0.3027 -0.1725 -0.0137  0.2991  0.7025
219. (0.00022) RY*( 7) C  4          s( 86.62%)p 0.13( 11.03%)d 0.03(  2.35%)
                                    0.0000 -0.0007  0.0199  0.9305 -0.0041
                                    0.0066  0.0041  0.0285  0.0016 -0.0059
                                    0.0856  0.2638  0.0075 -0.0429 -0.1750
                                   -0.0769 -0.0511 -0.0980  0.0591 -0.0433
220. (0.00013) RY*( 8) C  4          s(  6.24%)p11.16( 69.58%)d 3.88( 24.19%)
                                    0.0000  0.0116  0.0275  0.2440  0.0439
                                    0.0015  0.0003  0.0597  0.1315  0.0143
                                   -0.0456 -0.4120 -0.0167  0.0613  0.7063
                                   -0.2006 -0.2204  0.3299  0.1616 -0.1346
221. (0.00010) RY*( 9) C  4          s(  3.39%)p 3.55( 12.03%)d24.98( 84.58%)
222. (0.00008) RY*(10) C  4          s(  0.56%)p12.53(  7.07%)d99.99( 92.37%)
223. (0.00005) RY*(11) C  4          s(  2.25%)p19.12( 43.02%)d24.32( 54.73%)
224. (0.00003) RY*(12) C  4          s(  2.93%)p23.99( 70.39%)d 9.09( 26.67%)
225. (0.00002) RY*(13) C  4          s(  0.91%)p95.91( 87.16%)d13.13( 11.93%)
226. (0.00000) RY*(14) C  4          s( 99.70%)p 0.00(  0.08%)d 0.00(  0.21%)
227. (0.00000) RY*(15) C  4          s( 96.96%)p 0.00(  0.11%)d 0.03(  2.93%)
228. (0.00308) RY*( 1) C  5          s( 14.74%)p 5.21( 76.75%)d 0.58(  8.51%)
                                    0.0000  0.0040  0.3830 -0.0256 -0.0009
                                   -0.0024 -0.0085  0.8553 -0.0476 -0.0087
                                    0.1274  0.0129 -0.0105  0.1268  0.0311
                                    0.1808  0.1956 -0.0219  0.0954 -0.0675
229. (0.00178) RY*( 2) C  5          s(  0.00%)p 1.00( 96.46%)d 0.04(  3.53%)
                                    0.0000  0.0001  0.0047  0.0006  0.0004
                                   -0.0007 -0.0001  0.0102  0.0110  0.0069
                                   -0.7157 -0.1127 -0.0053  0.6552  0.1001
                                   -0.1269  0.1043  0.0025  0.0461  0.0789
230. (0.00090) RY*( 3) C  5          s( 27.48%)p 2.58( 70.98%)d 0.06(  1.54%)
                                    0.0000 -0.0066  0.5219 -0.0479 -0.0042
                                    0.0042 -0.0128 -0.3986  0.1425  0.0151
                                    0.4717 -0.1272  0.0150  0.5209 -0.1418
                                    0.0361  0.0376  0.0020  0.0751 -0.0838
231. (0.00052) RY*( 4) C  5          s( 54.09%)p 0.78( 42.31%)d 0.07(  3.60%)
                                    0.0000 -0.0031  0.7336  0.0511  0.0078
                                    0.0031  0.0114 -0.1595  0.0813  0.0072
                                   -0.3832  0.1757  0.0063 -0.4251  0.1801
                                   -0.1346 -0.1067  0.0718  0.0004 -0.0364
232. (0.00037) RY*( 5) C  5          s(  0.31%)p 3.02(  0.92%)d99.99( 98.77%)
                                    0.0000 -0.0011  0.0551  0.0045  0.0018
                                    0.0009  0.0003 -0.0171  0.0252 -0.0065
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                                    0.0052 -0.0807  0.0063 -0.0387  0.0137
                                    0.3073 -0.2460 -0.0647  0.4599  0.7855
233. (0.00015) RY*( 6) C  5          s( 24.52%)p 1.38( 33.87%)d 1.70( 41.61%)
                                    0.0000  0.0064  0.1249  0.4744 -0.0339
                                    0.0573  0.0030  0.0378 -0.5459  0.0139
                                    0.1328  0.0174  0.0148  0.1375  0.0449
                                   -0.1543 -0.1501  0.1114 -0.4993  0.3287
234. (0.00011) RY*( 7) C  5          s(  5.32%)p 6.41( 34.08%)d11.40( 60.60%)
                                    0.0000  0.0010  0.0431  0.2227 -0.0400
                                   -0.0102  0.0150  0.0549 -0.3492 -0.0161
                                   -0.0533 -0.3278 -0.0172 -0.0690 -0.3163
                                   -0.3110 -0.3037 -0.3578  0.4523 -0.2907
235. (0.00008) RY*( 8) C  5          s(  7.58%)p 8.97( 68.01%)d 3.22( 24.41%)
236. (0.00006) RY*( 9) C  5          s(  0.21%)p27.23(  5.84%)d99.99( 93.95%)
237. (0.00002) RY*(10) C  5          s(  2.32%)p 2.88(  6.66%)d39.30( 91.02%)
238. (0.00002) RY*(11) C  5          s(  8.44%)p 2.85( 24.01%)d 8.00( 67.55%)
239. (0.00002) RY*(12) C  5          s( 56.65%)p 0.74( 42.15%)d 0.02(  1.20%)
240. (0.00000) RY*(13) C  5          s(  0.15%)p99.99( 97.79%)d13.31(  2.05%)
241. (0.00000) RY*(14) C  5          s( 99.49%)p 0.00(  0.25%)d 0.00(  0.26%)
242. (0.00000) RY*(15) C  5          s( 98.75%)p 0.00(  0.14%)d 0.01(  1.11%)
243. (0.01383) RY*( 1) C  6          s( 38.95%)p 1.56( 60.84%)d 0.01(  0.21%)
                                    0.0000 -0.0744  0.6183  0.0400  0.0062
                                    0.0039 -0.0704 -0.5711  0.0845  0.0444
                                    0.3971 -0.0598  0.0360  0.3233 -0.0316
                                    0.0052 -0.0307  0.0042  0.0325  0.0055
244. (0.00533) RY*( 2) C  6          s(  0.68%)p99.99( 96.04%)d 4.81(  3.28%)
                                    0.0000  0.0039  0.0824  0.0036  0.0007
                                    0.0010 -0.0023  0.6944  0.0741  0.0150
                                    0.5106  0.1005  0.0102  0.4450  0.0590
                                   -0.0218  0.0818 -0.0863  0.0936 -0.0971
245. (0.00381) RY*( 3) C  6          s( 44.26%)p 0.74( 32.93%)d 0.52( 22.81%)
                                    0.0000 -0.0117  0.6617 -0.0662  0.0067
                                    0.0113 -0.0623  0.3244  0.0293  0.0626
                                   -0.4474 -0.0143  0.0238 -0.1201 -0.0054
                                   -0.2938  0.1783  0.0616 -0.2978 -0.1321
246. (0.00295) RY*( 4) C  6          s(  6.72%)p 9.43( 63.37%)d 4.45( 29.90%)
                                    0.0000 -0.0021  0.2574  0.0311 -0.0002
                                    0.0024 -0.0173  0.2091 -0.0201  0.0068
                                    0.3969  0.0666  0.0324 -0.6519 -0.0359
                                    0.1582 -0.3646  0.1773 -0.0214  0.3305
247. (0.00172) RY*( 5) C  6          s(  3.10%)p12.93( 40.08%)d18.33( 56.82%)
                                    0.0000  0.0007  0.1760 -0.0020 -0.0039
                                   -0.0003 -0.0177  0.1416 -0.0733 -0.0133
                                   -0.4406 -0.0235  0.0405  0.3933  0.1545
                                    0.3488 -0.5016  0.0519  0.2513  0.3591
248. (0.00149) RY*( 6) C  6          s(  4.90%)p 2.36( 11.58%)d17.06( 83.52%)
                                    0.0000 -0.0020  0.2180  0.0375 -0.0040
                                   -0.0018 -0.0462  0.0205 -0.1132 -0.0171
                                   -0.0826  0.0464 -0.0160 -0.2952  0.0613
                                    0.1969  0.1628 -0.3616  0.7170 -0.3536
249. (0.00025) RY*( 7) C  6          s( 83.48%)p 0.11(  8.87%)d 0.09(  7.65%)
                                    0.0000  0.0011  0.0098  0.9134 -0.0194
                                   -0.0059  0.0076  0.0147 -0.2635 -0.0014
                                   -0.0331  0.1110 -0.0025  0.0373  0.0647
                                   -0.0482  0.0577  0.2566  0.0008 -0.0711
250. (0.00010) RY*( 8) C  6          s( 13.83%)p 2.88( 39.79%)d 3.35( 46.38%)
                                    0.0000  0.0100  0.0144  0.3622  0.0746
                                    0.0351 -0.0067  0.0458  0.5964  0.0046
                                   -0.0741 -0.1577  0.0027 -0.0619 -0.0762
                                    0.3243  0.1382 -0.4999 -0.2201  0.2028
251. (0.00008) RY*( 9) C  6          s(  2.10%)p26.16( 54.90%)d20.49( 43.00%)
252. (0.00009) RY*(10) C  6          s(  1.97%)p 8.44( 16.58%)d41.45( 81.45%)
253. (0.00006) RY*(11) C  6          s(  0.35%)p12.51(  4.37%)d99.99( 95.28%)
254. (0.00003) RY*(12) C  6          s(  0.22%)p99.99( 95.45%)d19.59(  4.33%)
255. (0.00004) RY*(13) C  6          s(  0.89%)p86.43( 76.89%)d24.98( 22.22%)
256. (0.00000) RY*(14) C  6          s( 99.64%)p 0.00(  0.10%)d 0.00(  0.26%)
257. (0.00000) RY*(15) C  6          s( 97.48%)p 0.00(  0.17%)d 0.02(  2.36%)
258. (0.00833) RY*( 1) C  7          s(  6.28%)p14.08( 88.44%)d 0.84(  5.27%)
                                    0.0000 -0.0019  0.2506 -0.0004 -0.0035
                                    0.0006  0.0169 -0.2179 -0.0876 -0.0140
                                   -0.5877  0.0293 -0.0105 -0.6935  0.0394
                                   -0.0415 -0.0086  0.1208 -0.1594  0.1046
259. (0.00512) RY*( 2) C  7          s(  0.03%)p99.99( 90.74%)d99.99(  9.24%)
                                    0.0000 -0.0012  0.0138 -0.0083  0.0003
                                   -0.0001 -0.0007  0.0527  0.0106  0.0322
                                   -0.7261  0.0950 -0.0332  0.5996 -0.0812
                                    0.2016 -0.1890  0.0073 -0.0877 -0.0910
260. (0.00343) RY*( 3) C  7          s(  1.95%)p48.68( 94.94%)d 1.59(  3.11%)
                                    0.0000 -0.0056  0.1141  0.0803 -0.0009
                                   -0.0019 -0.0034 -0.9081 -0.2265  0.0152
                                    0.1309 -0.0197  0.0143  0.2339 -0.0297
                                   -0.1029 -0.1345 -0.0379  0.0260 -0.0161
261. (0.00110) RY*( 4) C  7          s( 74.53%)p 0.18( 13.38%)d 0.16( 12.09%)
                                    0.0000 -0.0012  0.8627  0.0323 -0.0027
                                   -0.0034  0.0152  0.1684 -0.1924  0.0182
                                    0.1957  0.0516  0.0106  0.1365  0.0903
                                    0.2133  0.1410  0.1022 -0.1417 -0.1582
262. (0.00101) RY*( 5) C  7          s(  4.97%)p 0.91(  4.50%)d18.23( 90.54%)
                                    0.0000 -0.0012  0.2218 -0.0211 -0.0007
                                   -0.0028  0.0029  0.0363  0.0164 -0.0074
                                   -0.1133  0.0172  0.0156  0.1724 -0.0146
                                   -0.1807  0.2354  0.0035  0.4920  0.7584
263. (0.00055) RY*( 6) C  7          s(  0.05%)p99.99(  5.10%)d99.99( 94.85%)
                                    0.0000  0.0006  0.0069  0.0210 -0.0014
                                    0.0010  0.0000 -0.0079  0.0326  0.0009
                                    0.1658  0.0045 -0.0013 -0.1460  0.0323
                                    0.6700 -0.6082 -0.0401  0.0912  0.3462
264. (0.00053) RY*( 7) C  7          s( 17.50%)p 2.55( 44.61%)d 2.16( 37.88%)
                                    0.0000 -0.0081  0.3312 -0.2549 -0.0157
                                    0.0069 -0.0090 -0.0506  0.6266  0.0091
                                   -0.0195 -0.1251  0.0083 -0.0619 -0.1757
                                   -0.2421 -0.3391 -0.0979  0.3432 -0.2792
265. (0.00019) RY*( 8) C  7          s( 69.36%)p 0.13(  9.04%)d 0.31( 21.60%)
                                    0.0000  0.0038  0.0952  0.8273 -0.0070
                                   -0.0006 -0.0097  0.0905  0.2621 -0.0056
                                    0.0264  0.0953 -0.0059  0.0334  0.0496
                                   -0.2920 -0.2304 -0.0915 -0.2283  0.1309
266. (0.00019) RY*( 9) C  7          s(  7.89%)p11.19( 88.29%)d 0.48(  3.82%)
                                    0.0000 -0.0007  0.0217  0.2788  0.0087
                                    0.0244  0.0058  0.0762 -0.2187  0.0006
                                   -0.0558 -0.6667  0.0000 -0.0537 -0.6154
                                    0.1180  0.0711 -0.0224  0.1217 -0.0631
267. (0.00012) RY*(10) C  7          s(  2.02%)p20.95( 42.37%)d27.50( 55.61%)
                                    0.0000 -0.0003  0.0017  0.1396  0.0227
                                    0.0150 -0.0088  0.1964 -0.5388  0.0062
                                   -0.0944  0.1006  0.0064 -0.0904  0.2597
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                                    -0.1940 -0.2936 -0.2683  0.5295 -0.2825
268. (0.00010) RY*(11) C  7          s(  8.86%)p 1.95( 17.30%)d 8.34( 73.84%)
269. (0.00003) RY*(12) C  7          s(  0.75%)p99.99( 98.77%)d 0.64(  0.48%)
270. (0.00002) RY*(13) C  7          s(  8.27%)p 0.23(  1.92%)d10.86( 89.81%)
271. (0.00000) RY*(14) C  7          s( 97.77%)p 0.01(  0.65%)d 0.02(  1.58%)
272. (0.00000) RY*(15) C  7          s( 99.77%)p 0.00(  0.21%)d 0.00(  0.02%)
273. (0.01434) RY*( 1) C  8          s( 57.19%)p 0.75( 42.71%)d 0.00(  0.10%)
                                     0.0000 -0.0805  0.7517  0.0154  0.0051
                                     0.0045  0.0583  0.3377 -0.0462  0.0740
                                     0.4645 -0.0531  0.0464  0.2826 -0.0374
                                     0.0231  0.0127  0.0173  0.0005 -0.0069
274. (0.00419) RY*( 2) C  8          s( 38.50%)p 1.43( 55.17%)d 0.16(  6.32%)
                                     0.0000  0.0016  0.6179 -0.0570 -0.0042
                                     0.0042  0.0314 -0.3834  0.0611  0.0572
                                    -0.4829  0.0708  0.0328 -0.3959  0.0273
                                     0.0331 -0.0412  0.1153 -0.2168 -0.0126
275. (0.00407) RY*( 3) C  8          s(  0.19%)p99.99( 94.82%)d26.79(  4.99%)
                                     0.0000  0.0029  0.0403 -0.0147  0.0034
                                     0.0007  0.0041 -0.8131 -0.1232  0.0036
                                     0.2606  0.0632  0.0017  0.4367  0.0960
                                     0.0841  0.0096 -0.1120  0.1363 -0.1079
276. (0.00310) RY*( 4) C  8          s(  0.40%)p99.99( 46.61%)d99.99( 52.99%)
                                     0.0000  0.0010  0.0241  0.0575 -0.0083
                                    -0.0046  0.0040 -0.1721  0.0086 -0.0184
                                     0.4029  0.0993  0.0190 -0.5115 -0.0442
                                    -0.1704  0.3698  0.1688  0.3908  0.4277
277. (0.00188) RY*( 5) C  8          s(  0.50%)p68.67( 34.62%)d99.99( 64.87%)
                                     0.0000 -0.0027 -0.0044  0.0700 -0.0092
                                    -0.0049  0.0150  0.0072  0.0978  0.0052
                                     0.3015  0.0950 -0.0431 -0.4810 -0.0570
                                     0.3737 -0.2289 -0.3441  0.1616 -0.5587
278. (0.00166) RY*( 6) C  8          s(  2.34%)p11.68( 27.28%)d30.13( 70.39%)
                                     0.0000  0.0029  0.1525  0.0058 -0.0056
                                    -0.0041  0.0439  0.1373  0.0683 -0.0150
                                    -0.4582 -0.0143  0.0114  0.1833  0.0568
                                     0.1327  0.2773 -0.2625  0.7334 -0.0507
279. (0.00022) RY*( 7) C  8          s( 87.14%)p 0.12( 10.46%)d 0.03(  2.40%)
                                     0.0000 -0.0004  0.0195  0.9333 -0.0041
                                     0.0061  0.0045 -0.0501 -0.1778  0.0057
                                    -0.0818 -0.2446  0.0066 -0.0012 -0.0618
                                    -0.0236 -0.0430  0.1296  0.0259 -0.0641
280. (0.00013) RY*( 8) C  8          s(  5.55%)p13.06( 72.48%)d 3.96( 21.97%)
                                     0.0000  0.0112  0.0312  0.2303  0.0369
                                    -0.0001 -0.0141  0.0193  0.6203 -0.0145
                                     0.0408  0.4101 -0.0074  0.0967  0.4000
                                    -0.3221 -0.3227  0.0223  0.1003  0.0366
281. (0.00009) RY*( 9) C  8          s(  3.01%)p 5.03( 15.15%)d27.20( 81.85%)
282. (0.00009) RY*(10) C  8          s(  0.92%)p 0.63(  0.58%)d99.99( 98.50%)
283. (0.00005) RY*(11) C  8          s(  3.17%)p12.01( 38.11%)d18.51( 58.72%)
284. (0.00003) RY*(12) C  8          s(  2.24%)p35.56( 79.82%)d 7.99( 17.94%)
285. (0.00003) RY*(13) C  8          s(  0.83%)p99.99( 83.80%)d18.42( 15.37%)
286. (0.00000) RY*(14) C  8          s( 99.72%)p 0.00(  0.08%)d 0.00(  0.20%)
287. (0.00000) RY*(15) C  8          s( 97.01%)p 0.00(  0.13%)d 0.03(  2.86%)
288. (0.00790) RY*( 1) C  9          s(  6.45%)p13.92( 89.80%)d 0.58(  3.75%)
                                     0.0000  0.0020  0.2537 -0.0119 -0.0008
                                     0.0009 -0.0006 -0.2855 -0.0425  0.0136
                                     0.6676 -0.0270  0.0143  0.6062 -0.0220
                                    -0.0435 -0.0427  0.1050 -0.1285  0.0792
289. (0.00432) RY*( 2) C  9          s(  0.01%)p 1.00( 98.33%)d 0.02(  1.66%)
                                     0.0000 -0.0007  0.0062 -0.0044 -0.0001
                                    -0.0003 -0.0013 -0.0616  0.0122  0.0063
                                    -0.6753  0.0812 -0.0064  0.7153 -0.0709
                                     0.0947 -0.0811  0.0036 -0.0138 -0.0297
290. (0.00276) RY*( 3) C  9          s(  2.08%)p45.58( 94.65%)d 1.58(  3.28%)
                                     0.0000  0.0019  0.1328  0.0558 -0.0024
                                    -0.0016 -0.0054 -0.8861 -0.2328 -0.0095
                                    -0.1971 -0.0150 -0.0056 -0.2604 -0.0042
                                     0.1262  0.1275  0.0088 -0.0215  0.0058
291. (0.00105) RY*( 4) C  9          s( 90.07%)p 0.10(  8.63%)d 0.01(  1.31%)
                                     0.0000 -0.0040  0.9488  0.0222 -0.0012
                                     0.0017  0.0003  0.1851  0.1040 -0.0103
                                    -0.1398 -0.0506 -0.0119 -0.1309 -0.0414
                                     0.0279 -0.0250  0.0301  0.0950 -0.0417
292. (0.00052) RY*( 5) C  9          s(  0.27%)p27.62(  7.35%)d99.99( 92.38%)
                                     0.0000  0.0014  0.0262  0.0443  0.0022
                                    -0.0025  0.0003  0.0311 -0.1329  0.0091
                                    -0.1104 -0.1487 -0.0060  0.0763 -0.1211
                                    -0.6736  0.5629  0.0024  0.1310  0.3690
293. (0.00050) RY*( 6) C  9          s(  2.47%)p25.55( 63.01%)d14.00( 34.52%)
                                     0.0000  0.0074 -0.0009  0.1562 -0.0012
                                    -0.0139  0.0050  0.1140 -0.5765  0.0073
                                    -0.0559 -0.3773  0.0097 -0.0664 -0.3671
                                    -0.1351 -0.5165  0.0501 -0.2156  0.1059
294. (0.00043) RY*( 7) C  9          s(  0.09%)p15.16(  1.37%)d99.99( 98.54%)
                                     0.0000  0.0005  0.0213  0.0209 -0.0030
                                    -0.0018  0.0011  0.0108 -0.0309 -0.0010
                                    -0.0267 -0.1054  0.0020  0.0142  0.0242
                                    -0.3049  0.2210  0.0118 -0.4727 -0.7874
295. (0.00021) RY*( 8) C  9          s(  5.71%)p14.97( 85.41%)d 1.56(  8.88%)
                                     0.0000 -0.0010 -0.0801  0.2249 -0.0061
                                    -0.0037 -0.0028 -0.1171  0.6661  0.0029
                                    -0.0177 -0.3963  0.0046 -0.0481 -0.4868
                                     0.1080  0.0439  0.0264 -0.2405  0.1292
296. (0.00014) RY*( 9) C  9          s( 77.77%)p 0.19( 15.12%)d 0.09(  7.11%)
                                     0.0000  0.0063  0.0274  0.8814  0.0048
                                    -0.0002 -0.0012  0.0299  0.0145  0.0028
                                     0.0081  0.3061  0.0027  0.0098  0.2371
                                    -0.0732 -0.0500 -0.1727 -0.1559  0.0955
297. (0.00012) RY*(10) C  9          s(  5.85%)p 4.88( 28.52%)d11.22( 65.63%)
                                     0.0000 -0.0001 -0.0239  0.2397  0.0145
                                     0.0157 -0.0155  0.2063 -0.3413 -0.0067
                                     0.0887 -0.3049 -0.0077  0.1138 -0.1098
                                     0.5802  0.5229 -0.0671  0.1654 -0.1199
298. (0.00008) RY*(11) C  9          s(  1.92%)p 5.97( 11.44%)d45.23( 86.65%)
299. (0.00004) RY*(12) C  9          s(  2.04%)p35.23( 71.70%)d12.90( 26.26%)
300. (0.00002) RY*(13) C  9          s(  6.49%)p 3.79( 24.58%)d10.62( 68.93%)
301. (0.00000) RY*(14) C  9          s( 99.06%)p 0.00(  0.19%)d 0.01(  0.75%)
302. (0.00000) RY*(15) C  9          s( 99.81%)p 0.00(  0.05%)d 0.00(  0.14%)
303. (0.01427) RY*( 1) C 10          s( 40.92%)p 1.44( 58.88%)d 0.00(  0.20%)
                                     0.0000 -0.0758  0.6340  0.0384  0.0066
                                     0.0041  0.0660 -0.5569 -0.0663 -0.0471
                                     0.3682  0.0549 -0.0499  0.3505  0.0610
                                    -0.0024 -0.0262 -0.0080  0.0352 -0.0035
304. (0.00540) RY*( 2) C 10          s(  2.79%)p34.00( 95.01%)d 0.79(  2.20%)
                                     0.0000  0.0031  0.1671 -0.0036  0.0011
                                     0.0021  0.0208 -0.0165  0.0189 -0.0212
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                                    0.4810 -0.0974 -0.0005 -0.8361  0.0927
                                    0.0521 -0.0585  0.0461 -0.0276  0.1139
305. (0.00407) RY*( 3) C 10          s( 46.40%)p 0.86( 39.97%)d 0.29( 13.63%)
                                    0.0000 -0.0115  0.6775 -0.0691  0.0063
                                    0.0108  0.0567  0.3240 -0.0133 -0.0561
                                   -0.5049  0.0164 -0.0458 -0.1754  0.0120
                                   -0.1928  0.1036  0.1660 -0.2259 -0.0990
306. (0.00283) RY*( 4) C 10          s(  3.77%)p13.77( 51.97%)d11.73( 44.25%)
                                    0.0000 -0.0019  0.1912  0.0344 -0.0008
                                    0.0017  0.0353  0.5928 -0.0011  0.0032
                                    0.3718 -0.0555  0.0056  0.1560 -0.0375
                                   -0.0398  0.0294 -0.2915  0.4609 -0.3778
307. (0.00203) RY*( 5) C 10          s(  0.60%)p77.00( 46.36%)d88.10( 53.04%)
                                    0.0000  0.0036  0.0710 -0.0310 -0.0017
                                   -0.0005  0.0333 -0.3741  0.1503  0.0209
                                   -0.4642  0.0277  0.0078 -0.2882  0.0124
                                    0.1597 -0.1383 -0.3442  0.5743 -0.1935
308. (0.00151) RY*( 6) C 10          s(  4.21%)p 2.87( 12.09%)d19.90( 83.71%)
                                    0.0000 -0.0024  0.2009  0.0408 -0.0036
                                   -0.0017  0.0057  0.2800  0.0963  0.0197
                                   -0.0635 -0.0473 -0.0477  0.1386 -0.0709
                                    0.4301 -0.4461 -0.0485  0.1225  0.6601
309. (0.00026) RY*( 7) C 10          s( 82.15%)p 0.14( 11.13%)d 0.08(  6.71%)
                                    0.0000  0.0002  0.0142  0.9060 -0.0206
                                   -0.0059 -0.0043 -0.0304  0.2528  0.0017
                                   -0.0427 -0.1161  0.0057 -0.0335 -0.1733
                                   -0.2541 -0.0366  0.0024 -0.0059  0.0341
310. (0.00011) RY*( 8) C 10          s( 15.32%)p 4.07( 62.35%)d 1.46( 22.33%)
                                    0.0000  0.0065 -0.0045  0.3868  0.0500
                                    0.0327  0.0102  0.0724 -0.5134 -0.0048
                                   -0.0926  0.1959 -0.0062 -0.0284  0.5538
                                    0.3703  0.2656 -0.1221 -0.0119  0.0237
311. (0.00009) RY*( 9) C 10          s(  2.83%)p 8.63( 24.47%)d25.64( 72.69%)
312. (0.00009) RY*(10) C 10          s(  0.24%)p72.28( 17.07%)d99.99( 82.69%)
313. (0.00007) RY*(11) C 10          s(  0.79%)p 2.22(  1.76%)d99.99( 97.45%)
314. (0.00004) RY*(12) C 10          s(  0.91%)p91.52( 83.42%)d17.19( 15.67%)
315. (0.00003) RY*(13) C 10          s(  0.42%)p99.99( 97.32%)d 5.39(  2.26%)
316. (0.00000) RY*(14) C 10          s( 99.63%)p 0.00(  0.11%)d 0.00(  0.26%)
317. (0.00000) RY*(15) C 10          s( 97.50%)p 0.00(  0.12%)d 0.02(  2.37%)
318. (0.00834) RY*( 1) C 11          s(  0.92%)p99.99( 97.38%)d 1.85(  1.70%)
                                    0.0000 -0.0278  0.0813 -0.0420 -0.0078
                                   -0.0016  0.0234  0.8224 -0.0040  0.0365
                                    0.0547  0.0099  0.0070  0.5406 -0.0068
                                    0.0903  0.0928  0.0068  0.0095 -0.0109
319. (0.00744) RY*( 2) C 11          s(  0.70%)p99.99( 98.77%)d 0.77(  0.54%)
                                    0.0000  0.0164  0.0817  0.0041 -0.0031
                                   -0.0015 -0.0203 -0.2454  0.0100  0.0109
                                   -0.8446  0.0149 -0.0369  0.4595 -0.0273
                                   -0.0246 -0.0459  0.0020 -0.0342 -0.0386
320. (0.00588) RY*( 3) C 11          s(  4.70%)p20.01( 94.11%)d 0.25(  1.19%)
                                    0.0000  0.0138  0.2149  0.0250 -0.0031
                                    0.0000 -0.0340  0.4712 -0.0079 -0.0055
                                   -0.4885 -0.0390  0.0073 -0.6905 -0.0267
                                   -0.0131 -0.0042  0.0559 -0.0847  0.0379
321. (0.00249) RY*( 4) C 11          s( 87.87%)p 0.10(  8.84%)d 0.04(  3.29%)
                                    0.0000 -0.0150  0.9370  0.0178 -0.0128
                                   -0.0056 -0.0131 -0.1617 -0.1486 -0.0392
                                    0.1771  0.0229 -0.0264  0.0700  0.0318
                                    0.1213 -0.0013  0.0737 -0.1027 -0.0466
322. (0.00050) RY*( 5) C 11          s(  2.27%)p 1.61(  3.66%)d41.44( 94.07%)
                                    0.0000 -0.0005  0.0715  0.1322  0.0106
                                    0.0040 -0.0001 -0.0190 -0.0619  0.0093
                                   -0.0292 -0.1355 -0.0185  0.0395  0.1058
                                   -0.0101  0.0294  0.0953  0.4399  0.8586
323. (0.00044) RY*( 6) C 11          s(  1.03%)p31.66( 32.71%)d64.13( 66.26%)
                                    0.0000  0.0006  0.0931  0.0406  0.0005
                                    0.0038 -0.0191  0.0216  0.2852  0.0073
                                    0.0047 -0.3269  0.0157 -0.0229 -0.3704
                                    0.3148 -0.4641 -0.2623  0.4894 -0.1995
324. (0.00037) RY*( 7) C 11          s(  7.91%)p 3.30( 26.13%)d 8.34( 65.97%)
                                    0.0000 -0.0001  0.0890  0.2666  0.0065
                                    0.0074 -0.0103 -0.0088 -0.0581  0.0093
                                    0.0040 -0.4941  0.0014  0.0163 -0.1149
                                   -0.5103  0.5197 -0.1355  0.2277 -0.2429
325. (0.00030) RY*( 8) C 11          s(  9.85%)p 7.85( 77.30%)d 1.30( 12.85%)
                                    0.0000  0.0032 -0.1701  0.2631 -0.0171
                                    0.0051  0.0147 -0.0053 -0.7785  0.0015
                                   -0.0086 -0.1928  0.0038  0.0107 -0.3596
                                    0.3052 -0.0642  0.0157 -0.1744  0.0241
326. (0.00024) RY*( 9) C 11          s( 78.41%)p 0.19( 14.82%)d 0.09(  6.77%)
                                    0.0000  0.0015 -0.0221  0.8850 -0.0143
                                   -0.0117  0.0047  0.0116  0.2808  0.0005
                                    0.0043  0.1918  0.0043  0.0127  0.1795
                                    0.2204  0.0392 -0.0501 -0.1162 -0.0395
327. (0.00013) RY*(10) C 11          s(  0.31%)p99.99( 67.45%)d99.99( 32.24%)
                                    0.0000 -0.0004  0.0317  0.0176  0.0395
                                    0.0143  0.0104 -0.0349  0.3991 -0.0042
                                    0.0681 -0.0478 -0.0124  0.0483 -0.7102
                                   -0.0989  0.1005  0.1956 -0.4229  0.2923
328. (0.00013) RY*(11) C 11          s(  1.29%)p53.39( 68.65%)d23.38( 30.07%)
                                    0.0000  0.0039  0.0725  0.0629  0.0584
                                    0.0148 -0.0110  0.0299 -0.1800  0.0121
                                   -0.0065  0.7141 -0.0028 -0.0352 -0.3764
                                   -0.2602  0.0543 -0.3750  0.2985  0.0152
329. (0.00007) RY*(12) C 11          s(  4.99%)p 0.72(  3.61%)d18.32( 91.40%)
330. (0.00002) RY*(13) C 11          s(  1.03%)p 6.17(  6.37%)d89.75( 92.60%)
331. (0.00000) RY*(14) C 11          s( 99.34%)p 0.00(  0.14%)d 0.01(  0.52%)
332. (0.00000) RY*(15) C 11          s( 99.35%)p 0.00(  0.35%)d 0.00(  0.30%)
333. (0.00634) RY*( 1) C 12          s(  7.69%)p11.03( 84.87%)d 0.97(  7.44%)
                                    0.0000  0.0037  0.2766 -0.0203  0.0017
                                   -0.0017 -0.0235 -0.0751  0.1174  0.0086
                                    0.5312 -0.0500  0.0140 -0.7331 -0.0795
                                    0.1208  0.0082 -0.1280 -0.0811  0.1917
334. (0.00511) RY*( 2) C 12          s(  1.40%)p65.72( 92.04%)d 4.69(  6.56%)
                                    0.0000 -0.0031  0.1155 -0.0255 -0.0014
                                   -0.0012  0.0082 -0.5300 -0.0679  0.0126
                                   -0.6855 -0.0892  0.0083 -0.3917 -0.0559
                                    0.0307  0.1126 -0.0088  0.2134  0.0799
335. (0.00238) RY*( 3) C 12          s( 24.28%)p 3.11( 75.53%)d 0.01(  0.20%)
                                    0.0000 -0.0105  0.4925 -0.0071  0.0084
                                   -0.0026 -0.0171 -0.6111  0.2237  0.0258
                                    0.2700 -0.1493 -0.0226  0.4847 -0.0155
                                   -0.0302 -0.0006 -0.0171 -0.0101 -0.0255
336. (0.00135) RY*( 4) C 12          s( 59.61%)p 0.54( 32.35%)d 0.13(  8.04%)
                                    0.0000 -0.0010  0.7493 -0.1863 -0.0022
                                   -0.0013  0.0040  0.4526 -0.0219 -0.0032
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                                    -0.3332  0.0796 -0.0134  0.0192  0.0145
                                    -0.0463 -0.0984 -0.0196 -0.2599  0.0252
337. (0.00063) RY*( 5) C 12          s(  4.70%)p 1.98(  9.31%)d18.29( 85.99%)
                                     0.0000 -0.0011  0.2161 -0.0167 -0.0036
                                     0.0013  0.0066  0.2205 -0.1407  0.0052
                                     0.1078  0.0232 -0.0014  0.0921  0.0632
                                     0.2571  0.1301 -0.2874  0.8308 -0.0624
338. (0.00031) RY*( 6) C 12          s(  5.00%)p 9.66( 48.30%)d 9.34( 46.70%)
                                     0.0000  0.0075 -0.0924  0.2020  0.0244
                                    -0.0004 -0.0105  0.1914  0.4937  0.0050
                                    -0.1654 -0.2608  0.0051  0.1108 -0.3078
                                     0.1417  0.4671 -0.4270 -0.1522  0.1526
339. (0.00013) RY*( 7) C 12          s( 40.35%)p 0.95( 38.32%)d 0.53( 21.33%)
                                     0.0000 -0.0003  0.0844  0.6284  0.0197
                                    -0.0331  0.0095  0.1105  0.2532 -0.0092
                                    -0.0914 -0.2747 -0.0018 -0.0414  0.4703
                                     0.1769 -0.2681  0.2712  0.0866  0.1706
340. (0.00011) RY*( 8) C 12          s( 24.40%)p 0.33(  8.00%)d 2.77( 67.60%)
                                     0.0000 -0.0008  0.1870  0.4570 -0.0013
                                     0.0141 -0.0123  0.0742 -0.1067  0.0099
                                     0.0876  0.0853 -0.0237 -0.1032 -0.1915
                                    -0.5353  0.4661  0.3136  0.1178 -0.2448
341. (0.00009) RY*( 9) C 12          s(  6.52%)p 8.07( 52.62%)d 6.27( 40.86%)
342. (0.00009) RY*(10) C 12          s(  2.10%)p 4.64(  9.73%)d42.03( 88.17%)
343. (0.00005) RY*(11) C 12          s( 15.88%)p 4.34( 68.99%)d 0.95( 15.13%)
344. (0.00002) RY*(12) C 12          s(  8.06%)p 9.19( 74.09%)d 2.21( 17.85%)
345. (0.00002) RY*(13) C 12          s(  1.46%)p 3.93(  5.73%)d63.75( 92.82%)
346. (0.00000) RY*(14) C 12          s( 98.74%)p 0.00(  0.24%)d 0.01(  1.01%)
347. (0.00000) RY*(15) C 12          s( 99.79%)p 0.00(  0.17%)d 0.00(  0.04%)
348. (0.00322) RY*( 1) C 13          s( 13.85%)p 5.69( 78.88%)d 0.52(  7.26%)
                                     0.0000  0.0040  0.3708 -0.0322  0.0001
                                    -0.0018 -0.0108  0.8752 -0.0449  0.0076
                                    -0.1205 -0.0188  0.0072 -0.0739 -0.0163
                                    -0.1439 -0.1259 -0.0648  0.1561 -0.0865
349. (0.00237) RY*( 2) C 13          s(  0.00%)p 1.00( 91.67%)d 0.09(  8.33%)
                                     0.0000  0.0006  0.0054  0.0005 -0.0001
                                    -0.0002  0.0007 -0.0376 -0.0007 -0.0001
                                    -0.6583 -0.1012 -0.0012  0.6805  0.0924
                                    -0.1812  0.1839 -0.0050  0.0535  0.1172
350. (0.00100) RY*( 3) C 13          s( 14.16%)p 5.97( 84.61%)d 0.09(  1.23%)
                                     0.0000 -0.0061  0.3713 -0.0606 -0.0028
                                     0.0029 -0.0104 -0.2938  0.1176 -0.0150
                                    -0.5895  0.1489 -0.0159 -0.5935  0.1531
                                     0.0163  0.0310 -0.0220  0.0965 -0.0362
351. (0.00069) RY*( 4) C 13          s( 69.54%)p 0.39( 27.24%)d 0.05(  3.22%)
                                     0.0000 -0.0034  0.8321  0.0545  0.0013
                                     0.0020  0.0112 -0.2454  0.0717 -0.0087
                                     0.2918 -0.1619 -0.0100  0.2608 -0.1653
                                     0.0534  0.0519  0.1328 -0.0844  0.0437
352. (0.00049) RY*( 5) C 13          s(  0.01%)p99.99(  3.47%)d99.99( 96.52%)
                                     0.0000 -0.0001  0.0107 -0.0057  0.0005
                                     0.0001 -0.0002 -0.0038 -0.0047  0.0053
                                    -0.1328 -0.0006 -0.0060  0.1221  0.0450
                                     0.1501 -0.1325  0.0007 -0.4777 -0.8348
353. (0.00012) RY*( 6) C 13          s(  2.61%)p 3.79(  9.88%)d33.56( 87.51%)
                                     0.0000  0.0001  0.0538  0.1513 -0.0100
                                    -0.0139  0.0125  0.0315 -0.1428  0.0202
                                     0.1044  0.1566  0.0205  0.0964  0.1781
                                     0.4923  0.5207 -0.2937  0.4609 -0.2509
354. (0.00012) RY*( 7) C 13          s( 27.84%)p 1.86( 51.66%)d 0.74( 20.50%)
                                     0.0000  0.0045  0.0725  0.5173 -0.0567
                                     0.0478  0.0072  0.0428 -0.6951 -0.0074
                                    -0.1019  0.0880 -0.0065 -0.1003  0.0578
                                     0.0568  0.0513  0.0248 -0.3833  0.2271
355. (0.00007) RY*( 8) C 13          s(  3.31%)p25.95( 85.79%)d 3.30( 10.90%)
356. (0.00003) RY*( 9) C 13          s(  4.66%)p 4.55( 21.19%)d15.92( 74.16%)
357. (0.00002) RY*(10) C 13          s(  2.34%)p 2.40(  5.61%)d39.32( 92.05%)
358. (0.00002) RY*(11) C 13          s( 59.29%)p 0.68( 40.25%)d 0.01(  0.46%)
359. (0.00003) RY*(12) C 13          s(  3.52%)p 6.56( 23.09%)d20.85( 73.39%)
360. (0.00000) RY*(13) C 13          s( 99.17%)p 0.00(  0.21%)d 0.01(  0.62%)
361. (0.00000) RY*(14) C 13          s(  0.16%)p99.99( 76.42%)d99.99( 23.42%)
362. (0.00000) RY*(15) C 13          s( 99.58%)p 0.00(  0.25%)d 0.00(  0.17%)
363. (0.00281) RY*( 1) C 14          s( 19.66%)p 3.65( 71.70%)d 0.44(  8.64%)
                                     0.0000  0.0018  0.4410 -0.0465 -0.0002
                                    -0.0011  0.0064 -0.6561  0.0676 -0.0104
                                     0.5222 -0.0375  0.0137 -0.0829 -0.0251
                                    -0.1687  0.1772 -0.0847 -0.0296 -0.1361
364. (0.00220) RY*( 2) C 14          s(  0.12%)p99.99( 94.14%)d45.95(  5.74%)
                                     0.0000 -0.0026  0.0351 -0.0030 -0.0012
                                     0.0002  0.0075 -0.5462 -0.0948  0.0102
                                    -0.7462 -0.1114  0.0061 -0.2437 -0.0726
                                     0.0087  0.1071  0.0520  0.1893  0.0855
365. (0.00111) RY*( 3) C 14          s(  2.68%)p35.94( 96.17%)d 0.43(  1.15%)
                                     0.0000  0.0001  0.1566 -0.0471  0.0047
                                    -0.0037  0.0184  0.3109 -0.1000 -0.0031
                                     0.0797 -0.0573 -0.0259 -0.8864  0.2423
                                    -0.0621  0.0747 -0.0147  0.0286 -0.0324
366. (0.00061) RY*( 4) C 14          s( 74.72%)p 0.29( 21.52%)d 0.05(  3.76%)
                                     0.0000 -0.0061  0.8639 -0.0279  0.0023
                                     0.0023 -0.0103  0.2870 -0.0824  0.0095
                                    -0.2675  0.0840 -0.0079  0.2166 -0.0170
                                    -0.0395 -0.1855  0.0381 -0.0049 -0.0110
367. (0.00035) RY*( 5) C 14          s(  0.08%)p 9.86(  0.78%)d99.99( 99.14%)
                                     0.0000  0.0005  0.0193  0.0201  0.0037
                                     0.0002  0.0035  0.0456  0.0230  0.0065
                                     0.0358  0.0152  0.0021  0.0163 -0.0578
                                    -0.3632  0.3175  0.6603 -0.2797  0.4944
368. (0.00012) RY*( 6) C 14          s( 20.04%)p 2.94( 58.81%)d 1.06( 21.15%)
                                     0.0000  0.0091  0.1079  0.4243  0.0740
                                    -0.0561 -0.0058 -0.0200  0.5518  0.0059
                                     0.0436 -0.5228 -0.0012 -0.0646  0.0615
                                     0.3068 -0.2405  0.2310  0.0379  0.0691
369. (0.00010) RY*( 7) C 14          s(  2.08%)p23.42( 48.62%)d23.74( 49.30%)
370. (0.00007) RY*( 8) C 14          s(  1.80%)p24.85( 44.75%)d29.68( 53.45%)
371. (0.00004) RY*( 9) C 14          s( 15.56%)p 2.39( 37.15%)d 3.04( 47.28%)
372. (0.00001) RY*(10) C 14          s( 10.88%)p 1.10( 11.94%)d 7.09( 77.17%)
373. (0.00002) RY*(11) C 14          s(  3.33%)p26.02( 86.64%)d 3.01( 10.03%)
374. (0.00001) RY*(12) C 14          s(  6.02%)p 4.12( 24.81%)d11.50( 69.17%)
375. (0.00000) RY*(13) C 14          s( 98.52%)p 0.01(  0.50%)d 0.01(  0.98%)
376. (0.00000) RY*(14) C 14          s( 98.91%)p 0.00(  0.18%)d 0.01(  0.90%)
377. (0.00001) RY*(15) C 14          s( 45.65%)p 0.05(  2.50%)d 1.14( 51.85%)
378. (0.00502) RY*( 1) C 15          s(  6.11%)p14.38( 87.84%)d 0.99(  6.05%)
                                     0.0000  0.0085  0.2428 -0.0455 -0.0013
                                    -0.0007  0.0215 -0.8171 -0.0803 -0.0007
                                     0.3002 -0.0813  0.0010  0.3181 -0.0765
                                    -0.1375 -0.1277 -0.0750  0.1207 -0.0710
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379. (0.00310) RY*( 2) C 15            s(  0.18%)p99.99( 96.16%)d20.71(  3.66%)
                                        0.0000 -0.0003  0.0393 -0.0148  0.0002
                                       -0.0002  0.0004  0.0090 -0.0038  0.0032
                                        0.7027  0.0937 -0.0032 -0.6715 -0.0897
                                       -0.0344  0.0453 -0.0077 -0.0878 -0.1600
380. (0.00160) RY*( 3) C 15            s( 11.71%)p 7.53( 88.15%)d 0.01(  0.14%)
                                        0.0000 -0.0014  0.3410 -0.0284 -0.0033
                                        0.0024 -0.0009  0.5403 -0.1207  0.0162
                                        0.4745 -0.1990  0.0167  0.5218 -0.1937
                                       -0.0190 -0.0290 -0.0072  0.0099 -0.0034
381. (0.00094) RY*( 4) C 15            s( 76.74%)p 0.30( 22.94%)d 0.00(  0.31%)
                                        0.0000 -0.0027  0.8678 -0.1193 -0.0004
                                        0.0112 -0.0207  0.0321 -0.0600 -0.0011
                                       -0.3514 -0.0196 -0.0018 -0.3167 -0.0134
                                       -0.0233 -0.0364  0.0254  0.0230 -0.0095
382. (0.00030) RY*( 5) C 15            s(  0.02%)p99.99(  3.33%)d99.99( 96.65%)
                                        0.0000 -0.0013  0.0111  0.0097  0.0011
                                       -0.0019  0.0000  0.0028  0.0656  0.0019
                                       -0.0920  0.0837 -0.0024  0.1161 -0.0061
                                        0.3311 -0.3063 -0.0153 -0.3948 -0.7791
383. (0.00022) RY*( 6) C 15            s(  4.55%)p14.30( 65.07%)d 6.68( 30.38%)
                                        0.0000 -0.0096  0.1743 -0.1184  0.0241
                                       -0.0202 -0.0074 -0.0046  0.6078 -0.0085
                                        0.1649  0.3409 -0.0060  0.1543  0.3374
                                        0.3465  0.2949  0.0257  0.3080 -0.0355
384. (0.00013) RY*( 7) C 15            s( 27.08%)p 1.47( 39.86%)d 1.22( 33.06%)
                                        0.0000  0.0083  0.0586  0.5149 -0.0241
                                        0.0397 -0.0150 -0.1165  0.2011 -0.0084
                                       -0.0584 -0.4201 -0.0090 -0.0643 -0.4002
                                        0.3778  0.3944 -0.1723 -0.0497  0.0131
385. (0.00007) RY*( 8) C 15            s(  3.66%)p 2.79( 10.19%)d23.55( 86.15%)
386. (0.00007) RY*( 9) C 15            s( 15.98%)p 1.37( 21.93%)d 3.89( 62.09%)
387. (0.00005) RY*(10) C 15            s(  6.93%)p 3.06( 21.18%)d10.37( 71.89%)
388. (0.00003) RY*(11) C 15            s( 42.76%)p 1.18( 50.67%)d 0.15(  6.57%)
389. (0.00001) RY*(12) C 15            s(  2.23%)p37.41( 83.32%)d 6.49( 14.45%)
390. (0.00002) RY*(13) C 15            s(  4.03%)p 2.24(  9.03%)d21.56( 86.94%)
391. (0.00000) RY*(14) C 15            s( 99.75%)p 0.00(  0.12%)d 0.00(  0.13%)
392. (0.00000) RY*(15) C 15            s( 98.31%)p 0.00(  0.46%)d 0.01(  1.23%)
393. (0.00830) RY*( 1) C 16            s(  0.65%)p99.99( 97.59%)d 2.71(  1.76%)
                                        0.0000 -0.0287  0.0614 -0.0432 -0.0072
                                       -0.0014  0.0003 -0.0475 -0.0025 -0.0339
                                       -0.1186 -0.0067  0.0288  0.9785 -0.0032
                                        0.0367  0.0457 -0.0804 -0.0359  0.0801
394. (0.00746) RY*( 2) C 16            s(  0.65%)p99.99( 99.03%)d 0.50(  0.32%)
                                        0.0000  0.0093  0.0795 -0.0049 -0.0038
                                       -0.0017 -0.0282  0.6718 -0.0243 -0.0175
                                        0.7226 -0.0183 -0.0277  0.1189 -0.0021
                                        0.0011 -0.0397  0.0065 -0.0282 -0.0281
395. (0.00567) RY*( 3) C 16            s(  0.71%)p99.99( 98.01%)d 1.79(  1.27%)
                                        0.0000  0.0186  0.0800  0.0193 -0.0017
                                       -0.0003  0.0196 -0.7321 -0.0306 -0.0028
                                        0.6623  0.0342 -0.0281  0.0476 -0.0045
                                       -0.0582  0.0521  0.0030 -0.0214 -0.0786
396. (0.00236) RY*( 4) C 16            s( 91.86%)p 0.04(  4.09%)d 0.04(  4.05%)
                                        0.0000 -0.0127  0.9579  0.0255 -0.0142
                                       -0.0059 -0.0149  0.0142  0.0885  0.0369
                                       -0.1068 -0.0171 -0.0286 -0.0804 -0.1109
                                       -0.0199  0.0331 -0.1596 -0.0856 -0.0789
397. (0.00045) RY*( 5) C 16            s(  1.00%)p19.61( 19.63%)d79.30( 79.37%)
                                        0.0000 -0.0007 -0.0192  0.0980  0.0057
                                        0.0007 -0.0236  0.0530  0.4269  0.0001
                                        0.0218 -0.0655  0.0014 -0.0040 -0.0770
                                       -0.3511  0.7440  0.1758  0.2186  0.1956
398. (0.00043) RY*( 6) C 16            s(  6.23%)p 4.55( 28.33%)d10.51( 65.44%)
                                        0.0000  0.0002  0.1423  0.2046  0.0109
                                        0.0075  0.0107  0.0019 -0.2438 -0.0101
                                        0.0200  0.4705 -0.0130  0.0125  0.0398
                                        0.1265 -0.0910  0.0740  0.7277  0.3085
399. (0.00036) RY*( 7) C 16            s(  4.57%)p 3.71( 16.94%)d17.19( 78.50%)
                                        0.0000  0.0000  0.0618  0.2045  0.0033
                                        0.0052  0.0055 -0.0021 -0.0748 -0.0085
                                       -0.0107  0.3760 -0.0062 -0.0013 -0.1489
                                       -0.1048 -0.0849  0.5092 -0.5603  0.4399
400. (0.00030) RY*( 8) C 16            s(  7.78%)p10.13( 78.75%)d 1.73( 13.47%)
                                        0.0000  0.0033 -0.1674  0.2222 -0.0173
                                        0.0051 -0.0033  0.0144  0.0477 -0.0010
                                        0.0093  0.1853  0.0145  0.0001 -0.8663
                                        0.1497  0.0479 -0.2949 -0.0118 -0.1513
401. (0.00024) RY*( 9) C 16            s( 79.96%)p 0.15( 12.35%)d 0.10(  7.69%)
                                        0.0000  0.0018 -0.0359  0.8932 -0.0159
                                       -0.0108  0.0009  0.0064 -0.0010 -0.0006
                                       -0.0043 -0.1840  0.0070  0.0167  0.2988
                                        0.1505  0.0592 -0.1837 -0.1218 -0.0469
402. (0.00012) RY*(10) C 16            s(  1.45%)p44.76( 64.72%)d23.40( 33.83%)
                                        0.0000  0.0036  0.0834  0.0633  0.0576
                                        0.0127  0.0046 -0.0525 -0.1432 -0.0120
                                        0.0192 -0.7208 -0.0116  0.0125 -0.3217
                                        0.2141 -0.1376  0.4206  0.2022  0.2361
403. (0.00013) RY*(11) C 16            s(  0.35%)p99.99( 69.96%)d85.77( 29.70%)
                                        0.0000 -0.0002  0.0246 -0.0008  0.0492
                                        0.0208 -0.0155  0.0505 -0.8303  0.0027
                                       -0.0658 -0.0351  0.0020 -0.0028 -0.0422
                                       -0.2098  0.4407  0.0362 -0.0719 -0.2285
404. (0.00007) RY*(12) C 16            s(  5.10%)p 0.84(  4.27%)d17.77( 90.63%)
405. (0.00003) RY*(13) C 16            s(  1.00%)p 6.05(  6.06%)d92.66( 92.93%)
406. (0.00000) RY*(14) C 16            s( 99.29%)p 0.00(  0.39%)d 0.00(  0.32%)
407. (0.00000) RY*(15) C 16            s( 99.39%)p 0.00(  0.15%)d 0.00(  0.46%)
408. (0.00258) RY*( 1) C 17            s( 12.60%)p 6.27( 78.96%)d 0.67(  8.43%)
                                        0.0000  0.0027  0.3518 -0.0476  0.0005
                                       -0.0003 -0.0145  0.6930 -0.0642 -0.0066
                                        0.3347 -0.0568 -0.0088  0.4333 -0.0438
                                        0.1883  0.2082  0.0016  0.0701 -0.0246
409. (0.00225) RY*( 2) C 17            s(  0.03%)p99.99( 94.04%)d99.99(  5.92%)
                                        0.0000  0.0000  0.0179 -0.0031  0.0001
                                        0.0001 -0.0019  0.0560 -0.0032 -0.0104
                                        0.7015  0.1026  0.0097 -0.6495 -0.1122
                                        0.1562 -0.1288  0.0045 -0.0526 -0.1245
410. (0.00138) RY*( 3) C 17            s(  2.68%)p36.11( 96.72%)d 0.22(  0.60%)
                                        0.0000 -0.0018  0.1636 -0.0020 -0.0004
                                       -0.0012 -0.0166 -0.6290  0.1651  0.0203
                                        0.5039 -0.1591  0.0195  0.4916 -0.1494
                                       -0.0427 -0.0195 -0.0262  0.0411 -0.0373
411. (0.00093) RY*( 4) C 17            s( 83.73%)p 0.16( 13.57%)d 0.03(  2.71%)
                                        0.0000 -0.0043  0.9106 -0.0901 -0.0018
                                        0.0028  0.0191 -0.1346  0.0250  0.0054
                                       -0.2373  0.0120  0.0048 -0.2449  0.0092
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                                    -0.1091 -0.1071  0.0599 -0.0031 -0.0091
412. (0.00043) RY*( 5) C 17          s(  0.00%)p 1.00(  0.28%)d99.99( 99.72%)
                                     0.0000  0.0002  0.0046 -0.0004 -0.0004
                                     0.0001  0.0001 -0.0060  0.0132  0.0054
                                    -0.0114 -0.0439 -0.0052  0.0202  0.0040
                                     0.4338 -0.4717  0.0218  0.4078  0.6479
413. (0.00010) RY*( 6) C 17          s(  4.43%)p 1.55(  6.86%)d20.02( 88.71%)
414. (0.00006) RY*( 7) C 17          s( 15.94%)p 3.03( 48.31%)d 2.24( 35.74%)
415. (0.00001) RY*( 8) C 17          s(  8.64%)p 2.90( 25.05%)d 7.68( 66.31%)
416. (0.00001) RY*( 9) C 17          s(  2.31%)p 1.37(  3.17%)d40.96( 94.53%)
417. (0.00001) RY*(10) C 17          s( 12.09%)p 7.27( 87.89%)d 0.00(  0.02%)
418. (0.00001) RY*(11) C 17          s( 13.66%)p 6.30( 86.04%)d 0.02(  0.30%)
419. (0.00001) RY*(12) C 17          s( 46.63%)p 1.14( 52.96%)d 0.01(  0.41%)
420. (0.00000) RY*(13) C 17          s( 98.57%)p 0.01(  0.82%)d 0.01(  0.61%)
421. (0.00000) RY*(14) C 17          s( 98.40%)p 0.00(  0.38%)d 0.01(  1.23%)
422. (0.00001) RY*(15) C 17          s(  0.34%)p15.35(  5.18%)d99.99( 94.48%)
423. (0.00484) RY*( 1) C 18          s(  5.79%)p15.19( 87.97%)d 1.08(  6.23%)
                                     0.0000  0.0084  0.2364 -0.0441 -0.0014
                                    -0.0009 -0.0097  0.6671 -0.0273  0.0006
                                    -0.3376  0.0763  0.0193 -0.5499 -0.1065
                                    -0.0041 -0.1729  0.1628  0.0769 -0.0041
424. (0.00292) RY*( 2) C 18          s(  0.15%)p99.99( 96.76%)d21.03(  3.09%)
                                     0.0000 -0.0003  0.0363 -0.0123  0.0001
                                    -0.0006  0.0056 -0.6080 -0.0779  0.0057
                                    -0.7051 -0.0942  0.0029 -0.2893 -0.0462
                                    -0.0099 -0.0380  0.0355 -0.1676  0.0057
425. (0.00161) RY*( 3) C 18          s( 11.78%)p 7.48( 88.11%)d 0.01(  0.11%)
                                     0.0000 -0.0015  0.3420 -0.0286 -0.0033
                                     0.0030  0.0154  0.1907 -0.1033 -0.0162
                                    -0.4535  0.1922  0.0070  0.7423 -0.1998
                                    -0.0044 -0.0188  0.0162  0.0130 -0.0171
426. (0.00094) RY*( 4) C 18          s( 77.77%)p 0.28( 21.92%)d 0.00(  0.31%)
                                     0.0000 -0.0028  0.8729 -0.1247 -0.0001
                                     0.0107  0.0074 -0.2801  0.0149  0.0007
                                     0.3445  0.0114 -0.0192 -0.1391 -0.0440
                                    -0.0317 -0.0416  0.0093  0.0173  0.0004
427. (0.00033) RY*( 5) C 18          s(  0.02%)p99.99(  2.62%)d99.99( 97.37%)
                                     0.0000 -0.0012  0.0067  0.0101  0.0010
                                    -0.0020  0.0056  0.0873 -0.0359  0.0065
                                     0.0753 -0.0781  0.0027  0.0471  0.0564
                                     0.1807 -0.5755 -0.3027 -0.6252 -0.3569
428. (0.00021) RY*( 6) C 18          s(  3.75%)p16.37( 61.36%)d 9.31( 34.90%)
                                     0.0000 -0.0094  0.1511 -0.1166  0.0243
                                    -0.0197 -0.0025  0.1381 -0.0243  0.0085
                                    -0.1639 -0.2978 -0.0105  0.0681  0.6881
                                     0.1597  0.0115 -0.3282  0.0354  0.4630
429. (0.00013) RY*( 7) C 18          s( 27.77%)p 1.55( 42.92%)d 1.06( 29.31%)
                                     0.0000  0.0088  0.0521  0.5221 -0.0250
                                     0.0410 -0.0011 -0.0088 -0.4501  0.0080
                                     0.0620  0.4486 -0.0167 -0.1357 -0.0517
                                     0.3381  0.2190 -0.2236 -0.1599  0.2352
430. (0.00007) RY*( 8) C 18          s(  9.72%)p 2.27( 22.08%)d 7.02( 68.21%)
431. (0.00007) RY*( 9) C 18          s( 11.74%)p 0.95( 11.16%)d 6.57( 77.10%)
432. (0.00004) RY*(10) C 18          s( 11.91%)p 1.23( 14.62%)d 6.17( 73.46%)
433. (0.00003) RY*(11) C 18          s( 36.52%)p 1.55( 56.47%)d 0.19(  7.02%)
434. (0.00002) RY*(12) C 18          s(  3.22%)p 1.83(  5.87%)d28.26( 90.91%)
435. (0.00000) RY*(13) C 18          s( 98.85%)p 0.00(  0.02%)d 0.01(  1.13%)
436. (0.00001) RY*(14) C 18          s(  1.37%)p64.19( 88.21%)d 7.58( 10.42%)
437. (0.00000) RY*(15) C 18          s( 99.69%)p 0.00(  0.16%)d 0.00(  0.15%)
438. (0.00314) RY*( 1) C 19          s( 17.31%)p 4.31( 74.71%)d 0.46(  7.98%)
                                     0.0000  0.0026  0.4112 -0.0634 -0.0024
                                     0.0002  0.0070 -0.0313  0.0053 -0.0135
                                     0.6208 -0.0379 -0.0133  0.5976 -0.0409
                                    -0.0545 -0.0518  0.1749 -0.1836  0.0991
439. (0.00182) RY*( 2) C 19          s(  0.00%)p 1.00( 93.62%)d 0.07(  6.38%)
                                     0.0000  0.0002  0.0020  0.0010  0.0000
                                     0.0001  0.0005 -0.0120 -0.0062  0.0087
                                    -0.6635 -0.1040 -0.0086  0.6884  0.1040
                                     0.0060 -0.0187  0.0060  0.1280  0.2168
440. (0.00121) RY*( 3) C 19          s(  1.64%)p60.03( 98.18%)d 0.11(  0.18%)
                                     0.0000  0.0003  0.1220 -0.0382  0.0010
                                     0.0005 -0.0310 -0.9501  0.2580 -0.0028
                                    -0.0676 -0.0037 -0.0047 -0.0824  0.0128
                                     0.0124  0.0197  0.0263 -0.0206  0.0136
441. (0.00062) RY*( 4) C 19          s( 77.98%)p 0.23( 18.18%)d 0.05(  3.84%)
                                     0.0000 -0.0068  0.8826 -0.0278  0.0059
                                    -0.0023 -0.0025  0.1381 -0.0740  0.0141
                                    -0.2684  0.0966  0.0121 -0.2620  0.0830
                                     0.0342  0.1409  0.0349  0.1186 -0.0455
442. (0.00053) RY*( 5) C 19          s(  0.50%)p 0.56(  0.28%)d99.99( 99.22%)
                                     0.0000 -0.0001  0.0706 -0.0014  0.0013
                                     0.0006 -0.0009  0.0031 -0.0103 -0.0054
                                    -0.0322 -0.0332  0.0068 -0.0055  0.0211
                                     0.6876 -0.7007  0.0194 -0.0424 -0.1623
443. (0.00011) RY*( 6) C 19          s(  2.15%)p 7.52( 16.18%)d37.98( 81.67%)
                                     0.0000 -0.0002 -0.0498  0.1362 -0.0217
                                    -0.0032  0.0337  0.1185  0.3627  0.0014
                                    -0.0078 -0.0971  0.0032 -0.0059 -0.0745
                                     0.6072  0.5683  0.1856 -0.2462  0.1731
444. (0.00009) RY*( 7) C 19          s( 15.21%)p 4.06( 61.68%)d 1.52( 23.11%)
445. (0.00004) RY*( 8) C 19          s(  2.56%)p27.56( 70.58%)d10.49( 26.86%)
446. (0.00001) RY*( 9) C 19          s( 65.28%)p 0.52( 34.20%)d 0.01(  0.52%)
447. (0.00001) RY*(10) C 19          s(  2.74%)p 6.79( 18.60%)d28.70( 78.66%)
448. (0.00000) RY*(11) C 19          s( 98.46%)p 0.01(  0.62%)d 0.01(  0.92%)
449. (0.00000) RY*(12) C 19          s( 13.10%)p 6.62( 86.76%)d 0.01(  0.14%)
450. (0.00001) RY*(13) C 19          s(  4.24%)p 4.41( 18.67%)d18.20( 77.09%)
451. (0.00000) RY*(14) C 19          s( 98.65%)p 0.01(  0.57%)d 0.01(  0.79%)
452. (0.00001) RY*(15) C 19          s(  0.23%)p32.17(  7.40%)d99.99( 92.37%)
453. (0.00833) RY*( 1) C 20          s(  6.18%)p14.35( 88.67%)d 0.83(  5.15%)
                                     0.0000 -0.0016  0.2485  0.0024 -0.0036
                                     0.0008 -0.0165 -0.5152  0.0745  0.0153
                                     0.5670 -0.0272  0.0099 -0.5382 -0.0574
                                    -0.1220  0.1397 -0.0234 -0.0223 -0.1267
454. (0.00511) RY*( 2) C 20          s(  0.05%)p99.99( 90.60%)d99.99(  9.35%)
                                     0.0000 -0.0015  0.0215 -0.0082  0.0003
                                    -0.0003 -0.0296  0.5080 -0.0757 -0.0327
                                     0.7369 -0.0959 -0.0153  0.2945 -0.0329
                                     0.0815 -0.1374 -0.1884 -0.0374 -0.1762
455. (0.00338) RY*( 3) C 20          s(  1.56%)p61.20( 95.23%)d 2.07(  3.21%)
                                     0.0000 -0.0057  0.0952  0.0803 -0.0002
                                    -0.0016  0.0144  0.6263  0.0830 -0.0140
                                    -0.1566  0.0151  0.0036 -0.6946 -0.2134
                                    -0.0227 -0.0915  0.1145  0.0600 -0.0808
456. (0.00109) RY*( 4) C 20          s( 64.61%)p 0.20( 13.13%)d 0.34( 22.26%)
                                     0.0000 -0.0011  0.8027  0.0422 -0.0018
                                    -0.0029 -0.0004  0.0205  0.1754 -0.0185
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                                    -0.2141 -0.0505  0.0166  0.1790 -0.1381
                                     0.0287 -0.0640 -0.2656 -0.3822 -0.0330
457. (0.00103) RY*( 5) C 20           s( 14.61%)p 0.35(  5.08%)d 5.50( 80.31%)
                                     0.0000 -0.0014  0.3821 -0.0102 -0.0010
                                    -0.0035  0.0125  0.1440  0.0177  0.0036
                                     0.0786 -0.0247  0.0135  0.1481 -0.0257
                                    -0.0809  0.4682  0.1257  0.6518  0.3698
458. (0.00055) RY*( 6) C 20           s(  1.34%)p 4.97(  6.64%)d68.83( 92.02%)
                                     0.0000  0.0026 -0.0805  0.0829  0.0020
                                    -0.0014 -0.0041 -0.1119  0.1247  0.0014
                                    -0.1665 -0.0420  0.0003 -0.0514 -0.0788
                                     0.3373 -0.0024 -0.6302  0.4933 -0.4074
459. (0.00055) RY*( 7) C 20           s( 16.89%)p 2.50( 42.18%)d 2.42( 40.93%)
                                     0.0000 -0.0074  0.3346 -0.2379 -0.0160
                                     0.0066  0.0113 -0.0561 -0.4269 -0.0097
                                    -0.0262  0.1342 -0.0034 -0.0923  0.4572
                                     0.0599 -0.5502  0.1092  0.2932 -0.0711
460. (0.00020) RY*( 8) C 20           s( 21.22%)p 2.62( 55.69%)d 1.09( 23.10%)
                                     0.0000  0.0031  0.0639  0.4557 -0.0111
                                    -0.0158  0.0012  0.0404  0.2161  0.0044
                                    -0.0532 -0.4911 -0.0120  0.0524  0.5114
                                    -0.0952  0.0810  0.2806  0.0357 -0.3679
461. (0.00018) RY*( 9) C 20           s( 55.74%)p 0.75( 41.73%)d 0.05(  2.53%)
                                     0.0000  0.0022  0.0709  0.7430  0.0012
                                     0.0176 -0.0026 -0.0651 -0.3971  0.0033
                                     0.0259  0.4530 -0.0033  0.0863 -0.2051
                                     0.0304  0.0107  0.1072  0.0203 -0.1113
462. (0.00012) RY*(10) C 20           s(  3.49%)p11.32( 39.52%)d16.32( 56.99%)
                                     0.0000  0.0004 -0.0057  0.1852  0.0192
                                     0.0143  0.0095 -0.1689  0.4801 -0.0071
                                     0.1102 -0.0979 -0.0025  0.1075 -0.3206
                                     0.1930 -0.5833  0.2884  0.2283  0.2389
463. (0.00010) RY*(11) C 20           s(  7.50%)p 2.72( 20.43%)d 9.60( 72.06%)
                                     0.0000  0.0039 -0.0329  0.2704 -0.0229
                                    -0.0178 -0.0014  0.0331 -0.0619 -0.0081
                                     0.0824 -0.1191  0.0218 -0.2273  0.3553
                                     0.5451  0.0500 -0.2395 -0.1801  0.5755
464. (0.00003) RY*(12) C 20           s(  0.71%)p99.99( 98.58%)d 0.99(  0.71%)
465. (0.00002) RY*(13) C 20           s(  8.34%)p 0.24(  1.97%)d10.75( 89.69%)
466. (0.00000) RY*(14) C 20           s( 97.98%)p 0.01(  0.62%)d 0.01(  1.40%)
467. (0.00000) RY*(15) C 20           s( 99.78%)p 0.00(  0.21%)d 0.00(  0.02%)
468. (0.00249) RY*( 1) C 21           s( 13.78%)p 5.53( 76.13%)d 0.73( 10.09%)
                                     0.0000  0.0024  0.3664 -0.0590 -0.0001
                                    -0.0026  0.0154 -0.6478  0.0434 -0.0063
                                     0.2962 -0.0155 -0.0146  0.5000 -0.0358
                                    -0.0449 -0.2318  0.1790  0.1097 -0.0332
469. (0.00153) RY*( 2) C 21           s(  0.76%)p99.99( 98.72%)d 0.69(  0.52%)
                                     0.0000 -0.0014  0.0870  0.0008 -0.0016
                                     0.0006 -0.0140 -0.2676  0.0587  0.0182
                                     0.5871 -0.0782 -0.0203 -0.7406  0.1092
                                     0.0238  0.0221 -0.0098  0.0134  0.0623
470. (0.00100) RY*( 3) C 21           s(  0.00%)p 1.00( 91.97%)d 0.09(  8.03%)
                                     0.0000 -0.0004  0.0026 -0.0008  0.0005
                                     0.0008  0.0062 -0.5661 -0.1025  0.0080
                                    -0.6740 -0.1445  0.0025 -0.3344 -0.0413
                                     0.1040 -0.0888 -0.1807  0.1081 -0.1315
471. (0.00076) RY*( 4) C 21           s( 84.63%)p 0.14( 12.08%)d 0.04(  3.29%)
                                     0.0000 -0.0045  0.9158 -0.0872 -0.0015
                                     0.0056 -0.0139  0.2779 -0.0165  0.0037
                                    -0.1690 -0.0076  0.0159 -0.1166  0.0254
                                    -0.0146  0.0710 -0.1344 -0.0769  0.0604
472. (0.00051) RY*( 5) C 21           s(  0.08%)p20.82(  1.65%)d99.99( 98.27%)
                                     0.0000 -0.0003  0.0274 -0.0065 -0.0006
                                     0.0008 -0.0058 -0.0416 -0.0091 -0.0081
                                    -0.0932  0.0424 -0.0024 -0.0153 -0.0625
                                    -0.0782  0.5233  0.3015  0.6728  0.3989
473. (0.00009) RY*( 6) C 21           s(  2.62%)p 2.08(  5.45%)d35.03( 91.93%)
474. (0.00005) RY*( 7) C 21           s( 20.43%)p 1.70( 34.83%)d 2.19( 44.73%)
475. (0.00003) RY*( 8) C 21           s(  2.36%)p38.66( 91.09%)d 2.78(  6.55%)
476. (0.00001) RY*( 9) C 21           s( 11.19%)p 1.36( 15.24%)d 6.58( 73.57%)
477. (0.00001) RY*(10) C 21           s( 40.75%)p 1.43( 58.42%)d 0.02(  0.83%)
478. (0.00001) RY*(11) C 21           s(  2.48%)p 2.78(  6.89%)d36.59( 90.64%)
479. (0.00002) RY*(12) C 21           s( 19.01%)p 0.78( 14.90%)d 3.48( 66.09%)
480. (0.00000) RY*(13) C 21           s( 97.95%)p 0.00(  0.48%)d 0.02(  1.57%)
481. (0.00000) RY*(14) C 21           s( 99.15%)p 0.00(  0.47%)d 0.00(  0.38%)
482. (0.00000) RY*(15) C 21           s(  4.87%)p18.89( 91.92%)d 0.66(  3.21%)
483. (0.00799) RY*( 1) C 22           s(  6.43%)p13.97( 89.81%)d 0.59(  3.76%)
                                     0.0000  0.0020  0.2533 -0.0118 -0.0007
                                     0.0009  0.0134  0.6618  0.0026 -0.0128
                                    -0.6731  0.0254  0.0071  0.0577 -0.0510
                                    -0.1103  0.0894 -0.0169 -0.0103 -0.1308
484. (0.00436) RY*( 2) C 22           s(  0.01%)p99.99( 98.48%)d99.99(  1.50%)
                                     0.0000 -0.0008  0.0089 -0.0059  0.0002
                                    -0.0003 -0.0061  0.6625 -0.0679 -0.0075
                                     0.6757 -0.0807 -0.0046  0.2786 -0.0222
                                     0.0392 -0.0590 -0.0821  0.0092 -0.0565
485. (0.00274) RY*( 3) C 22           s(  1.52%)p62.68( 95.16%)d 2.19(  3.32%)
                                     0.0000  0.0018  0.1104  0.0547 -0.0021
                                    -0.0015 -0.0020  0.2069  0.1109  0.0090
                                     0.1725  0.0049 -0.0076 -0.9073 -0.2084
                                     0.0559  0.0822 -0.1164 -0.0584  0.0799
486. (0.00104) RY*( 4) C 22           s( 90.64%)p 0.09(  8.12%)d 0.01(  1.24%)
                                     0.0000 -0.0037  0.9516  0.0285 -0.0013
                                     0.0015 -0.0103 -0.2010 -0.0835  0.0101
                                     0.1468  0.0623 -0.0055  0.0775  0.0467
                                    -0.0152 -0.0775 -0.0359  0.0459  0.0525
487. (0.00051) RY*( 5) C 22           s(  3.06%)p22.44( 68.75%)d 9.20( 28.19%)
                                     0.0000  0.0077 -0.0138  0.1738 -0.0012
                                    -0.0134  0.0051 -0.0928 -0.0475 -0.0093
                                     0.0847  0.3865  0.0081  0.0808 -0.7165
                                    -0.1934  0.0408  0.2362  0.1434 -0.4079
488. (0.00044) RY*( 6) C 22           s(  0.13%)p18.02(  2.34%)d99.99( 97.53%)
                                     0.0000 -0.0004  0.0332  0.0139  0.0001
                                     0.0001 -0.0006  0.0703 -0.0048  0.0000
                                     0.0864  0.0964 -0.0008  0.0404  0.0065
                                    -0.3023  0.3198  0.5919 -0.4850  0.4428
489. (0.00041) RY*( 7) C 22           s(  0.03%)p24.37(  0.77%)d99.99( 99.20%)
                                     0.0000  0.0006  0.0097  0.0144 -0.0033
                                    -0.0018  0.0007 -0.0364  0.0510  0.0005
                                    -0.0245  0.0540  0.0021 -0.0105 -0.0117
                                     0.0383 -0.5049 -0.1030 -0.7844 -0.3313
490. (0.00021) RY*( 8) C 22           s(  3.77%)p23.23( 87.51%)d 2.31(  8.72%)
                                     0.0000 -0.0011 -0.0793  0.1770 -0.0061
                                    -0.0045  0.0051  0.0182 -0.7448 -0.0030
                                     0.0158  0.4337 -0.0002 -0.1288  0.3394
                                     0.0366  0.2090 -0.1260 -0.0768 -0.1429
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491. (0.00014) RY*( 9) C 22            s( 75.64%)p 0.20( 15.21%)d 0.12(  9.15%)
                                        0.0000  0.0064  0.0265  0.8693  0.0039
                                       -0.0013  0.0035 -0.0067  0.1586 -0.0035
                                        0.0006 -0.3084  0.0010  0.0127  0.1779
                                        0.1041  0.1302  0.1520 -0.0109 -0.2013
492. (0.00012) RY*(10) C 22            s(  8.46%)p 3.11( 26.30%)d 7.72( 65.25%)
                                        0.0000  0.0004 -0.0304  0.2883  0.0158
                                        0.0163  0.0005  0.0018  0.0781  0.0063
                                       -0.0881  0.2736 -0.0172  0.2358 -0.3439
                                        0.3605  0.1130 -0.4591 -0.1796  0.5164
493. (0.00008) RY*(11) C 22            s(  2.25%)p 4.90( 11.04%)d38.50( 86.71%)
494. (0.00004) RY*(12) C 22            s(  2.25%)p31.47( 70.72%)d12.03( 27.03%)
495. (0.00002) RY*(13) C 22            s(  7.02%)p 3.66( 25.67%)d 9.59( 67.30%)
496. (0.00000) RY*(14) C 22            s( 99.82%)p 0.00(  0.06%)d 0.00(  0.12%)
497. (0.00000) RY*(15) C 22            s( 99.03%)p 0.00(  0.19%)d 0.01(  0.78%)
498. (0.00304) RY*( 1) C 23            s( 14.33%)p 5.38( 77.09%)d 0.60(  8.58%)
                                        0.0000  0.0041  0.3776 -0.0259 -0.0010
                                       -0.0027 -0.0051 -0.2877  0.0498  0.0086
                                       -0.1145 -0.0138 -0.0128  0.8194 -0.0275
                                        0.1050  0.0213 -0.1440 -0.0654  0.2222
499. (0.00178) RY*( 2) C 23            s(  0.00%)p 1.00( 96.59%)d 0.04(  3.40%)
                                        0.0000  0.0002  0.0055  0.0018  0.0005
                                       -0.0008 -0.0045  0.5673  0.0882 -0.0068
                                        0.7275  0.1169 -0.0020  0.3009  0.0526
                                       -0.0595  0.0966  0.1136  0.0293  0.0860
500. (0.00090) RY*( 3) C 23            s( 26.58%)p 2.71( 71.95%)d 0.06(  1.47%)
                                        0.0000 -0.0067  0.5133 -0.0472 -0.0040
                                        0.0042  0.0191  0.6558 -0.1872 -0.0151
                                       -0.4757  0.1270 -0.0041 -0.0910  0.0562
                                        0.0116 -0.0648 -0.0272 -0.0263  0.0948
501. (0.00051) RY*( 4) C 23            s( 55.24%)p 0.75( 41.17%)d 0.06(  3.59%)
                                        0.0000 -0.0030  0.7413  0.0533  0.0077
                                        0.0030  0.0008 -0.2947  0.1280 -0.0075
                                        0.3630 -0.1780  0.0131 -0.3431  0.1645
                                       -0.1300 -0.0809  0.0812  0.0134 -0.0754
502. (0.00037) RY*( 5) C 23            s(  0.35%)p 2.88(  1.01%)d99.99( 98.64%)
                                        0.0000 -0.0011  0.0589  0.0035  0.0019
                                        0.0012  0.0058 -0.0256 -0.0020  0.0066
                                       -0.0018  0.0867  0.0033 -0.0331  0.0268
                                        0.1982  0.2340 -0.2168  0.9194  0.0113
503. (0.00015) RY*( 6) C 23            s( 24.05%)p 1.34( 32.15%)d 1.82( 43.80%)
                                        0.0000  0.0062  0.1215  0.4704 -0.0326
                                        0.0579  0.0118  0.0905  0.2588 -0.0136
                                       -0.1262 -0.0001  0.0098  0.1043 -0.4681
                                       -0.1772  0.3721  0.0682 -0.0235 -0.5128
504. (0.00010) RY*( 7) C 23            s(  6.09%)p 4.54( 27.65%)d10.89( 66.27%)
                                        0.0000  0.0016  0.0423  0.2391 -0.0425
                                       -0.0104 -0.0228 -0.0730 -0.0707  0.0164
                                        0.0401  0.2758  0.0055  0.0175 -0.4328
                                        0.1791 -0.5914  0.4713  0.2030  0.1325
505. (0.00008) RY*( 8) C 23            s(  8.10%)p 9.15( 74.11%)d 2.20( 17.79%)
506. (0.00006) RY*( 9) C 23            s(  0.12%)p44.99(  5.52%)d99.99( 94.36%)
507. (0.00003) RY*(10) C 23            s(  8.03%)p 3.51( 28.20%)d 7.95( 63.77%)
508. (0.00002) RY*(11) C 23            s( 11.78%)p 3.49( 41.09%)d 4.00( 47.13%)
509. (0.00001) RY*(12) C 23            s( 39.51%)p 0.58( 22.94%)d 0.95( 37.55%)
510. (0.00000) RY*(13) C 23            s( 98.63%)p 0.00(  0.19%)d 0.01(  1.18%)
511. (0.00001) RY*(14) C 23            s(  7.81%)p10.28( 80.27%)d 1.53( 11.92%)
512. (0.00000) RY*(15) C 23            s( 99.43%)p 0.00(  0.31%)d 0.00(  0.25%)
513. (0.00313) RY*( 1) C 24            s( 17.26%)p 4.33( 74.77%)d 0.46(  7.98%)
                                        0.0000  0.0025  0.4104 -0.0641 -0.0024
                                        0.0002 -0.0146  0.5312 -0.0377  0.0141
                                       -0.6260  0.0379 -0.0003  0.2646 -0.0156
                                       -0.1769  0.1238 -0.0422 -0.0293 -0.1746
514. (0.00183) RY*( 2) C 24            s(  0.00%)p 1.00( 92.67%)d 0.08(  7.33%)
                                        0.0000  0.0001  0.0040  0.0008 -0.0002
                                        0.0001 -0.0055  0.6196  0.0938 -0.0060
                                        0.6561  0.1011 -0.0024  0.3023  0.0440
                                       -0.0315  0.1332  0.0433  0.2161  0.0773
515. (0.00121) RY*( 3) C 24            s(  1.40%)p70.17( 98.40%)d 0.14(  0.20%)
                                        0.0000  0.0004  0.1121 -0.0381  0.0009
                                        0.0005  0.0108  0.3801 -0.1108  0.0025
                                        0.0434  0.0076 -0.0292 -0.8786  0.2290
                                       -0.0168  0.0316 -0.0220 -0.0136 -0.0015
516. (0.00061) RY*( 4) C 24            s( 78.40%)p 0.23( 17.88%)d 0.05(  3.72%)
                                        0.0000 -0.0067  0.8849 -0.0286  0.0057
                                       -0.0022  0.0128 -0.2917  0.1050 -0.0132
                                        0.2683 -0.0973  0.0040 -0.0181 -0.0233
                                       -0.0114 -0.0117 -0.0445 -0.0164  0.1862
517. (0.00051) RY*( 5) C 24            s(  0.43%)p 2.80(  1.20%)d99.99( 98.38%)
                                        0.0000 -0.0001  0.0653 -0.0019  0.0010
                                        0.0005 -0.0062  0.0462  0.0290 -0.0080
                                        0.0817  0.0402 -0.0036  0.0219  0.0096
                                        0.2971 -0.4841 -0.6180  0.1950 -0.4911
518. (0.00011) RY*( 6) C 24            s(  2.26%)p 7.41( 16.75%)d35.82( 80.99%)
                                        0.0000 -0.0001 -0.0456  0.1417 -0.0210
                                       -0.0041 -0.0131 -0.0620 -0.2491 -0.0009
                                        0.0097  0.1132  0.0311  0.1007  0.2784
                                        0.1460  0.5257 -0.6214 -0.2588  0.2430
519. (0.00008) RY*( 7) C 24            s( 14.95%)p 4.07( 60.89%)d 1.62( 24.17%)
520. (0.00004) RY*( 8) C 24            s(  1.79%)p40.71( 72.99%)d14.07( 25.22%)
521. (0.00001) RY*( 9) C 24            s( 58.82%)p 0.08(  4.89%)d 0.62( 36.29%)
522. (0.00001) RY*(10) C 24            s( 24.49%)p 1.90( 46.61%)d 1.18( 28.90%)
523. (0.00001) RY*(11) C 24            s(  0.29%)p99.99( 42.07%)d99.99( 57.64%)
524. (0.00000) RY*(12) C 24            s( 98.77%)p 0.01(  0.95%)d 0.00(  0.28%)
525. (0.00001) RY*(13) C 24            s(  2.47%)p25.10( 62.03%)d14.36( 35.50%)
526. (0.00000) RY*(14) C 24            s(  0.01%)p99.99(  7.12%)d99.99( 92.87%)
527. (0.00000) RY*(15) C 24            s( 98.71%)p 0.01(  1.03%)d 0.00(  0.27%)
528. (0.00320) RY*( 1) C 25            s( 13.91%)p 5.66( 78.75%)d 0.53(  7.34%)
                                        0.0000  0.0040  0.3716 -0.0312  0.0001
                                       -0.0019  0.0107 -0.4836  0.0078 -0.0084
                                        0.1366  0.0172 -0.0061  0.7295 -0.0468
                                       -0.0173 -0.1960  0.1627  0.0880  0.0212
529. (0.00215) RY*( 2) C 25            s(  0.01%)p99.99( 93.59%)d99.99(  6.40%)
                                        0.0000  0.0006  0.0105  0.0005 -0.0001
                                       -0.0005 -0.0110  0.6307  0.0848 -0.0105
                                        0.6601  0.1020 -0.0046  0.2875  0.0432
                                       -0.0745  0.1327  0.1548 -0.0265  0.1272
530. (0.00100) RY*( 3) C 25            s( 14.77%)p 5.69( 83.99%)d 0.08(  1.24%)
                                        0.0000 -0.0063  0.3798 -0.0580 -0.0029
                                        0.0031 -0.0093 -0.3678  0.0747  0.0143
                                        0.5833 -0.1467 -0.0172 -0.5521  0.1786
                                        0.0259 -0.0486 -0.0026  0.0233  0.0940
531. (0.00069) RY*( 4) C 25            s( 68.72%)p 0.41( 28.04%)d 0.05(  3.25%)
                                        0.0000 -0.0033  0.8272  0.0542  0.0014
                                        0.0017 -0.0138  0.3427 -0.1802  0.0089
                                       -0.3091  0.1663  0.0050 -0.0820 -0.0153
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                                    -0.0906  0.1035 -0.1111 -0.0293 -0.0191
532. (0.00051) RY*( 5) C 25          s(  0.07%)p20.46(  1.46%)d99.99( 98.47%)
                                     0.0000 -0.0003  0.0263 -0.0047  0.0005
                                     0.0003  0.0061  0.0748  0.0311  0.0073
                                     0.0816 -0.0073  0.0025  0.0318  0.0141
                                     0.0904 -0.4916 -0.1638 -0.7911 -0.2866
533. (0.00013) RY*( 6) C 25          s( 15.00%)p 2.14( 32.12%)d 3.53( 52.89%)
                                     0.0000  0.0039  0.0385  0.3798 -0.0442
                                     0.0472 -0.0138 -0.1253  0.2170  0.0164
                                     0.1423 -0.0028 -0.0077 -0.0492 -0.4850
                                    -0.2303  0.3533  0.0692 -0.0479 -0.5865
534. (0.00011) RY*( 7) C 25          s( 16.10%)p 1.77( 28.44%)d 3.45( 55.46%)
                                     0.0000  0.0023  0.0826  0.3907 -0.0365
                                     0.0124  0.0057  0.0046  0.3744 -0.0136
                                    -0.0388 -0.1781  0.0199  0.0597 -0.3268
                                     0.4364  0.0875 -0.2763 -0.1239  0.5145
535. (0.00007) RY*( 8) C 25          s(  3.04%)p28.30( 86.03%)d 3.59( 10.93%)
536. (0.00002) RY*( 9) C 25          s(  6.52%)p 2.91( 18.97%)d11.42( 74.51%)
537. (0.00003) RY*(10) C 25          s(  3.34%)p 8.68( 29.00%)d20.24( 67.66%)
538. (0.00002) RY*(11) C 25          s( 58.06%)p 0.58( 33.75%)d 0.14(  8.19%)
539. (0.00002) RY*(12) C 25          s(  1.62%)p 6.20( 10.05%)d54.52( 88.33%)
540. (0.00000) RY*(13) C 25          s( 99.19%)p 0.00(  0.21%)d 0.01(  0.60%)
541. (0.00000) RY*(14) C 25          s(  0.12%)p99.99( 75.57%)d99.99( 24.31%)
542. (0.00000) RY*(15) C 25          s( 99.58%)p 0.00(  0.25%)d 0.00(  0.17%)
543. (0.00258) RY*( 1) C 26          s( 12.37%)p 6.40( 79.17%)d 0.68(  8.46%)
                                     0.0000  0.0027  0.3484 -0.0477  0.0004
                                    -0.0003 -0.0009  0.0358 -0.0069  0.0064
                                    -0.3249  0.0544 -0.0173  0.8217 -0.0790
                                     0.0927  0.0618 -0.1649 -0.0539  0.2052
544. (0.00225) RY*( 2) C 26          s(  0.02%)p99.99( 94.07%)d99.99(  5.91%)
                                     0.0000 -0.0001  0.0130 -0.0024  0.0001
                                     0.0003  0.0091 -0.6066 -0.1006  0.0096
                                    -0.6952 -0.1038  0.0028 -0.2557 -0.0544
                                     0.0593 -0.1434 -0.1172 -0.1091 -0.0970
545. (0.00138) RY*( 3) C 26          s(  2.96%)p32.58( 96.44%)d 0.20(  0.60%)
                                     0.0000 -0.0019  0.1720 -0.0029 -0.0004
                                    -0.0010  0.0241  0.7259 -0.2066 -0.0214
                                    -0.5187  0.1629 -0.0051 -0.3056  0.0693
                                     0.0018 -0.0552  0.0505  0.0096  0.0188
546. (0.00093) RY*( 4) C 26          s( 83.68%)p 0.16( 13.64%)d 0.03(  2.68%)
                                     0.0000 -0.0042  0.9103 -0.0905 -0.0018
                                     0.0028 -0.0051 -0.1539 -0.0034 -0.0050
                                     0.2370 -0.0114  0.0191 -0.2351  0.0259
                                    -0.1057 -0.0625  0.0668  0.0307 -0.0797
547. (0.00042) RY*( 5) C 26          s(  0.00%)p 1.00(  0.30%)d99.99( 99.69%)
                                     0.0000  0.0002  0.0061  0.0005 -0.0004
                                     0.0000  0.0056 -0.0168 -0.0081  0.0060
                                    -0.0259  0.0404  0.0026 -0.0130  0.0113
                                     0.1701  0.0213 -0.3908  0.8871 -0.1671
548. (0.00010) RY*( 6) C 26          s(  4.71%)p 1.57(  7.39%)d18.68( 87.90%)
549. (0.00006) RY*( 7) C 26          s( 15.51%)p 3.13( 48.47%)d 2.32( 36.02%)
550. (0.00001) RY*( 8) C 26          s(  1.17%)p49.67( 58.03%)d34.92( 40.80%)
551. (0.00001) RY*( 9) C 26          s(  1.80%)p53.68( 96.81%)d 0.77(  1.39%)
552. (0.00002) RY*(10) C 26          s(  6.80%)p 3.15( 21.45%)d10.55( 71.75%)
553. (0.00001) RY*(11) C 26          s( 19.26%)p 1.87( 36.11%)d 2.32( 44.63%)
554. (0.00000) RY*(12) C 26          s( 97.16%)p 0.01(  1.40%)d 0.01(  1.44%)
555. (0.00001) RY*(13) C 26          s(  1.59%)p 4.39(  7.00%)d57.32( 91.41%)
556. (0.00000) RY*(14) C 26          s( 54.57%)p 0.72( 39.02%)d 0.12(  6.41%)
557. (0.00000) RY*(15) C 26          s( 98.45%)p 0.01(  0.93%)d 0.01(  0.62%)
558. (0.00138) RY*( 1) H 27          s( 97.51%)p 0.03(  2.49%)
                                    -0.0057  0.9874 -0.0087  0.1255  0.0412
                                     0.0866
559. (0.00056) RY*( 2) H 27          s( 97.84%)p 0.02(  2.16%)
                                    -0.0002  0.0277  0.9887 -0.0609  0.0104
                                    -0.1335
560. (0.00021) RY*( 3) H 27          s(  0.98%)p99.99( 99.02%)
                                     0.0014 -0.0313  0.0940  0.1238 -0.8056
                                     0.5708
561. (0.00007) RY*( 4) H 27          s(  1.33%)p74.07( 98.67%)
562. (0.00005) RY*( 5) H 27          s(  2.46%)p39.72( 97.54%)
563. (0.00043) RY*( 1) H 28          s( 96.49%)p 0.04(  3.51%)
                                    -0.0058  0.9769 -0.1026 -0.1192 -0.0087
                                    -0.1441
564. (0.00038) RY*( 2) H 28          s(  0.94%)p99.99( 99.06%)
                                    -0.0007  0.0926 -0.0286  0.0137 -0.7263
                                     0.6803
565. (0.00033) RY*( 3) H 28          s( 64.93%)p 0.54( 35.07%)
                                     0.0116  0.1770  0.7860  0.2902  0.3513
                                     0.3782
566. (0.00009) RY*( 4) H 28          s(  7.40%)p12.51( 92.60%)
567. (0.00002) RY*( 5) H 28          s( 30.30%)p 2.30( 69.70%)
568. (0.00156) RY*( 1) H 29          s( 93.90%)p 0.07(  6.10%)
                                    -0.0095  0.9689 -0.0035 -0.0267 -0.0138
                                     0.2452
569. (0.00056) RY*( 2) H 29          s( 85.87%)p 0.16( 14.13%)
                                    -0.0026  0.0261  0.9263 -0.3027 -0.1787
                                    -0.1333
570. (0.00033) RY*( 3) H 29          s( 11.75%)p 7.51( 88.25%)
                                     0.0050 -0.0347  0.3410  0.4800  0.7717
                                     0.2380
571. (0.00015) RY*( 4) H 29          s(  2.65%)p36.75( 97.35%)
                                     0.0072  0.1032  0.1256  0.8092 -0.4484
                                    -0.3430
572. (0.00005) RY*( 5) H 29          s(  5.93%)p15.87( 94.07%)
573. (0.00055) RY*( 1) H 30          s( 13.68%)p 6.31( 86.32%)
                                    -0.0026  0.3650 -0.0602 -0.1366 -0.6349
                                     0.6644
574. (0.00051) RY*( 2) H 30          s( 79.32%)p 0.26( 20.68%)
                                    -0.0081  0.8830 -0.1161 -0.2230  0.3152
                                    -0.2402
575. (0.00033) RY*( 3) H 30          s( 75.06%)p 0.33( 24.94%)
                                     0.0096  0.2351  0.8338  0.3750 -0.2499
                                    -0.2152
576. (0.00011) RY*( 4) H 30          s(  2.56%)p37.99( 97.44%)
                                     0.0057  0.0803  0.1385  0.4226  0.6167
                                     0.6446
577. (0.00002) RY*( 5) H 30          s( 29.43%)p 2.40( 70.57%)
578. (0.00050) RY*( 1) H 31          s(  5.39%)p17.56( 94.61%)
                                     0.0004  0.2079  0.1032 -0.6386 -0.6541
                                    -0.3323
579. (0.00037) RY*( 2) H 31          s( 85.18%)p 0.17( 14.82%)
                                     0.0054  0.9105  0.1506 -0.0369  0.3788
                                    -0.0582
580. (0.00025) RY*( 3) H 31          s( 79.12%)p 0.26( 20.88%)
                                     0.0110 -0.3052  0.8354 -0.2295  0.3511
                                    -0.1813
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581. (0.00004) RY*( 4) H 31            s(  0.42%)p99.99( 99.58%)
582. (0.00002) RY*( 5) H 31            s( 29.95%)p 2.34( 70.05%)
583. (0.00116) RY*( 1) H 32            s( 93.23%)p 0.07(  6.77%)
                                      -0.0084  0.9654 -0.0174 -0.1928  0.0660
                                       0.1616
584. (0.00054) RY*( 2) H 32            s( 98.81%)p 0.01(  1.19%)
                                       0.0001  0.0415  0.9932  0.0368 -0.0799
                                      -0.0646
585. (0.00034) RY*( 3) H 32            s(  0.35%)p99.99( 99.65%)
                                       0.0002  0.0253  0.0537  0.6179  0.7263
                                       0.2954
586. (0.00012) RY*( 4) H 32            s(  0.12%)p99.99( 99.88%)
                                      -0.0020 -0.0220  0.0259 -0.4349  0.6301
                                      -0.6423
587. (0.00003) RY*( 5) H 32            s(  7.57%)p12.21( 92.43%)
588. (0.00117) RY*( 1) H 33            s( 93.16%)p 0.07(  6.84%)
                                      -0.0085  0.9650 -0.0182  0.2359 -0.0602
                                      -0.0954
589. (0.00053) RY*( 2) H 33            s( 98.62%)p 0.01(  1.38%)
                                       0.0003  0.0442  0.9921 -0.0811  0.0846
                                       0.0034
590. (0.00034) RY*( 3) H 33            s(  0.40%)p99.99( 99.60%)
                                       0.0004  0.0282  0.0566 -0.0167 -0.7220
                                       0.6887
591. (0.00011) RY*( 4) H 33            s(  0.15%)p99.99( 99.85%)
                                      -0.0018 -0.0236  0.0303 -0.3422 -0.6431
                                      -0.6840
592. (0.00003) RY*( 5) H 33            s(  7.75%)p11.91( 92.25%)
593. (0.00062) RY*( 1) H 34            s(  0.05%)p99.99( 99.95%)
                                      -0.0005  0.0197 -0.0108  0.0257  0.6984
                                      -0.7149
594. (0.00046) RY*( 2) H 34            s( 91.32%)p 0.10(  8.68%)
                                      -0.0076  0.9363 -0.1913 -0.2335 -0.1382
                                      -0.1147
595. (0.00033) RY*( 3) H 34            s( 70.00%)p 0.43( 30.00%)
                                       0.0094  0.3291  0.7692  0.4280  0.2379
                                       0.2453
596. (0.00005) RY*( 4) H 34            s(  0.04%)p99.99( 99.96%)
597. (0.00001) RY*( 5) H 34            s( 38.62%)p 1.59( 61.38%)
598. (0.00051) RY*( 1) H 35            s(  0.09%)p99.99( 99.91%)
                                       0.0002  0.0295 -0.0076 -0.0353 -0.7036
                                       0.7091
599. (0.00037) RY*( 2) H 35            s( 98.94%)p 0.01(  1.06%)
                                      -0.0007  0.9939  0.0405 -0.0798  0.0626
                                       0.0172
600. (0.00028) RY*( 3) H 35            s( 51.63%)p 0.94( 48.37%)
                                       0.0132 -0.0723  0.7148 -0.0492  0.4883
                                       0.4928
601. (0.00005) RY*( 4) H 35            s(  1.76%)p55.92( 98.24%)
602. (0.00001) RY*( 5) H 35            s( 47.61%)p 1.10( 52.39%)
603. (0.00050) RY*( 1) H 36            s(  0.08%)p99.99( 99.92%)
                                       0.0001  0.0214 -0.0180  0.6433  0.7060
                                       0.2950
604. (0.00037) RY*( 2) H 36            s( 98.74%)p 0.01(  1.26%)
                                      -0.0004  0.9924  0.0505  0.0693 -0.0691
                                      -0.0545
605. (0.00028) RY*( 3) H 36            s( 52.15%)p 0.92( 47.85%)
                                       0.0132 -0.0902  0.7164  0.4538 -0.4791
                                       0.2073
606. (0.00005) RY*( 4) H 36            s(  1.76%)p55.87( 98.24%)
607. (0.00001) RY*( 5) H 36            s( 47.30%)p 1.11( 52.70%)
608. (0.00040) RY*( 1) H 37            s( 97.44%)p 0.03(  2.56%)
                                      -0.0050  0.9825 -0.0951  0.0976 -0.0998
                                      -0.0782
609. (0.00034) RY*( 2) H 37            s(  1.52%)p64.78( 98.48%)
                                       0.0014 -0.0158  0.1223 -0.6506 -0.7016
                                      -0.2632
610. (0.00030) RY*( 3) H 37            s( 57.75%)p 0.73( 42.25%)
                                       0.0117  0.1752  0.7394 -0.3792  0.3187
                                       0.4209
611. (0.00004) RY*( 4) H 37            s(  0.15%)p99.99( 99.85%)
612. (0.00001) RY*( 5) H 37            s( 43.18%)p 1.32( 56.82%)
613. (0.00044) RY*( 1) H 38            s( 98.07%)p 0.02(  1.93%)
                                      -0.0054  0.9868 -0.0833 -0.0168  0.0446
                                      -0.1306
614. (0.00036) RY*( 2) H 38            s(  0.35%)p99.99( 99.65%)
                                       0.0007 -0.0116  0.0577 -0.5928 -0.7440
                                      -0.3025
615. (0.00032) RY*( 3) H 38            s( 63.04%)p 0.59( 36.96%)
                                       0.0120  0.1455  0.7804  0.2348 -0.3169
                                       0.4626
616. (0.00009) RY*( 4) H 38            s(  8.23%)p11.16( 91.77%)
617. (0.00002) RY*( 5) H 38            s( 30.38%)p 2.29( 69.62%)
618. (0.00055) RY*( 1) H 39            s(  7.95%)p11.58( 92.05%)
                                      -0.0019  0.2765 -0.0554  0.6638  0.6574
                                       0.2182
619. (0.00051) RY*( 2) H 39            s( 86.04%)p 0.16( 13.96%)
                                      -0.0078  0.9212 -0.1087 -0.0563 -0.2493
                                      -0.2726
620. (0.00033) RY*( 3) H 39            s( 73.44%)p 0.36( 26.56%)
                                       0.0099  0.2183  0.8286 -0.3694  0.2738
                                       0.2328
621. (0.00011) RY*( 4) H 39            s(  2.63%)p36.97( 97.37%)
                                       0.0062  0.0793  0.1414  0.3517 -0.6069
                                       0.6940
622. (0.00002) RY*( 5) H 39            s( 30.00%)p 2.33( 70.00%)
623. (0.00061) RY*( 1) H 40            s(  0.04%)p99.99( 99.96%)
                                      -0.0004  0.0206 -0.0043 -0.6498 -0.6956
                                      -0.3057
624. (0.00046) RY*( 2) H 40            s( 91.36%)p 0.09(  8.64%)
                                      -0.0076  0.9364 -0.1915  0.0108  0.1337
                                      -0.2615
625. (0.00033) RY*( 3) H 40            s( 70.07%)p 0.43( 29.93%)
                                       0.0094  0.3287  0.7698  0.0119 -0.2252
                                       0.4985
626. (0.00005) RY*( 4) H 40            s(  0.03%)p99.99( 99.97%)
627. (0.00001) RY*( 5) H 40            s( 38.53%)p 1.60( 61.47%)
628. (0.00041) RY*( 1) H 41            s( 96.10%)p 0.04(  3.90%)
                                      -0.0058  0.9723 -0.1250 -0.1627  0.0805
                                       0.0778
629. (0.00035) RY*( 2) H 41            s(  0.64%)p99.99( 99.36%)
                                       0.0007  0.0107  0.0796  0.0217  0.7123
                                      -0.6969
630. (0.00031) RY*( 3) H 41            s( 60.43%)p 0.65( 39.57%)
                                       0.0112  0.2223  0.7448  0.5479 -0.2625
                                      -0.1628
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631. (0.00005) RY*( 4) H 41            s(  0.07%)p99.99( 99.93%)
632. (0.00001) RY*( 5) H 41            s( 42.79%)p 1.34( 57.21%)
633. (0.00048) RY*( 1) H 42            s(  5.22%)p18.17( 94.78%)
                                        0.0004  0.2105  0.0885 -0.0132  0.6520
                                       -0.7229
634. (0.00036) RY*( 2) H 42            s( 86.74%)p 0.15( 13.26%)
                                        0.0048  0.9208  0.1396 -0.0197 -0.3614
                                       -0.0404
635. (0.00024) RY*( 3) H 42            s( 77.24%)p 0.29( 22.76%)
                                        0.0114 -0.2829  0.8320 -0.0364 -0.3631
                                       -0.3073
636. (0.00004) RY*( 4) H 42            s(  0.79%)p99.99( 99.21%)
637. (0.00002) RY*( 5) H 42            s( 30.07%)p 2.33( 69.93%)
638. (0.00165) RY*( 1) H 43            s( 63.65%)p 0.57( 36.35%)
                                        0.0016  0.7896 -0.1139  0.3194 -0.2074
                                       -0.4674
639. (0.00113) RY*( 2) H 43            s( 42.22%)p 1.37( 57.78%)
                                       -0.0083  0.6080  0.2289 -0.3507  0.1919
                                        0.6465
640. (0.00054) RY*( 3) H 43            s(  1.05%)p94.16( 98.95%)
                                        0.0006  0.0368  0.0957  0.2219  0.9425
                                       -0.2278
641. (0.00042) RY*( 4) H 43            s( 61.19%)p 0.63( 38.81%)
                                        0.0043 -0.0159  0.7821 -0.4121 -0.0925
                                       -0.4580
642. (0.00012) RY*( 5) H 43            s( 31.90%)p 2.13( 68.10%)
                                       -0.0032 -0.0719  0.5602  0.7456 -0.1525
                                        0.3190
643. (0.00268) RY*( 1) O 44            s(  0.27%)p99.99( 98.73%)d 3.63(  0.99%)
                                        0.0000  0.0008  0.0495 -0.0167 -0.0015
                                        0.0015  0.0037  0.5904 -0.0443  0.0022
                                        0.6376 -0.0385  0.0048  0.4764 -0.0428
                                        0.0247 -0.0562  0.0030 -0.0385 -0.0684
644. (0.00195) RY*( 2) O 44            s(  0.01%)p 1.00( 99.34%)d 0.01(  0.65%)
                                        0.0000  0.0006  0.0080 -0.0002 -0.0006
                                       -0.0001  0.0045  0.7813 -0.0602 -0.0027
                                       -0.3429  0.0337 -0.0021 -0.5094  0.0340
                                        0.0312 -0.0537 -0.0011  0.0205  0.0471
645. (0.00097) RY*( 3) O 44            s( 77.78%)p 0.07(  5.26%)d 0.22( 16.96%)
                                        0.0000  0.0134  0.8718 -0.1324  0.0055
                                       -0.0034  0.0057 -0.0469 -0.0290 -0.0418
                                       -0.0004  0.1506  0.0420 -0.0501 -0.1444
                                        0.0172 -0.0563  0.3510  0.1806 -0.1013
646. (0.00020) RY*( 4) O 44            s(  2.60%)p33.44( 86.89%)d 4.05( 10.51%)
                                        0.0000  0.0334 -0.1039  0.1169  0.0175
                                       -0.0106  0.0059  0.1523 -0.0080 -0.0301
                                       -0.6340  0.0374  0.0309  0.6623 -0.0415
                                        0.0676 -0.0228  0.2788  0.1217 -0.0868
647. (0.00005) RY*( 5) O 44            s(  9.96%)p 1.07( 10.62%)d 7.98( 79.42%)
648. (0.00002) RY*( 6) O 44            s(  1.13%)p17.48( 19.75%)d70.03( 79.12%)
649. (0.00002) RY*( 7) O 44            s( 12.64%)p 3.38( 42.70%)d 3.53( 44.66%)
650. (0.00002) RY*( 8) O 44            s(  1.85%)p16.66( 30.83%)d36.38( 67.32%)
651. (0.00000) RY*( 9) O 44            s( 99.64%)p 0.00(  0.16%)d 0.00(  0.20%)
652. (0.00000) RY*(10) O 44            s(  4.07%)p13.91( 56.59%)d 9.67( 39.34%)
653. (0.00000) RY*(11) O 44            s( 85.92%)p 0.04(  3.41%)d 0.12( 10.67%)
654. (0.00001) RY*(12) O 44            s(  0.11%)p10.26(  1.18%)d99.99( 98.71%)
655. (0.00000) RY*(13) O 44            s(  0.16%)p99.99( 98.02%)d11.49(  1.82%)
656. (0.00000) RY*(14) O 44            s( 98.61%)p 0.00(  0.49%)d 0.01(  0.90%)
657. (0.00000) RY*(15) O 44            s(  5.33%)p 8.93( 47.61%)d 8.83( 47.06%)
658. (0.00499) RY*( 1) O 45            s( 26.86%)p 2.69( 72.26%)d 0.03(  0.88%)
                                        0.0000 -0.0198  0.5170 -0.0312  0.0015
                                       -0.0005  0.0153 -0.5643  0.0032 -0.0063
                                       -0.0458 -0.0003 -0.0009 -0.6338  0.0087
                                        0.0455 -0.0274 -0.0025 -0.0769  0.0049
659. (0.00420) RY*( 2) O 45            s(  1.14%)p86.01( 98.29%)d 0.50(  0.57%)
                                        0.0000 -0.0028  0.1067  0.0059  0.0022
                                        0.0003 -0.0072 -0.6719  0.0196 -0.0105
                                       -0.1901 -0.0036  0.0076  0.7030 -0.0184
                                        0.0244 -0.0063  0.0578 -0.0195  0.0364
660. (0.00345) RY*( 3) O 45            s(  0.43%)p99.99( 98.62%)d 2.19(  0.95%)
                                        0.0000 -0.0034  0.0657 -0.0028  0.0012
                                        0.0003  0.0099 -0.1487  0.0216  0.0170
                                        0.9742  0.0208 -0.0015  0.1164 -0.0131
                                       -0.0281 -0.0209 -0.0827 -0.0083  0.0371
661. (0.00130) RY*( 4) O 45            s( 68.96%)p 0.43( 29.56%)d 0.02(  1.47%)
                                        0.0000  0.0172  0.8299 -0.0240  0.0059
                                        0.0008 -0.0372  0.4493 -0.0484  0.0058
                                       -0.0222 -0.0036 -0.0242  0.2938 -0.0508
                                        0.0208 -0.0560  0.0067 -0.1046 -0.0137
662. (0.00013) RY*( 5) O 45            s(  0.00%)p 1.00(  2.78%)d34.94( 97.22%)
                                        0.0000 -0.0001  0.0010  0.0010  0.0013
                                        0.0002  0.0001  0.0233 -0.0160  0.0018
                                        0.1008 -0.1251 -0.0013 -0.0168  0.0303
                                        0.5515  0.0877  0.7700  0.1740 -0.1927
663. (0.00010) RY*( 6) O 45            s(  7.82%)p 0.17(  1.33%)d11.62( 90.85%)
664. (0.00008) RY*( 7) O 45            s(  2.95%)p 1.55(  4.56%)d31.39( 92.49%)
665. (0.00006) RY*( 8) O 45            s(  0.68%)p 1.21(  0.82%)d99.99( 98.49%)
666. (0.00004) RY*( 9) O 45            s(  1.17%)p 3.25(  3.79%)d81.55( 95.05%)
667. (0.00002) RY*(10) O 45            s( 33.91%)p 1.57( 53.31%)d 0.38( 12.78%)
668. (0.00001) RY*(11) O 45            s(  5.85%)p15.57( 91.02%)d 0.54(  3.13%)
669. (0.00002) RY*(12) O 45            s(  0.76%)p99.99( 95.86%)d 4.44(  3.38%)
670. (0.00000) RY*(13) O 45            s( 99.98%)p 0.00(  0.01%)d 0.00(  0.01%)
671. (0.00000) RY*(14) O 45            s( 49.97%)p 0.95( 47.70%)d 0.05(  2.33%)
672. (0.00000) RY*(15) O 45            s( 99.55%)p 0.00(  0.40%)d 0.00(  0.05%)
673. (0.00272) RY*( 1) O 46            s(  0.06%)p99.99( 98.15%)d31.35(  1.79%)
                                        0.0000 -0.0008  0.0234 -0.0049  0.0012
                                        0.0000 -0.0001 -0.0256  0.0090 -0.0030
                                       -0.6248  0.0368  0.0056  0.7653 -0.0579
                                       -0.0503  0.1063 -0.0073 -0.0342 -0.0538
674. (0.00198) RY*( 2) O 46            s(  3.13%)p30.48( 95.38%)d 0.48(  1.49%)
                                        0.0000  0.0004  0.1747 -0.0277  0.0005
                                        0.0006 -0.0137 -0.5949  0.0682 -0.0001
                                       -0.5850  0.0221 -0.0026 -0.5017  0.0252
                                        0.0019  0.0061  0.0083 -0.0879  0.0842
675. (0.00131) RY*( 3) O 46            s( 78.05%)p 0.11(  8.78%)d 0.17( 13.17%)
                                        0.0000  0.0104  0.8757 -0.1164  0.0034
                                       -0.0025 -0.0436  0.2258  0.1165  0.0280
                                        0.0624 -0.1071  0.0216  0.0178 -0.0663
                                        0.2422  0.2054 -0.0922 -0.1149  0.0956
676. (0.00021) RY*( 4) O 46            s(  0.99%)p83.14( 82.14%)d17.07( 16.87%)
                                        0.0000  0.0345 -0.0341  0.0846  0.0161
                                       -0.0100 -0.0408 -0.7013  0.0635  0.0241
                                        0.4573 -0.0272  0.0186  0.3350 -0.0300
                                        0.2758  0.2191 -0.0934 -0.1689  0.0857
677. (0.00006) RY*( 5) O 46            s(  8.37%)p 1.05(  8.82%)d 9.89( 82.81%)
678. (0.00004) RY*( 6) O 46            s(  1.70%)p 2.47(  4.19%)d55.45( 94.11%)
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679. (0.00002) RY*( 7) O 46            s(  1.97%)p17.23( 33.87%)d32.64( 64.17%)
680. (0.00003) RY*( 8) O 46            s(  1.99%)p 5.36( 10.68%)d43.78( 87.32%)
681. (0.00002) RY*( 9) O 46            s(  3.90%)p 4.47( 17.44%)d20.17( 78.66%)
682. (0.00000) RY*(10) O 46            s(  0.64%)p99.99( 93.73%)d 8.78(  5.63%)
683. (0.00000) RY*(11) O 46            s( 95.27%)p 0.02(  1.59%)d 0.03(  3.14%)
684. (0.00001) RY*(12) O 46            s(  3.24%)p19.63( 63.65%)d10.21( 33.11%)
685. (0.00000) RY*(13) O 46            s( 99.53%)p 0.00(  0.15%)d 0.00(  0.32%)
686. (0.00000) RY*(14) O 46            s(  1.36%)p60.91( 83.03%)d11.45( 15.61%)
687. (0.00000) RY*(15) O 46            s( 99.87%)p 0.00(  0.04%)d 0.00(  0.09%)
688. (0.00268) RY*( 1) O 47            s(  0.28%)p99.99( 98.71%)d 3.62(  1.01%)
                                        0.0000  0.0008  0.0501 -0.0167 -0.0015
                                        0.0014  0.0022  0.1613 -0.0189 -0.0023
                                       -0.6461  0.0382  0.0058  0.7337 -0.0578
                                        0.0127 -0.0645 -0.0249 -0.0465 -0.0546
689. (0.00193) RY*( 2) O 47            s(  0.00%)p 1.00( 99.38%)d 0.01(  0.61%)
                                        0.0000  0.0001  0.0055 -0.0006 -0.0007
                                        0.0001 -0.0039 -0.8077  0.0585  0.0021
                                        0.3351 -0.0334  0.0030  0.4723 -0.0389
                                        0.0161 -0.0028 -0.0268  0.0624 -0.0354
690. (0.00097) RY*( 3) O 47            s( 77.50%)p 0.07(  5.26%)d 0.22( 17.23%)
                                        0.0000  0.0136  0.8702 -0.1328  0.0054
                                       -0.0034  0.0354 -0.0248 -0.1161  0.0416
                                        0.0047 -0.1503  0.0244 -0.0609 -0.0930
                                       -0.3066 -0.1812 -0.1779  0.0587  0.1021
691. (0.00020) RY*( 4) O 47            s(  2.66%)p32.77( 87.14%)d 3.84( 10.20%)
                                        0.0000  0.0332 -0.1060  0.1176  0.0175
                                       -0.0106  0.0252  0.5206 -0.0337  0.0295
                                        0.6311 -0.0348  0.0189  0.4441 -0.0252
                                       -0.2156 -0.1226 -0.1820  0.0157  0.0844
692. (0.00005) RY*( 5) O 47            s( 10.39%)p 1.00( 10.42%)d 7.62( 79.19%)
693. (0.00002) RY*( 6) O 47            s(  9.88%)p 4.30( 42.46%)d 4.83( 47.66%)
694. (0.00002) RY*( 7) O 47            s(  2.28%)p 2.35(  5.36%)d40.56( 92.37%)
695. (0.00002) RY*( 8) O 47            s(  2.01%)p23.42( 47.01%)d25.40( 50.98%)
696. (0.00000) RY*( 9) O 47            s( 99.74%)p 0.00(  0.17%)d 0.00(  0.09%)
697. (0.00000) RY*(10) O 47            s(  1.35%)p56.86( 76.91%)d16.07( 21.74%)
698. (0.00000) RY*(11) O 47            s( 88.80%)p 0.04(  3.90%)d 0.08(  7.30%)
699. (0.00001) RY*(12) O 47            s(  0.90%)p 1.34(  1.21%)d99.99( 97.88%)
700. (0.00000) RY*(13) O 47            s(  1.94%)p34.94( 67.65%)d15.71( 30.41%)
701. (0.00000) RY*(14) O 47            s( 98.99%)p 0.01(  0.54%)d 0.00(  0.47%)
702. (0.00001) RY*(15) O 47            s(  3.38%)p16.42( 55.46%)d12.19( 41.16%)
703. (0.00289) RY*( 1) O 48            s(  0.13%)p99.99( 97.90%)d14.95(  1.96%)
                                        0.0000 -0.0001  0.0359 -0.0044  0.0020
                                       -0.0004  0.0060  0.6872 -0.0565  0.0025
                                        0.6040 -0.0336  0.0024  0.3704 -0.0195
                                       -0.0127  0.0425  0.0489 -0.1059  0.0638
704. (0.00205) RY*( 2) O 48            s(  3.01%)p31.72( 95.47%)d 0.51(  1.52%)
                                        0.0000  0.0002  0.1714 -0.0268  0.0006
                                        0.0005  0.0041 -0.1603 -0.0107  0.0014
                                        0.6206 -0.0225 -0.0138 -0.7337  0.0689
                                       -0.0115  0.1011  0.0022 -0.0070 -0.0695
705. (0.00134) RY*( 3) O 48            s( 77.29%)p 0.13(  9.78%)d 0.17( 12.93%)
                                        0.0000  0.0095  0.8717 -0.1141  0.0033
                                       -0.0024  0.0399 -0.1265 -0.1107 -0.0261
                                       -0.0643  0.1065 -0.0283  0.2130  0.0753
                                        0.1822  0.2396 -0.1615 -0.0999  0.0511
706. (0.00022) RY*( 4) O 48            s(  0.72%)p99.99( 82.26%)d23.64( 17.02%)
                                        0.0000  0.0347 -0.0026  0.0753  0.0153
                                       -0.0094  0.0360  0.6252 -0.0596 -0.0250
                                       -0.4411  0.0277 -0.0283 -0.4777  0.0432
                                        0.2159  0.2551 -0.2062 -0.1253  0.0183
707. (0.00006) RY*( 5) O 48            s(  8.35%)p 1.03(  8.63%)d 9.94( 83.01%)
708. (0.00003) RY*( 6) O 48            s(  5.60%)p 1.40(  7.81%)d15.47( 86.59%)
709. (0.00004) RY*( 7) O 48            s(  0.06%)p24.78(  1.39%)d99.99( 98.56%)
710. (0.00002) RY*( 8) O 48            s(  0.03%)p99.99(  4.58%)d99.99( 95.40%)
711. (0.00001) RY*( 9) O 48            s(  1.65%)p 1.77(  2.92%)d57.72( 95.42%)
712. (0.00000) RY*(10) O 48            s(  1.27%)p77.05( 97.98%)d 0.59(  0.75%)
713. (0.00000) RY*(11) O 48            s( 98.69%)p 0.00(  0.42%)d 0.01(  0.89%)
714. (0.00001) RY*(12) O 48            s(  2.00%)p48.22( 96.52%)d 0.74(  1.48%)
715. (0.00000) RY*(13) O 48            s( 99.93%)p 0.00(  0.03%)d 0.00(  0.04%)
716. (0.00000) RY*(14) O 48            s(  1.36%)p70.31( 95.95%)d 1.96(  2.68%)
717. (0.00000) RY*(15) O 48            s( 99.97%)p 0.00(  0.00%)d 0.00(  0.02%)
718. (0.01012) RY*( 1) N 49            s(  3.09%)p30.73( 94.95%)d 0.64(  1.96%)
                                        0.0000  0.0220  0.1676  0.0479 -0.0044
                                        0.0009 -0.0413 -0.9086  0.0080  0.0199
                                        0.1394  0.0091  0.0243  0.3186  0.0077
                                        0.0991  0.0905  0.0230 -0.0282  0.0177
719. (0.00673) RY*( 2) N 49            s(  0.41%)p99.99( 99.38%)d 0.53(  0.22%)
                                        0.0000 -0.0023  0.0554 -0.0314 -0.0052
                                        0.0021 -0.0016  0.1509  0.0048  0.0218
                                       -0.6807 -0.0009 -0.0265  0.7115 -0.0133
                                       -0.0226 -0.0030  0.0155  0.0198  0.0318
720. (0.00501) RY*( 3) N 49            s(  4.17%)p22.37( 93.39%)d 0.58(  2.43%)
                                        0.0000  0.0080  0.1963  0.0561 -0.0018
                                        0.0001 -0.0237  0.3472 -0.0321 -0.0083
                                        0.6942 -0.0010 -0.0050  0.5743 -0.0006
                                       -0.0361 -0.0316  0.0834 -0.0974  0.0746
721. (0.00202) RY*( 4) N 49            s( 90.89%)p 0.08(  7.18%)d 0.02(  1.93%)
                                        0.0000 -0.0140  0.9523 -0.0339 -0.0256
                                        0.0049 -0.0211  0.0653 -0.0563  0.0173
                                       -0.1277  0.0085  0.0257 -0.2156 -0.0081
                                       -0.0225 -0.1171  0.0365  0.0594  0.0144
722. (0.00049) RY*( 5) N 49            s(  0.12%)p 3.56(  0.42%)d99.99( 99.46%)
                                        0.0000 -0.0001 -0.0204  0.0272  0.0055
                                       -0.0012  0.0025 -0.0101 -0.0217  0.0014
                                        0.0161 -0.0007  0.0016 -0.0348 -0.0466
                                       -0.2071  0.2422 -0.0344  0.4563  0.8268
723. (0.00031) RY*( 6) N 49            s(  1.98%)p 1.67(  3.31%)d47.78( 94.71%)
                                        0.0000 -0.0022  0.0638  0.1241  0.0181
                                       -0.0046 -0.0025 -0.0041 -0.0481  0.0225
                                       -0.0128 -0.1236 -0.0179 -0.0154  0.1193
                                       -0.6813  0.6126  0.1011 -0.0727 -0.3035
724. (0.00032) RY*( 7) N 49            s(  0.94%)p32.13( 30.21%)d73.23( 68.85%)
                                        0.0000 -0.0026 -0.0625  0.0741  0.0010
                                        0.0012  0.0227 -0.0839 -0.1731  0.0257
                                       -0.0758 -0.3410  0.0268 -0.0701 -0.3692
                                       -0.2876 -0.3240  0.3892 -0.5146  0.2908
725. (0.00014) RY*( 8) N 49            s( 74.01%)p 0.09(  6.85%)d 0.26( 19.14%)
                                        0.0000  0.0116 -0.0072  0.8600 -0.0163
                                        0.0101  0.0061 -0.0067 -0.2248 -0.0039
                                       -0.0450  0.1168 -0.0027  0.0028  0.0464
                                       -0.1003 -0.2346 -0.3542  0.0242 -0.0151
726. (0.00012) RY*( 9) N 49            s(  1.18%)p42.47( 50.00%)d41.47( 48.82%)
                                        0.0000  0.0016 -0.0184  0.1051  0.0115
                                        0.0157 -0.0104 -0.0540  0.6225 -0.0002
                                        0.0568 -0.2281  0.0006  0.0470 -0.2280
                                       -0.2871 -0.3609  0.1107  0.4644 -0.2183
```

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727. (0.00008) RY*(10) N 49            s( 22.46%)p 0.41(  9.24%)d 3.04( 68.30%)
728. (0.00004) RY*(11) N 49            s(  0.55%)p99.99( 58.74%)d74.62( 40.72%)
729. (0.00005) RY*(12) N 49            s(  0.78%)p66.14( 51.56%)d61.13( 47.66%)
730. (0.00002) RY*(13) N 49            s(  1.45%)p64.70( 93.91%)d 3.20(  4.64%)
731. (0.00000) RY*(14) N 49            s( 99.50%)p 0.00(  0.23%)d 0.00(  0.28%)
732. (0.00000) RY*(15) N 49            s( 98.45%)p 0.01(  1.10%)d 0.00(  0.45%)
733. (0.01050) RY*( 1) N 50            s(  3.19%)p29.82( 95.04%)d 0.56(  1.78%)
                                        0.0000  0.0216  0.1734  0.0362 -0.0048
                                        0.0014  0.0426  0.6799  0.0011 -0.0218
                                       -0.1521 -0.0072 -0.0232 -0.6797  0.0103
                                        0.0253  0.0730 -0.0908 -0.0392  0.0450
734. (0.00662) RY*( 2) N 50            s(  0.32%)p99.99( 99.54%)d 0.46(  0.15%)
                                        0.0000 -0.0023  0.0442 -0.0345 -0.0047
                                        0.0021 -0.0225  0.5609 -0.0147 -0.0228
                                        0.7160  0.0008 -0.0128  0.4082  0.0014
                                       -0.0170  0.0108  0.0096  0.0294  0.0101
735. (0.00490) RY*( 3) N 50            s(  4.36%)p21.36( 93.04%)d 0.60(  2.60%)
                                        0.0000  0.0085  0.1993  0.0612 -0.0029
                                        0.0002  0.0064  0.3895  0.0156  0.0065
                                       -0.6534 -0.0004 -0.0250  0.5916 -0.0295
                                       -0.0895  0.0839 -0.0171  0.0058 -0.1031
736. (0.00190) RY*( 4) N 50            s( 90.45%)p 0.08(  7.50%)d 0.02(  2.06%)
                                        0.0000 -0.0144  0.9501 -0.0293 -0.0244
                                        0.0054  0.0326 -0.2259  0.0113 -0.0188
                                        0.1331 -0.0005 -0.0048 -0.0334 -0.0598
                                       -0.0509 -0.0730  0.0078  0.0951 -0.0594
737. (0.00048) RY*( 5) N 50            s(  0.18%)p 3.43(  0.61%)d99.99( 99.22%)
                                        0.0000 -0.0002 -0.0208  0.0362  0.0052
                                       -0.0011 -0.0003 -0.0265 -0.0340 -0.0037
                                       -0.0094  0.0190  0.0042 -0.0264 -0.0551
                                       -0.0947  0.5617  0.2699  0.6964  0.3314
738. (0.00032) RY*( 6) N 50            s(  0.63%)p16.85( 10.65%)d99.99( 88.72%)
                                        0.0000 -0.0032  0.0126  0.0763  0.0178
                                       -0.0031 -0.0063 -0.0170 -0.0300 -0.0333
                                        0.0442  0.2808  0.0084 -0.0594 -0.1405
                                       -0.5960  0.2288  0.4925 -0.4868  0.0080
739. (0.00032) RY*( 7) N 50            s(  1.20%)p18.86( 22.59%)d63.63( 76.21%)
                                        0.0000  0.0018  0.1026  0.0368  0.0088
                                       -0.0035 -0.0190  0.0149  0.2969  0.0095
                                       -0.0557 -0.2262 -0.0338  0.0854  0.2726
                                        0.2071 -0.1345  0.2634 -0.2738  0.7461
740. (0.00014) RY*( 8) N 50            s( 87.12%)p 0.03(  2.95%)d 0.11(  9.94%)
                                        0.0000  0.0069 -0.0122  0.9332 -0.0047
                                        0.0060 -0.0030  0.0029  0.0571  0.0018
                                        0.0541 -0.0330  0.0032 -0.0135 -0.1482
                                        0.1374 -0.1750  0.1694  0.0915 -0.1132
741. (0.00011) RY*( 9) N 50            s(  0.07%)p99.99( 54.37%)d99.99( 45.56%)
                                        0.0000  0.0017 -0.0152  0.0022  0.0135
                                        0.0163  0.0060  0.0680 -0.4948  0.0002
                                       -0.0661  0.2421 -0.0100 -0.0182  0.4805
                                       -0.2359 -0.5237  0.2033  0.2752  0.0925
742. (0.00008) RY*(10) N 50            s( 10.54%)p 0.83(  8.77%)d 7.65( 80.68%)
743. (0.00005) RY*(11) N 50            s(  2.11%)p19.93( 42.00%)d26.52( 55.89%)
744. (0.00005) RY*(12) N 50            s(  0.56%)p99.99( 68.85%)d54.70( 30.59%)
745. (0.00002) RY*(13) N 50            s(  1.33%)p69.92( 93.29%)d 4.03(  5.37%)
746. (0.00000) RY*(14) N 50            s( 99.48%)p 0.00(  0.22%)d 0.00(  0.30%)
747. (0.00000) RY*(15) N 50            s( 98.45%)p 0.01(  1.06%)d 0.00(  0.49%)
748. (0.00794) RY*( 1)Ru 51            s( 46.47%)p 0.45( 21.14%)d 0.70( 32.39%)
                                        0.0000  0.0000  0.0000  0.0000 -0.0283
                                        0.6785 -0.0586 -0.0025  0.0071  0.0033
                                       -0.0035  0.0011 -0.0006 -0.0002 -0.0002
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000 -0.2298 -0.1193  0.0249 -0.0004
                                        0.0000  0.0000  0.0000  0.0000  0.1623
                                        0.2463 -0.0421 -0.0005  0.0000  0.0000
                                        0.0000  0.0000 -0.1138 -0.2031 -0.0279
                                        0.0021 -0.0001  0.0000  0.0059  0.0649
                                       -0.0474 -0.0040  0.0000  0.0000  0.0080
                                       -0.0289  0.0224  0.0061  0.0001  0.0000
                                        0.0051  0.3426 -0.1321 -0.0180 -0.0006
                                        0.0000  0.0020  0.0990 -0.0294 -0.0110
                                       -0.0001  0.0000  0.0114  0.3902  0.1324
                                        0.0040  0.0004
749. (0.00722) RY*( 2)Ru 51            s(  0.11%)p19.17(  2.14%)d99.99( 97.74%)
                                        0.0000  0.0000  0.0000  0.0000 -0.0035
                                        0.0240  0.0129 -0.0070 -0.0172  0.0004
                                       -0.0043  0.0008 -0.0002 -0.0001 -0.0001
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000  0.0128 -0.0871  0.0112 -0.0010
                                        0.0000  0.0000  0.0000  0.0000  0.0582
                                       -0.0277  0.0037 -0.0006  0.0000  0.0000
                                        0.0000  0.0000 -0.0736 -0.0625  0.0074
                                        0.0001  0.0000  0.0000  0.0022  0.5704
                                        0.0325 -0.0050  0.0001  0.0000 -0.0027
                                        0.0597  0.0023  0.0015  0.0000  0.0000
                                        0.0037 -0.4245 -0.0588 -0.0075  0.0003
                                        0.0000  0.0020  0.6801  0.0090  0.0014
                                       -0.0004  0.0000 -0.0005 -0.0293  0.0111
                                       -0.0004  0.0002
750. (0.00563) RY*( 3)Ru 51            s( 11.22%)p 1.03( 11.53%)d 6.88( 77.25%)
                                        0.0000  0.0000  0.0000  0.0000 -0.0276
                                        0.3306  0.0262 -0.0339 -0.0146 -0.0045
                                        0.0094 -0.0003 -0.0001  0.0001  0.0000
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000  0.0175 -0.0311  0.0390 -0.0020
                                        0.0002  0.0000  0.0000  0.0000  0.2623
                                        0.1390 -0.0324  0.0026 -0.0001  0.0000
                                        0.0000  0.0000  0.1506 -0.0243 -0.0090
                                       -0.0008  0.0001  0.0000  0.0059 -0.6528
                                       -0.0068  0.0025  0.0001  0.0000  0.0085
                                        0.0345 -0.0203 -0.0007  0.0002  0.0000
                                       -0.0010 -0.4621 -0.0174 -0.0006  0.0000
                                        0.0000 -0.0008  0.2226 -0.0016 -0.0049
                                        0.0002  0.0000 -0.0089 -0.2844 -0.0149
                                        0.0000 -0.0001
751. (0.00456) RY*( 4)Ru 51            s(  0.27%)p68.21( 18.39%)d99.99( 81.34%)
                                        0.0000  0.0000  0.0000  0.0000  0.0163
                                        0.0353  0.0256 -0.0144 -0.0125  0.0030
                                       -0.0125  0.0016 -0.0004 -0.0002 -0.0001
                                        0.0000  0.0000  0.0000  0.0000  0.0000
                                        0.0000 -0.2658 -0.0695 -0.0093  0.0007
                                        0.0000  0.0000  0.0000  0.0000  0.0831
                                       -0.1176  0.0181 -0.0013 -0.0001  0.0000
                                        0.0000  0.0000  0.2595 -0.1411  0.0012
                                        0.0010  0.0000  0.0000 -0.0079  0.1094
                                       -0.0279 -0.0137  0.0003  0.0000  0.0041
```

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                                    0.5858  0.0271 -0.0065  0.0004  0.0000
                                    0.0012  0.3825 -0.0392 -0.0165 -0.0003
                                    0.0000 -0.0002  0.0666 -0.0346  0.0014
                                   -0.0006  0.0000 -0.0111 -0.5492  0.0314
                                    0.0048  0.0000
752. (0.00420) RY*( 5)Ru 51         s(  5.31%)p10.90( 57.91%)d 6.92( 36.77%)
                                    0.0000  0.0000  0.0000  0.0000  0.0030
                                    0.0739  0.2157 -0.0243  0.0210  0.0101
                                    0.0018 -0.0016  0.0013 -0.0001  0.0003
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.2099 -0.0086 -0.0208  0.0001
                                   -0.0001  0.0000  0.0000  0.0000  0.6865
                                   -0.2354  0.0045  0.0020  0.0000  0.0000
                                    0.0000  0.0000  0.0295  0.0789  0.0289
                                   -0.0014 -0.0001  0.0000 -0.0057  0.2854
                                    0.0493 -0.0007  0.0007  0.0000 -0.0120
                                   -0.0536 -0.0116 -0.0022  0.0002  0.0000
                                    0.0108 -0.2601  0.0323  0.0148  0.0007
                                    0.0000  0.0067 -0.4558 -0.0195  0.0070
                                    0.0004  0.0000 -0.0084  0.0221 -0.0530
                                   -0.0025 -0.0002
753. (0.00393) RY*( 6)Ru 51         s(  0.12%)p99.99( 60.45%)d99.99( 39.44%)
                                    0.0000  0.0000  0.0000  0.0000  0.0100
                                    0.0224 -0.0179 -0.0125 -0.0095 -0.0009
                                   -0.0018 -0.0009  0.0005  0.0005  0.0001
                                    0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.0368 -0.1112  0.0440 -0.0026
                                    0.0001  0.0000  0.0000  0.0000 -0.0053
                                    0.0182  0.0238 -0.0014  0.0001  0.0000
                                    0.0000  0.0000  0.7666  0.0073 -0.0146
                                    0.0022 -0.0001  0.0000  0.0108  0.1306
                                   -0.0113  0.0007 -0.0001  0.0000  0.0001
                                   -0.5741 -0.0504  0.0031  0.0003  0.0000
                                   -0.0140  0.1545  0.0258 -0.0013 -0.0014
                                    0.0000 -0.0141  0.1069  0.0116 -0.0079
                                   -0.0004  0.0000  0.0004 -0.0836 -0.0360
                                    0.0009  0.0003
754. (0.00310) RY*( 7)Ru 51         s(  5.20%)p14.34( 74.63%)d 3.88( 20.17%)
                                    0.0000  0.0000  0.0000  0.0000  0.0173
                                    0.1558 -0.1544  0.0463 -0.0314  0.0209
                                   -0.0083 -0.0002  0.0007  0.0002  0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.7652 -0.0200 -0.0029  0.0004
                                    0.0000  0.0000  0.0000  0.0000  0.0885
                                    0.1742  0.0649 -0.0058  0.0003  0.0000
                                    0.0000  0.0000  0.1670 -0.2997  0.0143
                                   -0.0007  0.0001  0.0000 -0.0024  0.2054
                                   -0.0031 -0.0001 -0.0010  0.0000 -0.0091
                                    0.1568  0.1096 -0.0004 -0.0007  0.0000
                                    0.0100 -0.0679 -0.1633 -0.0126 -0.0002
                                    0.0000  0.0028 -0.2777 -0.0242 -0.0055
                                    0.0002  0.0000 -0.0012 -0.0792  0.0851
                                    0.0012  0.0003
755. (0.00270) RY*( 8)Ru 51         s( 10.74%)p 2.29( 24.60%)d 6.02( 64.65%)
                                    0.0000  0.0000  0.0000  0.0000 -0.0108
                                    0.3249 -0.0077  0.0390  0.0125  0.0009
                                   -0.0047  0.0002  0.0001  0.0002  0.0001
                                   -0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.0287 -0.0963  0.0468 -0.0009
                                    0.0000  0.0000  0.0000  0.0000 -0.2396
                                    0.0220 -0.0329  0.0003 -0.0001  0.0000
                                    0.0000  0.0000 -0.4074  0.0861 -0.0365
                                    0.0011 -0.0001  0.0000  0.0048  0.1821
                                   -0.0183 -0.0032 -0.0003  0.0000  0.0009
                                   -0.4066 -0.0501  0.0005 -0.0002  0.0000
                                   -0.0070 -0.0090 -0.0538  0.0021  0.0001
                                    0.0000 -0.0087 -0.1897 -0.0707  0.0043
                                   -0.0001  0.0000 -0.0095 -0.6331 -0.0127
                                    0.0003  0.0002
756. (0.00220) RY*( 9)Ru 51         s(  4.93%)p10.64( 52.50%)d 8.63( 42.57%)
                                    0.0000  0.0000  0.0000  0.0000 -0.0241
                                    0.1784 -0.0971  0.0771  0.0369 -0.0080
                                    0.0093 -0.0035  0.0012 -0.0002  0.0004
                                   -0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.3796  0.1330 -0.0912  0.0009
                                   -0.0001  0.0000  0.0000  0.0000 -0.4897
                                    0.1778 -0.0040  0.0017 -0.0001  0.0000
                                    0.0000  0.0000  0.2868 -0.0330 -0.0067
                                    0.0008 -0.0001  0.0000 -0.0128  0.1468
                                    0.0094  0.0162  0.0000  0.0000 -0.0168
                                    0.2048  0.1509  0.0118  0.0003  0.0000
                                    0.0142 -0.4633 -0.0306  0.0152  0.0006
                                    0.0000  0.0235 -0.3295 -0.0374  0.0068
                                    0.0004  0.0000 -0.0023  0.1011  0.0407
                                   -0.0082 -0.0004
757. (0.00126) RY*(10)Ru 51         s( 26.07%)p 2.27( 59.14%)d 0.57( 14.79%)
                                    0.0000  0.0000  0.0000  0.0000 -0.0084
                                    0.3880  0.3303  0.0085 -0.0252 -0.0173
                                   -0.0017 -0.0005  0.0011  0.0012  0.0004
                                    0.0001  0.0000  0.0000  0.0000  0.0000
                                    0.0000  0.2564 -0.3218  0.1187 -0.0003
                                   -0.0001  0.0000  0.0000  0.0000 -0.2784
                                   -0.4953 -0.0470  0.0046 -0.0002  0.0000
                                    0.0000  0.0000  0.1089  0.2658 -0.0219
                                   -0.0050  0.0002  0.0000  0.0043 -0.0179
                                    0.0383 -0.0206  0.0005  0.0000  0.0049
                                    0.1786 -0.0208 -0.0239 -0.0005  0.0000
                                    0.0031 -0.0116  0.2897  0.0292  0.0019
                                    0.0000 -0.0063 -0.0071  0.0657  0.0260
                                    0.0000  0.0000  0.0017  0.1507  0.0008
                                   -0.0031 -0.0012
758. (0.00077) RY*(11)Ru 51         s(  6.85%)p 8.05( 55.15%)d 5.55( 38.00%)
                                    0.0000  0.0000  0.0000  0.0000  0.0015
                                   -0.1022  0.2267  0.0675 -0.0249  0.0257
                                   -0.0281  0.0013  0.0005 -0.0010 -0.0002
                                    0.0003  0.0000  0.0000  0.0000  0.0000
                                    0.0000 -0.0869 -0.1715 -0.0166 -0.0050
                                    0.0003  0.0000  0.0000  0.0000 -0.1481
                                   -0.3994  0.1292 -0.0009  0.0001  0.0000
                                    0.0000  0.0000 -0.0329 -0.5308  0.1822
                                   -0.0051  0.0003  0.0000  0.0084 -0.1407
                                   -0.2881 -0.0188  0.0006  0.0000  0.0008
                                   -0.1203 -0.1551 -0.0096  0.0001  0.0000
                                    0.0108 -0.1052 -0.4358 -0.0296 -0.0005
                                    0.0000 -0.0052 -0.0359 -0.1617 -0.0130
                                   -0.0009  0.0000 -0.0034  0.0751  0.0513
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                                0.0180 -0.0003
759. (0.00053) RY*(12)Ru 51     s( 14.79%)p 4.77( 70.59%)d 0.99( 14.61%)
                                0.0000  0.0000  0.0000  0.0000  0.0115
                                0.2245  0.2520  0.1647 -0.0774 -0.0261
                                0.0063 -0.0072  0.0013 -0.0010  0.0004
                               -0.0002  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0682  0.7239 -0.2477 -0.0033
                                0.0005  0.0000  0.0000  0.0000 -0.0367
                               -0.1474  0.0366  0.0079 -0.0004  0.0000
                                0.0000  0.0000  0.0061 -0.2736  0.1280
                                0.0118 -0.0007  0.0000 -0.0066  0.0276
                                0.0702  0.0164  0.0016  0.0000 -0.0028
                               -0.0839 -0.0995  0.0274  0.0019  0.0000
                               -0.0004  0.0773  0.2729 -0.0545  0.0008
                                0.0000 -0.0002  0.1035  0.1334 -0.0159
                               -0.0001  0.0000 -0.0014 -0.0538 -0.0845
                                0.0164 -0.0010
760. (0.00036) RY*(13)Ru 51     s( 75.06%)p 0.14( 10.77%)d 0.19( 14.17%)
                                0.0000  0.0000  0.0000  0.0000  0.0035
                               -0.0439  0.1887  0.8442  0.0086  0.0114
                               -0.0036  0.0107 -0.0056 -0.0006 -0.0018
                                0.0004  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0059 -0.0949  0.1477  0.0041
                               -0.0001  0.0000  0.0000  0.0000  0.0453
                                0.2351 -0.0079  0.0072 -0.0003  0.0000
                                0.0000  0.0000  0.0245  0.1366 -0.0081
                               -0.0070  0.0005  0.0000 -0.0014  0.0147
                               -0.0312 -0.0226  0.0008  0.0000 -0.0001
                                0.0842 -0.1809 -0.0202 -0.0006  0.0000
                               -0.0020  0.0315 -0.1148 -0.0089  0.0020
                                0.0000  0.0021  0.0109  0.0005  0.0017
                               -0.0002  0.0000  0.0026  0.0244 -0.2910
                               -0.0088 -0.0006
761. (0.00029) RY*(14)Ru 51     s(  2.87%)p 9.70( 27.88%)d24.10( 69.25%)
                                0.0000  0.0000  0.0000  0.0000  0.0071
                               -0.0199  0.1561 -0.0382 -0.0369  0.0068
                                0.0283 -0.0150  0.0054  0.0014  0.0016
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0054 -0.2390 -0.2843 -0.0076
                                0.0005  0.0000  0.0000  0.0000  0.0052
                                0.1755  0.2105  0.0010  0.0001  0.0000
                                0.0000  0.0000 -0.0556 -0.1064  0.2262
                                0.0064 -0.0002  0.0000  0.0044 -0.0144
                               -0.1123 -0.0144 -0.0001  0.0000  0.0004
                               -0.0390  0.4547  0.0169  0.0010  0.0000
                                0.0005  0.0332  0.3427 -0.0407 -0.0002
                                0.0000  0.0011  0.0395 -0.4232 -0.0143
                               -0.0017  0.0000  0.0009  0.0032 -0.4115
                                0.0214  0.0000
762. (0.00022) RY*(15)Ru 51     s( 11.55%)p 1.43( 16.55%)d 6.22( 71.89%)
                                0.0000  0.0000  0.0000  0.0000  0.0025
                                0.0537  0.2193 -0.1753  0.1526  0.0873
                                0.0538 -0.0050  0.0017 -0.0004  0.0002
                               -0.0002  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0760  0.0989 -0.2160 -0.0040
                                0.0000  0.0000  0.0000  0.0000 -0.0067
                                0.0814 -0.1645  0.0129 -0.0004  0.0000
                                0.0000  0.0000  0.0329  0.2606  0.0211
                               -0.0013  0.0001  0.0000 -0.0046  0.0484
                               -0.5900  0.0702 -0.0007  0.0000 -0.0024
                                0.0307  0.1908  0.0453  0.0011  0.0000
                               -0.0057  0.0395 -0.3140  0.0641  0.0003
                                0.0000 -0.0009  0.0240  0.4012  0.0094
                               -0.0002  0.0000  0.0014 -0.0156 -0.2388
                               -0.0311  0.0011
763. (0.00018) RY*(16)Ru 51     s( 15.84%)p 1.22( 19.38%)d 4.09( 64.78%)
                                0.0000  0.0000  0.0000  0.0000  0.0059
                                0.0114  0.3603 -0.1398 -0.0861 -0.0316
                               -0.0162  0.0105 -0.0080 -0.0007 -0.0020
                               -0.0005 -0.0001 -0.0001  0.0000  0.0000
                                0.0000  0.0679  0.1962  0.0250  0.0106
                               -0.0001  0.0000  0.0000  0.0000 -0.0565
                                0.0408 -0.2919  0.0162 -0.0009  0.0000
                                0.0000  0.0000  0.0623  0.2119  0.1039
                               -0.0066  0.0004  0.0000  0.0004 -0.0152
                                0.4551  0.0246 -0.0013  0.0000  0.0075
                                0.0012  0.1760 -0.0018  0.0002  0.0000
                               -0.0078  0.0838 -0.4935  0.0313 -0.0001
                                0.0000 -0.0051  0.0530 -0.3897  0.0059
                                0.0000  0.0000  0.0038  0.0179 -0.0464
                               -0.0010 -0.0007
764. (0.00016) RY*(17)Ru 51     s( 14.99%)p 0.42(  6.25%)d 5.26( 78.77%)
                                0.0000  0.0000  0.0000  0.0000  0.0066
                               -0.0593  0.0503  0.3676  0.0513 -0.0761
                               -0.0081 -0.0101  0.0041  0.0011  0.0017
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0002  0.0822 -0.0839 -0.0066
                                0.0007  0.0000  0.0000  0.0000  0.0873
                               -0.1330 -0.0101 -0.0003  0.0008  0.0000
                                0.0000  0.0000 -0.0034  0.1368 -0.0663
                                0.0087 -0.0005  0.0000  0.0033 -0.0539
                               -0.1889 -0.0153 -0.0004  0.0000  0.0005
                               -0.1121  0.5370 -0.0249  0.0008  0.0000
                               -0.0108  0.0165  0.0314  0.0105 -0.0015
                                0.0000 -0.0079  0.0821 -0.0995  0.0498
                               -0.0007  0.0000 -0.0032 -0.0481  0.6514
                               -0.0084  0.0006
765. (0.00011) RY*(18)Ru 51     s(  6.78%)p 3.69( 25.01%)d10.06( 68.21%)
                                0.0000  0.0000  0.0000  0.0000 -0.0051
                               -0.0774  0.1542  0.0719  0.1784 -0.0217
                                0.0234  0.0008 -0.0009  0.0025  0.0001
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000 -0.0648 -0.2338 -0.1126  0.0118
                               -0.0010  0.0000  0.0000  0.0000 -0.0309
                               -0.0269 -0.0164 -0.0111  0.0003  0.0000
                                0.0000  0.0000 -0.0617 -0.3347 -0.2459
                                0.0062 -0.0008  0.0000  0.0040 -0.0701
                                0.4739 -0.0001  0.0023  0.0000 -0.0008
                               -0.0915  0.3726 -0.0041 -0.0017  0.0000
                                0.0033  0.0106 -0.0735  0.0424  0.0023
                                0.0000 -0.0068 -0.0176  0.5299 -0.0028
                               -0.0012  0.0000 -0.0002 -0.0333 -0.1255
                               -0.0039 -0.0004
766. (0.00007) RY*(19)Ru 51     s( 39.43%)p 0.96( 38.03%)d 0.57( 22.54%)
767. (0.00003) RY*(20)Ru 51     s( 82.11%)p 0.11(  9.21%)d 0.11(  8.68%)
768. (0.00001) RY*(21)Ru 51     s(  5.61%)p13.85( 77.75%)d 2.97( 16.64%)
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769. (0.00002) RY*(22)Ru 51            s( 17.01%)p 4.45( 75.68%)d 0.43(  7.32%)
770. (0.00001) RY*(23)Ru 51            s(  6.68%)p10.73( 71.70%)d 3.24( 21.62%)
771. (0.00000) RY*(24)Ru 51            s(100.00%)p 0.00(  0.00%)d 0.00(  0.00%)
772. (0.00000) RY*(25)Ru 51            s(100.00%)p 0.00(  0.00%)
773. (0.00000) RY*(26)Ru 51            s(100.00%)
774. (0.00000) RY*(27)Ru 51            s(  0.01%)p99.99( 99.97%)d 1.58(  0.02%)
775. (0.00000) RY*(28)Ru 51            s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
776. (0.00001) RY*(29)Ru 51            s( 92.10%)p 0.05(  4.44%)d 0.04(  3.46%)
777. (0.00000) RY*(30)Ru 51            s( 97.48%)p 0.01(  1.01%)d 0.02(  1.51%)
778. (0.00000) RY*(31)Ru 51            s(  0.34%)p 3.62(  1.25%)d99.99( 98.41%)
779. (0.00000) RY*(32)Ru 51            s(  0.00%)p 0.00(  0.01%)d 1.00( 99.99%)
780. (0.00000) RY*(33)Ru 51            s( 99.66%)p 0.00(  0.18%)d 0.00(  0.16%)
781. (0.00000) RY*(34)Ru 51            s(  0.01%)p 1.00( 99.95%)d 0.00(  0.05%)
782. (0.00000) RY*(35)Ru 51            s(  0.15%)p 8.57(  1.29%)d99.99( 98.56%)
783. (0.00000) RY*(36)Ru 51            s(  0.00%)p 0.00(  0.00%)d 1.00( 99.99%)
784. (0.00000) RY*(37)Ru 51            s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
785. (0.00000) RY*(38)Ru 51            s( 99.95%)p 0.00(  0.02%)d 0.00(  0.02%)
786. (0.00000) RY*(39)Ru 51            s(  0.34%)p 4.98(  1.71%)d99.99( 97.94%)
787. (0.00000) RY*(40)Ru 51            s(  0.00%)p 1.00(  0.02%)d99.99( 99.98%)
788. (0.00000) RY*(41)Ru 51            s( 99.99%)p 0.00(  0.01%)d 0.00(  0.00%)
789. (0.00000) RY*(42)Ru 51            s( 99.99%)p 0.00(  0.00%)d 0.00(  0.00%)
790. (0.00000) RY*(43)Ru 51            s(  0.04%)p82.32(  3.20%)d99.99( 96.77%)
791. (0.00000) RY*(44)Ru 51            s(  0.00%)p 1.00(  0.02%)d99.99( 99.98%)
792. (0.00000) RY*(45)Ru 51            s(  0.06%)p99.99( 99.86%)d 1.42(  0.08%)
793. (0.00000) RY*(46)Ru 51            s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
794. (0.00000) RY*(47)Ru 51            s(  0.06%)p 6.95(  0.42%)d99.99( 99.52%)
795. (0.00000) RY*(48)Ru 51            s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
796. (0.00849) RY*( 1)Ru 52            s( 24.10%)p 0.44( 10.64%)d 2.71( 65.26%)
                                        0.0000  0.0000  0.0000  0.0000 -0.0187
                                        0.4904  0.0023 -0.0127  0.0055  0.0004
                                       -0.0057  0.0015 -0.0002 -0.0002  0.0000
                                        0.0000 -0.0003  0.0003  0.0000  0.0000
                                        0.0000 -0.0346 -0.1207 -0.0152  0.0009
                                        0.0000  0.0000  0.0000  0.0000 -0.1053
                                       -0.1113  0.0252  0.0002  0.0001  0.0000
                                        0.0000  0.0000 -0.2058 -0.1545  0.0066
                                        0.0014 -0.0001  0.0000 -0.0040 -0.6144
                                        0.0479  0.0104  0.0006  0.0000  0.0065
                                        0.4694  0.0920  0.0072  0.0001  0.0000
                                       -0.0054 -0.1349  0.0728  0.0124 -0.0001
                                        0.0000  0.0014 -0.0148  0.0246 -0.0003
                                        0.0000  0.0000  0.0062 -0.1365 -0.0257
                                       -0.0066  0.0001
797. (0.00721) RY*( 2)Ru 52            s( 29.32%)p 0.55( 16.04%)d 1.86( 54.64%)
                                        0.0000  0.0000  0.0000  0.0000 -0.0344
                                        0.5343 -0.0800 -0.0058 -0.0020  0.0046
                                        0.0052 -0.0005 -0.0001 -0.0001  0.0000
                                        0.0000 -0.0002  0.0002  0.0000  0.0000
                                        0.0000  0.0901 -0.0638 -0.0339  0.0014
                                        0.0000  0.0000  0.0000  0.0000 -0.1771
                                       -0.2973  0.0439  0.0004 -0.0001  0.0000
                                        0.0000  0.0000 -0.1073 -0.1170  0.0147
                                       -0.0012  0.0001  0.0000  0.0054  0.3547
                                        0.1130  0.0093  0.0004  0.0000  0.0057
                                       -0.2623  0.0397  0.0082  0.0004  0.0000
                                       -0.0062  0.0748  0.0661  0.0000  0.0005
                                        0.0000  0.0049  0.5551  0.0612 -0.0104
                                        0.0003  0.0000  0.0057  0.1227  0.0070
                                        0.0029 -0.0002
798. (0.00517) RY*( 3)Ru 52            s(  5.28%)p 1.66(  8.79%)d16.27( 85.93%)
                                        0.0000  0.0000  0.0000  0.0000 -0.0147
                                        0.2271  0.0275 -0.0153 -0.0005 -0.0049
                                        0.0058 -0.0003 -0.0001 -0.0001  0.0000
                                        0.0000 -0.0001  0.0001  0.0000  0.0000
                                        0.0000  0.2027  0.0048 -0.0182 -0.0004
                                        0.0000  0.0000  0.0000  0.0000 -0.1174
                                       -0.0452  0.0352 -0.0023  0.0002  0.0000
                                        0.0000  0.0000 -0.1673  0.0369 -0.0066
                                        0.0001  0.0001  0.0000  0.0006 -0.1359
                                       -0.0164 -0.0007  0.0000  0.0000 -0.0051
                                       -0.2237 -0.0112 -0.0022  0.0001  0.0000
                                        0.0038  0.5930 -0.0004 -0.0008 -0.0002
                                        0.0000 -0.0114 -0.5227  0.0023  0.0010
                                       -0.0002  0.0000  0.0114  0.4060  0.0193
                                       -0.0004  0.0004
799. (0.00477) RY*( 4)Ru 52            s(  3.01%)p 9.04( 27.20%)d23.19( 69.79%)
                                        0.0000  0.0000  0.0000  0.0000 -0.0149
                                        0.0097  0.1713 -0.0127  0.0119  0.0039
                                        0.0112 -0.0028  0.0004  0.0004  0.0001
                                        0.0000  0.0004 -0.0004  0.0000  0.0000
                                        0.0000  0.2609  0.1433 -0.0043 -0.0017
                                        0.0000  0.0000  0.0000  0.0000 -0.4010
                                        0.1079  0.0123 -0.0035  0.0001  0.0000
                                        0.0000  0.0000  0.0630  0.0774  0.0286
                                       -0.0016  0.0000  0.0000  0.0035  0.0443
                                       -0.0851 -0.0139 -0.0001  0.0000  0.0007
                                        0.0531 -0.1031 -0.0059 -0.0004  0.0000
                                       -0.0072  0.4135 -0.0977 -0.0145 -0.0004
                                        0.0000 -0.0034  0.0807 -0.0367 -0.0028
                                        0.0000  0.0000 -0.0069 -0.6960 -0.0434
                                        0.0041  0.0004
800. (0.00417) RY*( 5)Ru 52            s(  1.23%)p48.22( 59.25%)d32.16( 39.52%)
                                        0.0000  0.0000  0.0000  0.0000 -0.0103
                                        0.0033  0.1102 -0.0023  0.0003  0.0021
                                        0.0035  0.0002 -0.0002 -0.0003 -0.0001
                                        0.0000  0.0000  0.0003  0.0000  0.0000
                                        0.0000 -0.6948 -0.0244  0.0314 -0.0032
                                        0.0001  0.0000  0.0000  0.0000 -0.3050
                                        0.0835  0.0101 -0.0020  0.0001  0.0000
                                        0.0000  0.0000 -0.0850  0.0298  0.0028
                                       -0.0004  0.0000  0.0000 -0.0171  0.3424
                                        0.0287 -0.0061 -0.0012  0.0000 -0.0069
                                        0.4272  0.0179 -0.0069 -0.0007  0.0000
                                       -0.0032  0.2636 -0.0200 -0.0006 -0.0010
                                        0.0000  0.0069 -0.0285 -0.0128  0.0054
                                        0.0002  0.0000  0.0057  0.1511  0.0059
                                       -0.0002  0.0003
801. (0.00382) RY*( 6)Ru 52            s(  3.01%)p 9.81( 29.53%)d22.40( 67.46%)
                                        0.0000  0.0000  0.0000  0.0000  0.0169
                                        0.1564  0.0716 -0.0006  0.0051  0.0115
                                       -0.0089 -0.0005  0.0003  0.0000  0.0000
                                        0.0000  0.0008 -0.0003  0.0000  0.0000
                                        0.0000  0.1776 -0.0379  0.0239  0.0013
                                       -0.0001  0.0000  0.0000  0.0000 -0.4803
                                        0.1208 -0.0219  0.0018 -0.0001  0.0000
                                        0.0000  0.0000 -0.1053 -0.0645 -0.0268
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                                    0.0002 -0.0001  0.0000 -0.0122  0.3417
                                    0.0545 -0.0011  0.0002  0.0000 -0.0184
                                   -0.0660  0.0656 -0.0001  0.0002  0.0000
                                    0.0060 -0.5660  0.0273  0.0053 -0.0001
                                    0.0000  0.0022 -0.4713 -0.0288  0.0036
                                    0.0001  0.0000 -0.0018 -0.0385  0.0101
                                    0.0011  0.0002
802. (0.00327) RY*( 7)Ru 52          s(  2.25%)p41.15( 92.54%)d 2.32(  5.21%)
                                    0.0000  0.0000  0.0000  0.0000  0.0164
                                    0.1132 -0.0805  0.0174 -0.0503  0.0048
                                   -0.0079  0.0017 -0.0001  0.0001  0.0001
                                    0.0000 -0.0004  0.0003  0.0000  0.0000
                                    0.0000  0.0110 -0.2020 -0.0118  0.0006
                                    0.0000  0.0000  0.0000  0.0000 -0.1295
                                   -0.1218 -0.0553  0.0035 -0.0001  0.0000
                                    0.0000  0.0000  0.8986 -0.1997  0.0481
                                   -0.0015  0.0001  0.0000 -0.0027 -0.0141
                                    0.0575  0.0117 -0.0001  0.0000  0.0012
                                    0.0826  0.1054  0.0008  0.0000  0.0000
                                   -0.0066  0.0756  0.0662  0.0130  0.0008
                                    0.0000 -0.0023 -0.1216  0.0135 -0.0023
                                    0.0002  0.0000 -0.0047  0.0637 -0.0327
                                   -0.0085 -0.0004
803. (0.00256) RY*( 8)Ru 52          s( 11.20%)p 3.35( 37.47%)d 4.58( 51.33%)
                                    0.0000  0.0000  0.0000  0.0000 -0.0141
                                    0.3212 -0.0627  0.0670  0.0125  0.0070
                                   -0.0027  0.0011  0.0000  0.0001 -0.0001
                                    0.0000 -0.0003  0.0001  0.0000  0.0000
                                    0.0000 -0.4800  0.0478 -0.0374 -0.0014
                                    0.0001  0.0000  0.0000  0.0000  0.3514
                                   -0.1234  0.0151  0.0006  0.0001  0.0000
                                    0.0000  0.0000  0.0123 -0.0282  0.0271
                                    0.0005 -0.0001  0.0000  0.0048  0.0635
                                    0.0822 -0.0036 -0.0007  0.0000 -0.0013
                                   -0.3935 -0.0151 -0.0005 -0.0004  0.0000
                                   -0.0036  0.0064  0.0545 -0.0059  0.0003
                                    0.0000 -0.0070 -0.3381 -0.0193 -0.0015
                                    0.0003  0.0000 -0.0050 -0.4759 -0.0553
                                    0.0021 -0.0001
804. (0.00219) RY*( 9)Ru 52          s(  3.98%)p10.01( 39.84%)d14.11( 56.18%)
                                    0.0000  0.0000  0.0000  0.0000  0.0209
                                   -0.1077  0.1454 -0.0734 -0.0342 -0.0020
                                   -0.0082  0.0040 -0.0006 -0.0002  0.0001
                                    0.0000 -0.0012  0.0009  0.0000  0.0000
                                    0.0000 -0.3427  0.1175 -0.0679  0.0019
                                    0.0000  0.0000  0.0000  0.0000 -0.4443
                                    0.2001  0.0236 -0.0002  0.0000  0.0000
                                    0.0000  0.0000  0.0680 -0.1072  0.0916
                                   -0.0015  0.0001  0.0000  0.0225 -0.4482
                                   -0.0427  0.0075  0.0008  0.0000  0.0192
                                   -0.5061 -0.1336 -0.0014  0.0007  0.0000
                                   -0.0047 -0.1162  0.0185  0.0235  0.0002
                                    0.0000 -0.0224  0.1874  0.0571  0.0062
                                   -0.0002  0.0000 -0.0029  0.1280 -0.1196
                                   -0.0093 -0.0004
805. (0.00118) RY*(10)Ru 52          s( 30.85%)p 1.93( 59.54%)d 0.31(  9.61%)
                                    0.0000  0.0000  0.0000  0.0000 -0.0098
                                    0.4027  0.3818 -0.0035 -0.0161 -0.0151
                                   -0.0051 -0.0004  0.0009  0.0011  0.0001
                                    0.0000  0.0009 -0.0014  0.0000  0.0000
                                    0.0000  0.0707  0.2960 -0.0868 -0.0022
                                    0.0002  0.0000  0.0000  0.0000  0.3077
                                    0.5750  0.0662 -0.0053  0.0003  0.0000
                                    0.0000  0.0000  0.1534 -0.1826  0.0924
                                   -0.0037  0.0000  0.0000  0.0001  0.1069
                                   -0.1565 -0.0277 -0.0006  0.0000  0.0030
                                    0.0851 -0.0811 -0.0269 -0.0004  0.0000
                                   -0.0056 -0.0344 -0.1036  0.0053 -0.0016
                                    0.0000 -0.0057  0.0640  0.0581  0.0245
                                   -0.0008  0.0000 -0.0003  0.1365  0.0778
                                    0.0061 -0.0003
806. (0.00087) RY*(11)Ru 52          s(  5.92%)p10.58( 62.60%)d 5.32( 31.48%)
                                    0.0000  0.0000  0.0000  0.0000  0.0020
                                   -0.1313  0.1829  0.0679 -0.0520  0.0214
                                   -0.0264  0.0018 -0.0003 -0.0008  0.0002
                                    0.0000  0.0007  0.0006  0.0000  0.0000
                                    0.0000  0.0705 -0.5471  0.1525  0.0007
                                    0.0000  0.0000  0.0000  0.0000  0.1110
                                    0.3586 -0.1089  0.0007 -0.0001  0.0000
                                    0.0000  0.0000 -0.1683 -0.3395  0.0445
                                   -0.0060  0.0004  0.0000 -0.0059  0.0545
                                    0.2444  0.0365  0.0012  0.0000 -0.0031
                                   -0.0810  0.0853  0.0108  0.0008  0.0000
                                   -0.0112  0.1612  0.3609  0.0371 -0.0001
                                    0.0000 -0.0061  0.0501 -0.0261  0.0045
                                   -0.0009  0.0000 -0.0013 -0.0860 -0.2614
                                   -0.0076 -0.0005
807. (0.00058) RY*(12)Ru 52          s(  6.30%)p10.69( 67.33%)d 4.18( 26.37%)
                                    0.0000  0.0000  0.0000  0.0000  0.0087
                                    0.1974  0.1086  0.0633 -0.0876 -0.0187
                                    0.0056 -0.0099  0.0013  0.0003 -0.0003
                                    0.0000  0.0025 -0.0017  0.0000  0.0000
                                    0.0000 -0.0561 -0.5867  0.2039  0.0064
                                   -0.0005  0.0000  0.0000  0.0000  0.0068
                                    0.1591 -0.0449 -0.0019  0.0001  0.0000
                                    0.0000  0.0000  0.0701  0.4711 -0.1735
                                    0.0054 -0.0001  0.0000 -0.0029 -0.0701
                                   -0.1107  0.0506  0.0002  0.0000 -0.0019
                                   -0.1168 -0.1763  0.0340  0.0001  0.0000
                                    0.0058 -0.0575 -0.3785  0.0010 -0.0012
                                    0.0000 -0.0003  0.0623  0.0188 -0.0083
                                   -0.0006  0.0000 -0.0025 -0.0081  0.2168
                                    0.0067  0.0011
808. (0.00039) RY*(13)Ru 52          s( 68.78%)p 0.12(  8.38%)d 0.33( 22.84%)
                                    0.0000  0.0000  0.0000  0.0000  0.0098
                                    0.0326  0.2611  0.7859  0.0215 -0.0167
                                    0.0025  0.0046 -0.0017 -0.0012  0.0003
                                    0.0000 -0.0018  0.0015  0.0000  0.0000
                                    0.0000  0.0152  0.0918  0.0969  0.0067
                                   -0.0004  0.0000  0.0000  0.0000 -0.0252
                                   -0.1905 -0.0468 -0.0146  0.0003  0.0000
                                    0.0000  0.0000  0.0330  0.1589  0.0068
                                   -0.0024  0.0005  0.0000  0.0022 -0.0132
                                   -0.2631  0.0159 -0.0010  0.0000 -0.0023
                                    0.0265 -0.1110  0.0040  0.0000  0.0000
                                    0.0047 -0.0568  0.2448  0.0304 -0.0021
```

```
                                    0.0000  0.0045  0.0217 -0.1274  0.0026
                                   -0.0012  0.0000  0.0013  0.0842 -0.2398
                                   -0.0168  0.0009
809. (0.00025) RY*(14)Ru 52         s(  2.98%)p 7.54( 22.46%)d25.03( 74.56%)
                                    0.0000  0.0000  0.0000  0.0000  0.0024
                                   -0.0519  0.1439  0.0454 -0.0335  0.0499
                                    0.0251 -0.0088  0.0012  0.0012 -0.0001
                                    0.0000  0.0004 -0.0003  0.0000  0.0000
                                    0.0000 -0.0294  0.0423  0.1833 -0.0010
                                    0.0003  0.0000  0.0000  0.0000 -0.0050
                                   -0.1292 -0.0881  0.0018  0.0001  0.0000
                                    0.0000  0.0000 -0.0266 -0.3899 -0.1054
                                   -0.0002 -0.0001  0.0000  0.0026 -0.0494
                                    0.0570  0.0201  0.0002  0.0000  0.0033
                                   -0.0575 -0.0683  0.0089  0.0016  0.0000
                                   -0.0052  0.0186 -0.1704  0.0181 -0.0008
                                    0.0000 -0.0018  0.0310 -0.7260  0.0009
                                   -0.0011  0.0000 -0.0001  0.0076  0.4162
                                    0.0204 -0.0021
810. (0.00024) RY*(15)Ru 52         s( 21.50%)p 1.05( 22.63%)d 2.60( 55.87%)
                                    0.0000  0.0000  0.0000  0.0000 -0.0049
                                   -0.0622 -0.1962  0.4014 -0.0914 -0.0282
                                   -0.0451  0.0170 -0.0014  0.0000  0.0002
                                    0.0000 -0.0034  0.0019  0.0000  0.0000
                                    0.0000  0.0302 -0.0668 -0.2983 -0.0116
                                    0.0006  0.0000  0.0000  0.0000 -0.0155
                                    0.0388 -0.0420  0.0128 -0.0004  0.0000
                                    0.0000  0.0000 -0.0871 -0.2346  0.2559
                                    0.0039 -0.0001  0.0000 -0.0023  0.0107
                                    0.2824 -0.0017  0.0002  0.0000  0.0010
                                    0.0333 -0.0736 -0.0292 -0.0015  0.0000
                                   -0.0048  0.0150 -0.6479  0.0730 -0.0003
                                    0.0000 -0.0012 -0.0242  0.0656  0.0296
                                    0.0005  0.0000  0.0028  0.0152 -0.1980
                                   -0.0288 -0.0020
811. (0.00018) RY*(16)Ru 52         s( 17.08%)p 1.51( 25.83%)d 3.34( 57.08%)
                                    0.0000  0.0000  0.0000  0.0000  0.0078
                                    0.0125  0.3888 -0.0967 -0.0636 -0.0755
                                   -0.0138  0.0098 -0.0025 -0.0015 -0.0005
                                    0.0000 -0.0039  0.0021  0.0000  0.0000
                                    0.0000  0.0324  0.1233  0.0723 -0.0043
                                    0.0000  0.0000  0.0000  0.0000  0.0488
                                   -0.0755  0.2892 -0.0208  0.0010  0.0000
                                    0.0000  0.0000  0.0854  0.3667  0.0534
                                    0.0052  0.0003  0.0000  0.0081 -0.0545
                                    0.5219 -0.0146  0.0003  0.0000  0.0075
                                   -0.0195  0.3726 -0.0147 -0.0001  0.0000
                                    0.0045 -0.0412 -0.1220 -0.0291  0.0008
                                    0.0000 -0.0027  0.0349 -0.2516  0.0077
                                   -0.0004  0.0000  0.0014  0.0525 -0.2664
                                    0.0026  0.0007
812. (0.00014) RY*(17)Ru 52         s( 17.04%)p 0.38(  6.50%)d 4.49( 76.46%)
                                    0.0000  0.0000  0.0000  0.0000  0.0024
                                   -0.0684 -0.0397  0.3882  0.1154 -0.0061
                                   -0.0001 -0.0075  0.0028  0.0026  0.0000
                                    0.0000  0.0019 -0.0029  0.0000  0.0000
                                    0.0000 -0.0334  0.0653 -0.0666 -0.0028
                                    0.0000  0.0000  0.0000  0.0000 -0.0769
                                    0.1838  0.0013  0.0105 -0.0011  0.0000
                                    0.0000  0.0000 -0.0071  0.0203 -0.1223
                                    0.0027 -0.0002  0.0000  0.0099 -0.0858
                                    0.1493 -0.0521 -0.0002  0.0000  0.0034
                                   -0.1046  0.5735 -0.0404 -0.0005  0.0000
                                    0.0006  0.0711  0.0710 -0.0222  0.0012
                                    0.0000 -0.0081  0.0519  0.2531  0.0260
                                    0.0001  0.0000 -0.0067 -0.0695  0.5546
                                    0.0097 -0.0007
813. (0.00010) RY*(18)Ru 52         s( 17.07%)p 1.04( 17.77%)d 3.82( 65.16%)
                                    0.0000  0.0000  0.0000  0.0000  0.0009
                                   -0.0760  0.2881 -0.1389  0.1636 -0.1887
                                   -0.0069 -0.0127  0.0025  0.0021 -0.0003
                                    0.0000  0.0029 -0.0058  0.0000  0.0000
                                    0.0000 -0.0374 -0.1768 -0.1566  0.0240
                                   -0.0016  0.0000  0.0000  0.0000  0.0420
                                   -0.2069 -0.0214 -0.0070  0.0004  0.0000
                                    0.0000  0.0000 -0.0594 -0.2192 -0.1523
                                    0.0075 -0.0003  0.0000  0.0003  0.0423
                                   -0.5253  0.0351  0.0004  0.0000 -0.0044
                                   -0.0782  0.4800 -0.0370  0.0011  0.0000
                                   -0.0047  0.0015 -0.2882  0.0421 -0.0032
                                    0.0000  0.0011 -0.0089  0.0261  0.0179
                                   -0.0004  0.0000  0.0005 -0.0269 -0.2193
                                    0.0074  0.0002
814. (0.00006) RY*(19)Ru 52         s( 31.07%)p 1.00( 31.10%)d 1.22( 37.83%)
815. (0.00003) RY*(20)Ru 52         s( 83.77%)p 0.10(  8.69%)d 0.09(  7.54%)
816. (0.00001) RY*(21)Ru 52         s(  2.74%)p30.76( 84.29%)d 4.73( 12.97%)
817. (0.00002) RY*(22)Ru 52         s( 11.99%)p 6.52( 78.11%)d 0.83(  9.90%)
818. (0.00001) RY*(23)Ru 52         s(  9.09%)p 7.66( 69.65%)d 2.34( 21.26%)
819. (0.00000) RY*(24)Ru 52         s(100.00%)
820. (0.00000) RY*(25)Ru 52         s( 99.97%)p 0.00(  0.02%)d 0.00(  0.01%)
821. (0.00000) RY*(26)Ru 52         s( 99.94%)p 0.00(  0.05%)d 0.00(  0.01%)
822. (0.00000) RY*(27)Ru 52         s(  0.01%)p99.99( 99.97%)d 1.64(  0.02%)
823. (0.00000) RY*(28)Ru 52         s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
824. (0.00001) RY*(29)Ru 52         s( 93.53%)p 0.02(  2.00%)d 0.05(  4.47%)
825. (0.00000) RY*(30)Ru 52         s( 96.86%)p 0.03(  2.65%)d 0.01(  0.49%)
826. (0.00000) RY*(31)Ru 52         s(  0.20%)p13.80(  2.70%)d99.99( 97.10%)
827. (0.00000) RY*(32)Ru 52         s(  0.00%)p 1.00(  0.01%)d99.99( 99.99%)
828. (0.00000) RY*(33)Ru 52         s( 99.51%)p 0.00(  0.33%)d 0.00(  0.17%)
829. (0.00000) RY*(34)Ru 52         s(  0.01%)p 1.00( 99.93%)d 0.00(  0.06%)
830. (0.00000) RY*(35)Ru 52         s(  0.08%)p18.78(  1.51%)d99.99( 98.41%)
831. (0.00000) RY*(36)Ru 52         s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
832. (0.00000) RY*(37)Ru 52         s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
833. (0.00000) RY*(38)Ru 52         s( 99.98%)p 0.00(  0.01%)d 0.00(  0.01%)
834. (0.00000) RY*(39)Ru 52         s(  0.38%)p 6.67(  2.53%)d99.99( 97.09%)
835. (0.00000) RY*(40)Ru 52         s(  0.00%)p 1.00(  0.02%)d99.99( 99.98%)
836. (0.00000) RY*(41)Ru 52         s( 99.98%)p 0.00(  0.02%)d 0.00(  0.00%)
837. (0.00000) RY*(42)Ru 52         s(100.00%)p 0.00(  0.00%)d 0.00(  0.00%)
838. (0.00000) RY*(43)Ru 52         s(  0.11%)p12.43(  1.38%)d99.99( 98.51%)
839. (0.00000) RY*(44)Ru 52         s(  0.00%)p 0.00(  0.01%)d 1.00( 99.99%)
840. (0.00000) RY*(45)Ru 52         s(  0.06%)p99.99( 99.83%)d 1.65(  0.10%)
841. (0.00000) RY*(46)Ru 52         s(  0.00%)p 1.00(100.00%)d 0.00(  0.00%)
842. (0.00000) RY*(47)Ru 52         s(  0.08%)p 7.33(  0.57%)d99.99( 99.36%)
843. (0.00000) RY*(48)Ru 52         s(  0.00%)p 1.00(  0.01%)d99.99( 99.99%)
844. (0.00413) RY*( 1)Cl 53         s(  0.04%)p99.99( 82.27%)d99.99( 17.69%)
                                    0.0000  0.0000 -0.0003  0.0194 -0.0032
                                   -0.0006 -0.0003  0.0000  0.0000 -0.0052
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                                    -0.7707 -0.0133  0.0013  0.0000  0.0042
                                     0.2340  0.0074 -0.0005  0.0000  0.0020
                                     0.4168  0.0046 -0.0012  0.0673 -0.2091
                                     0.0927 -0.2110  0.2748
845. (0.00368) RY*( 2)Cl 53           s(  2.07%)p26.14( 53.99%)d21.28( 43.94%)
                                     0.0000  0.0000 -0.0058  0.1412 -0.0260
                                     0.0033 -0.0029  0.0003  0.0000 -0.0029
                                    -0.3253 -0.0148  0.0008  0.0000 -0.0002
                                    -0.0181  0.0008  0.0000  0.0000 -0.0058
                                    -0.6581 -0.0226  0.0017  0.1573 -0.2681
                                    -0.1105 -0.3948 -0.4179
846. (0.00137) RY*( 3)Cl 53           s( 44.22%)p 0.08(  3.66%)d 1.18( 52.12%)
                                     0.0000  0.0000  0.0006  0.6569 -0.1024
                                    -0.0079 -0.0109  0.0004  0.0000 -0.0060
                                     0.0989 -0.0467 -0.0011  0.0000  0.0005
                                     0.0543 -0.0019 -0.0004  0.0000 -0.0100
                                     0.1259 -0.0753 -0.0022  0.5813 -0.0694
                                    -0.3407  0.2329  0.0900
847. (0.00128) RY*( 4)Cl 53           s(  0.15%)p99.99( 97.29%)d17.06(  2.56%)
                                     0.0000  0.0000  0.0000  0.0376 -0.0093
                                     0.0016 -0.0003  0.0001  0.0000 -0.0006
                                    -0.1885  0.0079  0.0006  0.0000 -0.0086
                                    -0.9583  0.0542 -0.0039  0.0000 -0.0002
                                     0.1254 -0.0115  0.0007 -0.0267 -0.0412
                                    -0.1223 -0.0332  0.0846
848. (0.00077) RY*( 5)Cl 53           s( 43.53%)p 0.08(  3.63%)d 1.21( 52.84%)
                                     0.0000  0.0000  0.0003  0.6497 -0.1139
                                     0.0126 -0.0039 -0.0004  0.0000 -0.0061
                                     0.0895 -0.0544  0.0006  0.0000  0.0009
                                    -0.0043 -0.0052 -0.0001  0.0000 -0.0100
                                     0.1285 -0.0930  0.0014 -0.4311  0.2884
                                     0.2937 -0.4090 -0.0765
849. (0.00039) RY*( 6)Cl 53           s(  0.09%)p48.51(  4.16%)d99.99( 95.76%)
                                     0.0000  0.0000  0.0002  0.0281  0.0078
                                     0.0021 -0.0006  0.0000  0.0000 -0.0101
                                     0.0336  0.0205  0.0066  0.0000 -0.0352
                                     0.1425  0.1322  0.0047  0.0000  0.0053
                                    -0.0274 -0.0060 -0.0034 -0.5058 -0.1129
                                    -0.7905 -0.1193  0.2234
850. (0.00028) RY*( 7)Cl 53           s( 11.76%)p 0.31(  3.63%)d 7.19( 84.61%)
                                     0.0000  0.0000  0.0103  0.2257  0.2579
                                     0.0064  0.0026 -0.0003  0.0000 -0.0141
                                     0.0622  0.0457 -0.0070  0.0000 -0.0005
                                    -0.0074  0.0101 -0.0032  0.0000 -0.0255
                                     0.1602  0.0592 -0.0092 -0.3226 -0.6977
                                     0.1736  0.3622 -0.3065
851. (0.00025) RY*( 8)Cl 53           s(  0.69%)p26.41( 18.22%)d99.99( 81.09%)
                                     0.0000  0.0000  0.0008  0.0448  0.0660
                                     0.0231  0.0005  0.0006  0.0000 -0.0116
                                     0.3186 -0.0052  0.0152  0.0000  0.0028
                                    -0.0464 -0.0742  0.0109  0.0000  0.0046
                                    -0.2688  0.0141 -0.0017  0.0779 -0.4210
                                     0.2540 -0.2885  0.6927
852. (0.00019) RY*( 9)Cl 53           s( 19.34%)p 1.76( 34.04%)d 2.41( 46.62%)
                                     0.0000  0.0000 -0.0008  0.2429  0.3573
                                     0.0812 -0.0105  0.0018  0.0000  0.0021
                                    -0.3535  0.0124  0.0061  0.0000  0.0004
                                     0.0047  0.0173 -0.0008  0.0000 -0.0005
                                    -0.4597  0.0583  0.0157 -0.1852  0.3087
                                     0.1043  0.4830  0.3041
853. (0.00009) RY*(10)Cl 53           s( 73.55%)p 0.10(  7.39%)d 0.26( 19.06%)
854. (0.00002) RY*(11)Cl 53           s(  1.50%)p65.76( 98.36%)d 0.10(  0.15%)
855. (0.00001) RY*(12)Cl 53           s(  4.90%)p19.38( 94.97%)d 0.03(  0.13%)
856. (0.00002) RY*(13)Cl 53           s(  0.01%)p99.99( 97.65%)d99.99(  2.34%)
857. (0.00000) RY*(14)Cl 53           s(  0.03%)p99.99( 99.94%)d 1.11(  0.03%)
858. (0.00000) RY*(15)Cl 53           s(100.00%)p 0.00(  0.00%)d 0.00(  0.00%)
859. (0.00000) RY*(16)Cl 53           s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
860. (0.00000) RY*(17)Cl 53           s( 99.23%)p 0.01(  0.71%)d 0.00(  0.07%)
861. (0.00001) RY*(18)Cl 53           s( 98.86%)p 0.00(  0.44%)d 0.01(  0.70%)
862. (0.00000) RY*(19)Cl 53           s(  0.01%)p99.99( 99.95%)d 3.69(  0.04%)
863. (0.02309) BD*( 1) C 12- C 14
             ( 50.00%)   0.7071* C 12 s( 37.81%)p 1.64( 62.10%)d 0.00(  0.09%)
                                    -0.0001  0.6149  0.0023  0.0039 -0.0001
                                     0.0000 -0.6016  0.0075 -0.0056  0.2665
                                    -0.0153  0.0023  0.4330  0.0169 -0.0014
                                    -0.0120 -0.0226  0.0093  0.0119  0.0010
             ( 50.00%)  -0.7071* C 14 s( 34.64%)p 1.88( 65.26%)d 0.00(  0.09%)
                                     0.0000  0.5886 -0.0006  0.0050 -0.0002
                                     0.0002  0.6003 -0.0088 -0.0051 -0.2623
                                    -0.0041  0.0024 -0.4721  0.0234 -0.0005
                                    -0.0159 -0.0214  0.0091  0.0123 -0.0023
864. (0.29507) BD*( 2) C 12- C 14
             ( 53.34%)   0.7304* C 12 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                     0.0000 -0.0008  0.0009 -0.0012  0.0001
                                    -0.0001  0.5750  0.0124  0.0047  0.7422
                                     0.0112  0.0032  0.3433  0.0044  0.0020
                                    -0.0079  0.0057  0.0118 -0.0072  0.0096
             ( 46.66%)  -0.6831* C 14 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                     0.0000 -0.0006  0.0018 -0.0008  0.0000
                                    -0.0001  0.5853  0.0107  0.0052  0.7388
                                     0.0117  0.0065  0.3330  0.0057  0.0037
                                     0.0045  0.0040 -0.0049  0.0169 -0.0005
865. (0.02395) BD*( 1) C 12- N 50
             ( 59.84%)   0.7735* C 12 s( 32.38%)p 2.09( 67.54%)d 0.00(  0.09%)
                                     0.0000  0.5685  0.0233  0.0037 -0.0002
                                     0.0003  0.5408 -0.0235  0.0047 -0.5493
                                     0.0163 -0.0055  0.2833  0.0054 -0.0002
                                    -0.0223  0.0117 -0.0131 -0.0011 -0.0077
             ( 40.16%)  -0.6337* N 50 s( 35.27%)p 1.83( 64.56%)d 0.00(  0.18%)
                                     0.0000  0.5932  0.0293 -0.0008  0.0004
                                    -0.0001 -0.5177 -0.0057 -0.0002  0.5439
                                     0.0128  0.0016 -0.2846 -0.0228 -0.0035
                                    -0.0359  0.0085 -0.0107  0.0042 -0.0160
866. (0.02408) BD*( 1) C 12- H 29
             ( 39.29%)   0.6268* C 12 s( 29.83%)p 2.35( 70.11%)d 0.00(  0.06%)
                                    -0.0004  0.5458 -0.0172 -0.0070  0.0002
                                    -0.0002  0.1153  0.0012 -0.0073  0.2735
                                    -0.0001 -0.0040 -0.7828 -0.0131  0.0084
                                     0.0024 -0.0065 -0.0123 -0.0020  0.0199
             ( 60.71%)  -0.7792* H 29 s( 99.91%)p 0.00(  0.09%)
                                     0.9995  0.0027  0.0025 -0.0052 -0.0126
                                     0.0270
867. (0.01458) BD*( 1) C 14- C 21
             ( 49.94%)   0.7067* C 14 s( 35.25%)p 1.83( 64.66%)d 0.00(  0.09%)
                                     0.0000 -0.5936 -0.0083 -0.0036  0.0002
                                    -0.0001  0.1012 -0.0181  0.0045  0.2591
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                                    0.0075 -0.0035 -0.7540  0.0169  0.0005
                                    0.0005  0.0032  0.0183  0.0030 -0.0238
              ( 50.06%)  -0.7076* C 21 s( 34.98%)p 1.86( 64.93%)d 0.00(  0.09%)
                                    0.0000 -0.5914 -0.0054 -0.0039 -0.0001
                                    0.0000 -0.0443 -0.0154  0.0027 -0.2956
                                    0.0168 -0.0002  0.7479 -0.0100 -0.0039
                                   -0.0008  0.0057  0.0161  0.0022 -0.0244
868. (0.01313) BD*( 1) C 14- H 31
              ( 38.35%)   0.6193* C 14 s( 30.05%)p 2.33( 69.88%)d 0.00(  0.07%)
                                   -0.0004  0.5481 -0.0050 -0.0080  0.0003
                                   -0.0002 -0.5344 -0.0075  0.0009  0.5634
                                    0.0036 -0.0050 -0.3094 -0.0025  0.0047
                                   -0.0190  0.0111 -0.0120 -0.0014 -0.0070
              ( 61.65%)  -0.7852* H 31 s( 99.95%)p 0.00(  0.05%)
                                    0.9997  0.0018 -0.0004  0.0136 -0.0161
                                    0.0077
869. (0.01316) BD*( 1) C 25- C 26
              ( 49.62%)   0.7044* C 25 s( 36.16%)p 1.76( 63.75%)d 0.00(  0.09%)
                                    0.0000 -0.6012 -0.0125 -0.0033 -0.0001
                                    0.0000 -0.5311 -0.0003  0.0015  0.5665
                                   -0.0091  0.0005 -0.1842  0.0208 -0.0040
                                    0.0256 -0.0049  0.0071  0.0005  0.0116
              ( 50.38%)  -0.7098* C 26 s( 35.56%)p 1.81( 64.35%)d 0.00(  0.09%)
                                    0.0000 -0.5963 -0.0064 -0.0037 -0.0001
                                    0.0001  0.5466 -0.0211 -0.0025 -0.5691
                                    0.0131  0.0037  0.1413  0.0148 -0.0034
                                    0.0255 -0.0071  0.0092  0.0017  0.0115
870. (0.31736) BD*( 2) C 25- C 26
              ( 51.09%)   0.7148* C 25 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                    0.0000 -0.0015  0.0016 -0.0001  0.0000
                                   -0.0001  0.6454  0.0102  0.0060  0.7014
                                    0.0115  0.0071  0.3014  0.0048  0.0031
                                    0.0015  0.0023 -0.0047  0.0150 -0.0007
              ( 48.91%)  -0.6994* C 26 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                    0.0000 -0.0012  0.0012 -0.0001  0.0000
                                    0.0000  0.6481  0.0109  0.0056  0.6986
                                    0.0111  0.0060  0.3020  0.0051  0.0027
                                    0.0017 -0.0086 -0.0036 -0.0121 -0.0050
871. (0.01662) BD*( 1) C 25- H 39
              ( 39.77%)   0.6306* C 25 s( 28.58%)p 2.50( 71.34%)d 0.00(  0.07%)
                                   -0.0003  0.5345 -0.0034 -0.0102 -0.0002
                                    0.0001 -0.5462 -0.0052  0.0067  0.2483
                                    0.0031 -0.0051  0.5944  0.0009 -0.0020
                                   -0.0093 -0.0210  0.0097  0.0077  0.0062
              ( 60.23%)  -0.7761* H 39 s( 99.94%)p 0.00(  0.06%)
                                    0.9997  0.0022  0.0002  0.0129 -0.0045
                                   -0.0198
872. (0.01445) BD*( 1) C 26- H 40
              ( 39.08%)   0.6251* C 26 s( 29.12%)p 2.43( 70.80%)d 0.00(  0.08%)
                                    0.0004 -0.5395  0.0090  0.0073  0.0001
                                   -0.0001 -0.0243  0.0001 -0.0010  0.3518
                                    0.0043 -0.0006 -0.7639 -0.0091  0.0038
                                   -0.0008 -0.0014  0.0180  0.0043 -0.0206
              ( 60.92%)  -0.7805* H 40 s( 99.96%)p 0.00(  0.04%)
                                   -0.9998 -0.0022 -0.0005  0.0011 -0.0081
                                    0.0174
873. (0.01279) BD*( 1) C  3- C  5
              ( 50.29%)   0.7091* C  3 s( 35.51%)p 1.81( 64.40%)d 0.00(  0.09%)
                                    0.0000  0.5958  0.0058  0.0039  0.0001
                                   -0.0001  0.0041 -0.0199  0.0023  0.5453
                                   -0.0124 -0.0038  0.5881 -0.0122 -0.0040
                                   -0.0019 -0.0023  0.0269 -0.0109  0.0086
              ( 49.71%)  -0.7051* C  5 s( 35.94%)p 1.78( 63.97%)d 0.00(  0.09%)
                                    0.0000  0.5993  0.0130  0.0032  0.0001
                                   -0.0001  0.0386 -0.0207  0.0048 -0.5478
                                    0.0065  0.0004 -0.5811  0.0080  0.0003
                                    0.0012  0.0008  0.0271 -0.0104  0.0079
874. (0.28773) BD*( 2) C  3- C  5
              ( 52.05%)   0.7215* C  3 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                    0.0000 -0.0009  0.0009 -0.0002  0.0000
                                    0.0000  0.0321  0.0004  0.0003 -0.7323
                                   -0.0099 -0.0071  0.6797  0.0085  0.0060
                                    0.0079 -0.0065 -0.0012  0.0083  0.0153
              ( 47.95%)  -0.6925* C  5 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                    0.0000 -0.0019  0.0009 -0.0002 -0.0001
                                   -0.0001  0.0336  0.0009  0.0007 -0.7269
                                   -0.0074 -0.0069  0.6856  0.0076  0.0066
                                    0.0075 -0.0077  0.0010 -0.0080 -0.0126
875. (0.01463) BD*( 1) C  3- H 41
              ( 38.65%)   0.6217* C  3 s( 29.33%)p 2.41( 70.59%)d 0.00(  0.08%)
                                    0.0003 -0.5415  0.0088  0.0070  0.0001
                                   -0.0001 -0.7353 -0.0118  0.0017  0.2590
                                    0.0035  0.0000  0.3131  0.0049  0.0000
                                    0.0130  0.0160 -0.0044 -0.0161  0.0081
              ( 61.35%)  -0.7832* H 41 s( 99.96%)p 0.00(  0.04%)
                                   -0.9998 -0.0022 -0.0002  0.0166 -0.0062
                                   -0.0069
876. (0.03150) BD*( 1) C  5- C  7
              ( 50.30%)   0.7092* C  5 s( 34.43%)p 1.90( 65.48%)d 0.00(  0.09%)
                                    0.0000  0.5867 -0.0070  0.0069  0.0002
                                   -0.0002 -0.6994  0.0067  0.0042  0.2606
                                   -0.0082 -0.0001  0.3122 -0.0096 -0.0002
                                   -0.0130 -0.0159  0.0065  0.0193 -0.0099
              ( 49.70%)  -0.7050* C  7 s( 35.53%)p 1.81( 64.41%)d 0.00(  0.07%)
                                   -0.0002  0.5961  0.0000 -0.0024  0.0001
                                    0.0000  0.7089 -0.0063  0.0023 -0.2388
                                    0.0119  0.0000 -0.2901  0.0140 -0.0001
                                   -0.0127 -0.0152  0.0044  0.0140 -0.0068
877. (0.01528) BD*( 1) C  5- H 28
              ( 38.85%)   0.6233* C  5 s( 29.59%)p 2.38( 70.34%)d 0.00(  0.07%)
                                    0.0004 -0.5439  0.0033  0.0092  0.0002
                                   -0.0002 -0.7121 -0.0040  0.0036 -0.3203
                                   -0.0025  0.0058 -0.3062 -0.0025  0.0061
                                   -0.0149 -0.0139 -0.0071 -0.0124  0.0075
              ( 61.15%)  -0.7820* H 28 s( 99.94%)p 0.00(  0.06%)
                                   -0.9997 -0.0021 -0.0002  0.0215  0.0084
                                    0.0077
878. (0.24546) BD*( 1) C  8- O 47
              ( 74.91%)   0.8655* C  8 s(  0.15%)p99.99( 99.61%)d 1.53(  0.23%)
                                    0.0000 -0.0382 -0.0081 -0.0009  0.0003
                                    0.0002  0.3206 -0.0025 -0.0018 -0.6404
                                    0.0067  0.0103  0.6950 -0.0086 -0.0067
                                    0.0081 -0.0254 -0.0074 -0.0299 -0.0261
              ( 25.09%)  -0.5009* O 47 s(  0.21%)p99.99( 99.40%)d 1.87(  0.39%)
                                    0.0000 -0.0456  0.0019  0.0000 -0.0001
                                    0.0000  0.2548  0.0015  0.0006 -0.7199
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                                    0.0014 -0.0004  0.6409  0.0010  0.0010
                                   -0.0158  0.0286  0.0060  0.0404  0.0340
879. (0.18542) BD*( 2) C  8- O 47
               ( 74.32%)   0.8621* C  8 s(  0.01%)p 1.00( 99.77%)d 0.00(  0.22%)
                                    0.0000  0.0072  0.0036 -0.0007  0.0001
                                    0.0000  0.7647 -0.0057 -0.0099 -0.2569
                                    0.0003  0.0023 -0.5889  0.0054  0.0068
                                   -0.0178 -0.0013  0.0245 -0.0282  0.0222
               ( 25.68%)  -0.5068* O 47 s(  0.01%)p99.99( 99.60%)d29.53(  0.39%)
                                    0.0000  0.0115 -0.0005  0.0000  0.0000
                                    0.0000  0.7803 -0.0006  0.0009 -0.2368
                                   -0.0002 -0.0003 -0.5753  0.0003 -0.0007
                                    0.0257  0.0019 -0.0310  0.0378 -0.0289
880. (0.01440) BD*( 3) C  8- O 47
               ( 68.08%)   0.8251* C  8 s( 39.04%)p 1.56( 60.90%)d 0.00(  0.06%)
                                   -0.0001  0.6097  0.1362 -0.0011 -0.0005
                                   -0.0005 -0.4299  0.0223 -0.0155 -0.5770
                                    0.0264 -0.0180 -0.2983  0.0199 -0.0124
                                    0.0170  0.0090  0.0127 -0.0051 -0.0067
               ( 31.92%)  -0.5650* O 47 s( 42.48%)p 1.34( 56.75%)d 0.02(  0.77%)
                                    0.0001  0.6513 -0.0236 -0.0025  0.0001
                                    0.0000  0.4295 -0.0173 -0.0036  0.4688
                                   -0.0212 -0.0045  0.4028 -0.0143 -0.0029
                                    0.0573  0.0415  0.0491 -0.0093 -0.0134
881. (0.34598) BD*( 1) C  8-Ru 52
               ( 33.41%)   0.5780* C  8 s( 62.09%)p 0.61( 37.90%)d 0.00(  0.01%)
                                   -0.0001 -0.7873  0.0332 -0.0003 -0.0001
                                   -0.0003 -0.3475 -0.0211 -0.0043 -0.4258
                                   -0.0295 -0.0057 -0.2747 -0.0114 -0.0016
                                   -0.0065 -0.0025 -0.0054  0.0018  0.0041
               ( 66.59%)  -0.8160*Ru 52 s( 35.82%)p 0.00(  0.09%)d 1.79( 64.09%)
                                    0.0000  0.0000  0.0001  0.0009 -0.5980
                                   -0.0230  0.0082  0.0024 -0.0004 -0.0002
                                    0.0008 -0.0004  0.0001  0.0001  0.0000
                                    0.0000  0.0001 -0.0001  0.0000  0.0000
                                   -0.0005 -0.0003  0.0084 -0.0016 -0.0004
                                    0.0000  0.0000  0.0000 -0.0007 -0.0042
                                    0.0053 -0.0130 -0.0003  0.0000  0.0000
                                    0.0000 -0.0006  0.0186  0.0161  0.0000
                                   -0.0003  0.0000  0.0000 -0.5358 -0.0240
                                    0.0034 -0.0021 -0.0001  0.0000 -0.4049
                                   -0.0236  0.0041 -0.0016 -0.0001  0.0000
                                   -0.4144 -0.0184  0.0014 -0.0009 -0.0001
                                    0.0000  0.0764  0.0042 -0.0048  0.0005
                                    0.0000  0.0000  0.1033  0.0077  0.0009
                                    0.0000  0.0000
882. (0.32004) BD*( 1) C  6-Ru 52
               ( 31.80%)   0.5639* C  6 s( 62.92%)p 0.59( 37.08%)d 0.00(  0.01%)
                                   -0.0001 -0.7923  0.0385 -0.0017 -0.0002
                                   -0.0003  0.4763  0.0313  0.0064 -0.3070
                                   -0.0175 -0.0042 -0.2197 -0.0105 -0.0017
                                    0.0055  0.0042 -0.0028 -0.0038  0.0027
               ( 68.20%)  -0.8258*Ru 52 s( 36.90%)p 0.00(  0.06%)d 1.71( 63.03%)
                                    0.0000  0.0000  0.0000  0.0009 -0.6070
                                   -0.0232  0.0047  0.0026  0.0001 -0.0009
                                    0.0000 -0.0002  0.0000  0.0000  0.0000
                                    0.0000  0.0001 -0.0001  0.0000  0.0000
                                    0.0005  0.0037 -0.0129  0.0061  0.0005
                                    0.0000  0.0000  0.0000 -0.0006 -0.0032
                                   -0.0002 -0.0139  0.0000  0.0000  0.0000
                                    0.0000 -0.0003  0.0096  0.0115 -0.0016
                                   -0.0003  0.0000  0.0000  0.4639  0.0164
                                   -0.0045  0.0016  0.0001  0.0000  0.4796
                                    0.0153 -0.0019  0.0012  0.0001  0.0000
                                   -0.2184 -0.0249  0.0019 -0.0001 -0.0001
                                    0.0000 -0.3402 -0.0229 -0.0009 -0.0007
                                   -0.0001  0.0000  0.1413  0.0068  0.0007
                                    0.0003  0.0001
883. (0.19883) BD*( 1) C  6- O 46
               ( 74.67%)   0.8641* C  6 s(  0.90%)p99.99( 98.87%)d 0.25(  0.23%)
                                    0.0000  0.0933  0.0183  0.0003 -0.0001
                                    0.0000  0.5398 -0.0146 -0.0039  0.0006
                                   -0.0043 -0.0024  0.8347 -0.0090 -0.0135
                                   -0.0128  0.0221 -0.0230  0.0183 -0.0277
               ( 25.33%)  -0.5033* O 46 s(  0.87%)p99.99( 98.72%)d 0.47(  0.41%)
                                    0.0000  0.0931 -0.0032 -0.0004  0.0000
                                    0.0000  0.3742  0.0009  0.0013  0.1119
                                   -0.0045 -0.0003  0.9136 -0.0024  0.0005
                                    0.0030 -0.0386  0.0330 -0.0213  0.0321
884. (0.21822) BD*( 2) C  6- O 46
               ( 74.88%)   0.8653* C  6 s(  0.13%)p99.99( 99.64%)d 1.85(  0.23%)
                                    0.0000  0.0344  0.0087  0.0010 -0.0003
                                    0.0000  0.4567 -0.0071 -0.0061  0.8352
                                   -0.0045 -0.0126 -0.3001 -0.0040  0.0040
                                    0.0193 -0.0183 -0.0069  0.0382  0.0107
               ( 25.12%)  -0.5012* O 46 s(  0.10%)p99.99( 99.50%)d 4.07(  0.40%)
                                    0.0000  0.0312 -0.0015 -0.0001  0.0000
                                    0.0000  0.4079  0.0011  0.0007  0.8673
                                   -0.0013  0.0004 -0.2766 -0.0035 -0.0002
                                   -0.0306  0.0223  0.0122 -0.0474 -0.0121
885. (0.01855) BD*( 3) C  6- O 46
               ( 68.70%)   0.8289* C  6 s( 37.49%)p 1.67( 62.45%)d 0.00(  0.06%)
                                   -0.0001  0.5970  0.1361 -0.0023 -0.0007
                                   -0.0006  0.5109 -0.0246  0.0240 -0.4489
                                    0.0169 -0.0156 -0.3998  0.0192 -0.0087
                                   -0.0162 -0.0139  0.0120  0.0016 -0.0039
               ( 31.30%)  -0.5594* O 46 s( 42.62%)p 1.33( 56.61%)d 0.02(  0.76%)
                                    0.0001  0.6524 -0.0251 -0.0028  0.0001
                                    0.0000 -0.6540  0.0223  0.0044  0.3347
                                   -0.0157 -0.0033  0.1596 -0.0097 -0.0023
                                   -0.0604 -0.0390  0.0242  0.0308 -0.0303
886. (0.01480) BD*( 1) C  1- C  3
               ( 50.03%)   0.7073* C  1 s( 35.25%)p 1.83( 64.66%)d 0.00(  0.09%)
                                    0.0000  0.5936  0.0088  0.0036 -0.0002
                                    0.0001  0.7075 -0.0239  0.0016  0.2800
                                    0.0069 -0.0036  0.2585  0.0080 -0.0039
                                    0.0171  0.0161  0.0094  0.0149 -0.0088
               ( 49.97%)  -0.7069* C  3 s( 35.11%)p 1.85( 64.80%)d 0.00(  0.09%)
                                    0.0000  0.5925  0.0056  0.0038  0.0001
                                    0.0000 -0.6758  0.0014  0.0048 -0.3129
                                    0.0172 -0.0001 -0.3044  0.0182 -0.0005
                                    0.0155  0.0148  0.0072  0.0169 -0.0100
887. (0.02264) BD*( 1) C  1- C  2
               ( 49.82%)   0.7058* C  1 s( 34.70%)p 1.88( 65.21%)d 0.00(  0.09%)
                                    0.0000 -0.5890  0.0011 -0.0051  0.0002
                                   -0.0001  0.7039 -0.0245 -0.0019 -0.2495
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                                    -0.0042  0.0027 -0.3063 -0.0027  0.0048
                                     0.0151  0.0185 -0.0091 -0.0152  0.0068
              ( 50.18%)  -0.7084* C  2 s( 37.50%)p 1.66( 62.40%)d 0.00(  0.09%)
                                     0.0001 -0.6124 -0.0048 -0.0039  0.0001
                                    -0.0001 -0.6705 -0.0114 -0.0009  0.2592
                                    -0.0162  0.0030  0.3266 -0.0147  0.0057
                                     0.0138  0.0172 -0.0053 -0.0180  0.0087
888. (0.28685) BD*( 2) C  1- C  2
              ( 45.85%)   0.6772* C  1 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                     0.0000  0.0004 -0.0013  0.0006  0.0000
                                     0.0001 -0.0388 -0.0004 -0.0010  0.7285
                                     0.0127  0.0066 -0.6834 -0.0132 -0.0067
                                    -0.0063  0.0048  0.0013 -0.0080 -0.0146
              ( 54.15%)  -0.7358* C  2 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                     0.0000  0.0029 -0.0002  0.0010 -0.0001
                                     0.0000 -0.0524  0.0015  0.0001  0.7297
                                     0.0095  0.0033 -0.6812 -0.0114 -0.0052
                                     0.0151 -0.0144 -0.0013 -0.0011  0.0013
889. (0.01334) BD*( 1) C  1- H 42
              ( 38.39%)   0.6196* C  1 s( 30.00%)p 2.33( 69.94%)d 0.00(  0.07%)
                                    -0.0004  0.5476 -0.0049 -0.0080  0.0003
                                    -0.0002 -0.0099  0.0023  0.0035 -0.5726
                                    -0.0037  0.0050 -0.6093 -0.0073  0.0031
                                     0.0011  0.0010  0.0225 -0.0106  0.0077
              ( 61.61%)  -0.7850* H 42 s( 99.95%)p 0.00(  0.05%)
                                     0.9997  0.0019 -0.0003  0.0009  0.0160
                                     0.0155
890. (0.02376) BD*( 1) C  2- N 49
              ( 60.10%)   0.7753* C  2 s( 31.64%)p 2.16( 68.27%)d 0.00(  0.09%)
                                     0.0000  0.5620  0.0244  0.0034 -0.0002
                                     0.0003 -0.0007  0.0148 -0.0024  0.5622
                                    -0.0167  0.0053  0.6047 -0.0180  0.0043
                                     0.0015  0.0018  0.0264 -0.0115  0.0084
              ( 39.90%)  -0.6316* N 49 s( 35.46%)p 1.81( 64.37%)d 0.00(  0.17%)
                                    -0.0001  0.5949  0.0280 -0.0010  0.0004
                                     0.0000 -0.0024 -0.0157 -0.0027 -0.5492
                                    -0.0129 -0.0017 -0.5843 -0.0155 -0.0018
                                    -0.0073 -0.0086  0.0361 -0.0118  0.0108
891. (0.02499) BD*( 1) C  2- H 27
              ( 37.44%)   0.6119* C  2 s( 30.88%)p 2.24( 69.06%)d 0.00(  0.06%)
                                    -0.0004  0.5553 -0.0188 -0.0066  0.0002
                                    -0.0002 -0.7389 -0.0130  0.0110 -0.2874
                                    -0.0017  0.0036 -0.2486 -0.0058 -0.0029
                                     0.0123  0.0098  0.0034  0.0147 -0.0098
              ( 62.56%)  -0.7909* H 27 s( 99.89%)p 0.00(  0.11%)
                                     0.9994  0.0009  0.0027  0.0315  0.0107
                                     0.0054
892. (0.03586) BD*( 1) C  7- N 49
              ( 59.29%)   0.7700* C  7 s( 29.91%)p 2.34( 70.02%)d 0.00(  0.07%)
                                    -0.0001  0.5465  0.0198 -0.0007  0.0005
                                     0.0002 -0.7001 -0.0120 -0.0016 -0.3352
                                    -0.0007 -0.0002 -0.3123  0.0008 -0.0003
                                     0.0151  0.0141  0.0079  0.0128 -0.0079
              ( 40.71%)  -0.6380* N 49 s( 33.99%)p 1.94( 65.84%)d 0.01(  0.17%)
                                    -0.0001  0.5828  0.0142 -0.0003  0.0007
                                    -0.0002  0.6872  0.0088  0.0005  0.3190
                                     0.0105  0.0018  0.2900  0.0120  0.0017
                                     0.0192  0.0156  0.0102  0.0272 -0.0166
893. (0.50057) BD*( 2) C  7- N 49
              ( 65.91%)   0.8119* C  7 s(  0.00%)p 1.00( 99.92%)d 0.00(  0.08%)
                                     0.0000 -0.0035 -0.0011 -0.0003  0.0000
                                     0.0000 -0.0382 -0.0025  0.0000  0.7189
                                     0.0285 -0.0021 -0.6923 -0.0283  0.0016
                                    -0.0137  0.0138 -0.0009  0.0117  0.0174
              ( 34.09%)  -0.5838* N 49 s(  0.00%)p 1.00( 99.91%)d 0.00(  0.09%)
                                     0.0000 -0.0011  0.0004 -0.0006  0.0001
                                     0.0000 -0.0477 -0.0045  0.0005  0.7267
                                     0.0239 -0.0012 -0.6838 -0.0238  0.0012
                                     0.0212 -0.0189 -0.0026  0.0017  0.0086
894. (0.03027) BD*( 1) C  7- C  9
              ( 49.11%)   0.7008* C  7 s( 34.57%)p 1.89( 65.38%)d 0.00(  0.05%)
                                     0.0003 -0.5878  0.0133 -0.0015  0.0004
                                     0.0000  0.0681 -0.0074 -0.0033 -0.5583
                                     0.0131  0.0011 -0.5805  0.0136  0.0015
                                     0.0038  0.0039 -0.0179  0.0093 -0.0055
              ( 50.89%)  -0.7134* C  9 s( 30.47%)p 2.28( 69.46%)d 0.00(  0.07%)
                                     0.0002 -0.5519  0.0084 -0.0013  0.0002
                                    -0.0003 -0.1337 -0.0023 -0.0023  0.5819
                                    -0.0104  0.0004  0.5813 -0.0108  0.0005
                                     0.0044  0.0043 -0.0223  0.0106 -0.0066
895. (0.02953) BD*( 1) C  9- C 13
              ( 49.11%)   0.7008* C  9 s( 34.63%)p 1.89( 65.30%)d 0.00(  0.07%)
                                     0.0003 -0.5885 -0.0065  0.0001 -0.0003
                                    -0.0001 -0.6363  0.0003 -0.0025 -0.3502
                                     0.0087 -0.0011 -0.3540  0.0069 -0.0013
                                    -0.0145 -0.0149 -0.0088 -0.0107  0.0058
              ( 50.89%)  -0.7134* C 13 s( 35.26%)p 1.83( 64.66%)d 0.00(  0.08%)
                                     0.0000 -0.5937  0.0062 -0.0078 -0.0002
                                     0.0002  0.6052 -0.0050 -0.0028  0.3608
                                    -0.0109 -0.0014  0.3872 -0.0102 -0.0011
                                    -0.0158 -0.0168 -0.0114 -0.0108  0.0058
896. (0.41082) BD*( 2) C  9- C 13
              ( 47.57%)   0.6897* C  9 s(  0.00%)p 1.00( 99.99%)d 0.00(  0.01%)
                                     0.0000  0.0035  0.0009  0.0000  0.0000
                                     0.0000 -0.0086  0.0026  0.0000 -0.7059
                                    -0.0074 -0.0025  0.7081  0.0079  0.0024
                                    -0.0055  0.0052  0.0004  0.0029  0.0054
              ( 52.43%)  -0.7241* C 13 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.02%)
                                     0.0000  0.0022  0.0013 -0.0002  0.0000
                                    -0.0001 -0.0281 -0.0006 -0.0001 -0.7073
                                    -0.0029 -0.0057  0.7061  0.0033  0.0058
                                     0.0108 -0.0106  0.0007 -0.0014 -0.0039
897. (0.03382) BD*( 1) C  9- C 11
              ( 46.46%)   0.6816* C  9 s( 34.84%)p 1.87( 65.09%)d 0.00(  0.06%)
                                     0.0001 -0.5903 -0.0028  0.0024  0.0000
                                     0.0002  0.7593 -0.0003 -0.0071 -0.1990
                                     0.0038 -0.0006 -0.1862  0.0046  0.0001
                                     0.0084  0.0079 -0.0048 -0.0187  0.0109
              ( 53.54%)  -0.7317* C 11 s( 35.14%)p 1.84( 64.76%)d 0.00(  0.10%)
                                     0.0001 -0.5927 -0.0126 -0.0013 -0.0004
                                    -0.0004 -0.7403 -0.0169 -0.0049  0.2290
                                     0.0071  0.0010  0.2159  0.0077  0.0021
                                     0.0096  0.0091 -0.0057 -0.0244  0.0150
898. (0.01320) BD*( 1) C 13- C 17
              ( 49.63%)   0.7045* C 13 s( 36.14%)p 1.76( 63.78%)d 0.00(  0.09%)
                                     0.0000 -0.6010 -0.0125 -0.0032 -0.0001
```

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                                    0.0000  0.1028  0.0183 -0.0042 -0.5623
                                    0.0095 -0.0006 -0.5572  0.0097 -0.0006
                                    0.0065  0.0061 -0.0257  0.0099 -0.0053
              ( 50.37%)  -0.7097* C 17 s( 35.55%)p 1.81( 64.36%)d 0.00(  0.09%)
                                    0.0000 -0.5962 -0.0063 -0.0038 -0.0001
                                    0.0001 -0.1484  0.0233 -0.0017  0.5636
                                   -0.0126 -0.0038  0.5506 -0.0117 -0.0039
                                    0.0046  0.0042 -0.0267  0.0114 -0.0062
899. (0.01659) BD*( 1) C 13- H 30
              ( 39.75%)   0.6305* C 13 s( 28.56%)p 2.50( 71.36%)d 0.00(  0.07%)
                                    0.0003 -0.5343  0.0035  0.0101  0.0002
                                   -0.0001 -0.7882 -0.0036  0.0050  0.2290
                                    0.0028 -0.0050  0.1997  0.0041 -0.0050
                                    0.0123  0.0103 -0.0033 -0.0182  0.0111
              ( 60.25%)  -0.7762* H 30 s( 99.94%)p 0.00(  0.06%)
                                   -0.9997 -0.0023 -0.0003  0.0235 -0.0043
                                   -0.0021
900. (0.02089) BD*( 1) C 11- C 15
              ( 51.97%)   0.7209* C 11 s( 37.24%)p 1.68( 62.67%)d 0.00(  0.09%)
                                   -0.0001  0.6092  0.0352 -0.0021  0.0003
                                    0.0000 -0.1577 -0.0174 -0.0047  0.5609
                                    0.0153  0.0048  0.5352  0.0130  0.0038
                                   -0.0009 -0.0009  0.0272 -0.0123  0.0060
              ( 48.03%)  -0.6930* C 15 s( 36.81%)p 1.71( 63.10%)d 0.00(  0.09%)
                                    0.0001  0.6066  0.0082  0.0016  0.0000
                                   -0.0004  0.0809  0.0148 -0.0024 -0.5707
                                    0.0093  0.0037 -0.5461  0.0101  0.0034
                                   -0.0063 -0.0057  0.0264 -0.0116  0.0050
901. (0.30039) BD*( 2) C 11- C 15
              ( 54.05%)   0.7352* C 11 s(  0.01%)p 1.00( 99.94%)d 0.00(  0.05%)
                                    0.0000  0.0064 -0.0030  0.0005  0.0000
                                    0.0000 -0.0107  0.0050 -0.0006 -0.6946
                                   -0.0246  0.0051  0.7176  0.0336 -0.0058
                                   -0.0083  0.0090  0.0010  0.0096  0.0169
              ( 45.95%)  -0.6778* C 15 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                   -0.0001 -0.0042  0.0001  0.0003  0.0000
                                    0.0000 -0.0142  0.0005  0.0003 -0.6945
                                    0.0012 -0.0040  0.7191 -0.0026  0.0048
                                   -0.0090  0.0091 -0.0006 -0.0059 -0.0093
902. (0.28627) BD*( 1) C 11-Ru 51
              ( 40.40%)   0.6356* C 11 s( 27.65%)p 2.62( 72.34%)d 0.00(  0.01%)
                                   -0.0001  0.5249 -0.0325  0.0025 -0.0006
                                   -0.0002 -0.6509  0.0371 -0.0030 -0.3835
                                    0.0394 -0.0012 -0.3860  0.0292  0.0005
                                    0.0053  0.0031  0.0036 -0.0005 -0.0015
              ( 59.60%)  -0.7720*Ru 51 s( 26.47%)p 0.00(  0.06%)d 2.78( 73.47%)
                                    0.0000  0.0000 -0.0001  0.0007  0.5143
                                    0.0116 -0.0086  0.0010  0.0008 -0.0013
                                    0.0016 -0.0004  0.0001  0.0000  0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0007 -0.0137  0.0053 -0.0029  0.0003
                                    0.0000  0.0000  0.0000 -0.0008 -0.0068
                                    0.0099 -0.0097  0.0002  0.0000  0.0000
                                    0.0000 -0.0010 -0.0027  0.0089 -0.0018
                                    0.0001  0.0000  0.0001  0.6055 -0.0009
                                   -0.0003  0.0013  0.0000  0.0000  0.3728
                                    0.0033  0.0001  0.0010  0.0000  0.0000
                                    0.4386 -0.0132  0.0017  0.0007  0.0000
                                    0.0000 -0.0922 -0.0051  0.0062  0.0000
                                    0.0000  0.0000 -0.1673  0.0060  0.0001
                                   -0.0002  0.0000
903. (0.01534) BD*( 1) C 17- C 19
              ( 49.80%)   0.7057* C 17 s( 35.29%)p 1.83( 64.62%)d 0.00(  0.09%)
                                    0.0000 -0.5940 -0.0051 -0.0041 -0.0001
                                    0.0001  0.7414 -0.0083 -0.0042 -0.2350
                                    0.0179 -0.0020 -0.2017  0.0174 -0.0021
                                    0.0119  0.0097 -0.0041 -0.0217  0.0129
              ( 50.20%)  -0.7085* C 19 s( 35.33%)p 1.83( 64.58%)d 0.00(  0.09%)
                                    0.0000 -0.5943 -0.0078 -0.0033  0.0000
                                   -0.0001 -0.7608  0.0222  0.0015  0.1971
                                    0.0098 -0.0026  0.1655  0.0103 -0.0027
                                    0.0136  0.0115 -0.0042 -0.0208  0.0126
904. (0.35553) BD*( 2) C 17- C 19
              ( 48.27%)   0.6947* C 17 s(  0.00%)p 1.00( 99.98%)d 0.00(  0.02%)
                                    0.0000  0.0000  0.0010 -0.0001  0.0000
                                    0.0000 -0.0291 -0.0002 -0.0001 -0.7022
                                   -0.0122 -0.0065  0.7110  0.0120  0.0064
                                    0.0104 -0.0106  0.0005 -0.0011 -0.0034
              ( 51.73%)  -0.7193* C 19 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                    0.0000  0.0003  0.0007 -0.0001  0.0000
                                    0.0000 -0.0266 -0.0006 -0.0003 -0.7004
                                   -0.0104 -0.0056  0.7128  0.0107  0.0062
                                   -0.0078  0.0084 -0.0005 -0.0063 -0.0102
905. (0.01446) BD*( 1) C 17- H 34
              ( 39.10%)   0.6253* C 17 s( 29.11%)p 2.43( 70.81%)d 0.00(  0.08%)
                                    0.0004 -0.5394  0.0090  0.0073  0.0001
                                   -0.0001 -0.6525 -0.0079  0.0038 -0.3644
                                   -0.0045  0.0007 -0.3865 -0.0042  0.0010
                                   -0.0166 -0.0174 -0.0083 -0.0098  0.0050
              ( 60.90%)  -0.7804* H 34 s( 99.96%)p 0.00(  0.04%)
                                   -0.9998 -0.0022 -0.0005  0.0146  0.0083
                                    0.0093
906. (0.01454) BD*( 1) C 19- H 35
              ( 39.12%)   0.6255* C 19 s( 28.61%)p 2.49( 71.31%)d 0.00(  0.08%)
                                    0.0004 -0.5348  0.0064  0.0085 -0.0001
                                    0.0001  0.1361  0.0001 -0.0029 -0.5971
                                   -0.0083  0.0018 -0.5813 -0.0077  0.0016
                                    0.0059  0.0058 -0.0232  0.0125 -0.0063
              ( 60.88%)  -0.7803* H 35 s( 99.96%)p 0.00(  0.04%)
                                   -0.9998 -0.0021  0.0000 -0.0034  0.0130
                                    0.0132
907. (0.02223) BD*( 1) C 15- C 19
              ( 50.11%)   0.7079* C 15 s( 35.02%)p 1.85( 64.88%)d 0.00(  0.10%)
                                   -0.0001  0.5917  0.0075  0.0045  0.0002
                                    0.0000  0.6167  0.0080  0.0001  0.3644
                                   -0.0147  0.0050  0.3676 -0.0146  0.0052
                                    0.0178  0.0182  0.0113  0.0126 -0.0072
              ( 49.89%)  -0.7063* C 19 s( 36.01%)p 1.77( 63.91%)d 0.00(  0.08%)
                                    0.0000  0.6001  0.0017  0.0056 -0.0001
                                    0.0001 -0.6322  0.0255  0.0032 -0.3363
                                   -0.0033  0.0034 -0.3543 -0.0026  0.0031
                                    0.0165  0.0173  0.0113  0.0095 -0.0049
908. (0.01908) BD*( 1) C 15- H 33
              ( 39.07%)   0.6250* C 15 s( 28.12%)p 2.55( 71.81%)d 0.00(  0.07%)
                                   -0.0004  0.5300 -0.0149 -0.0061 -0.0001
                                    0.0003 -0.7818 -0.0105  0.0076  0.2411
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                                    0.0039  0.0007  0.2205  0.0028 -0.0002
                                   -0.0120 -0.0105  0.0029  0.0177 -0.0106
              ( 60.93%)  -0.7806* H 33 s( 99.92%)p 0.00(  0.08%)
                                    0.9996  0.0013  0.0025  0.0259 -0.0077
                                   -0.0083
909. (0.24641) BD*( 1) C  4- O 44
              ( 74.95%)   0.8658* C  4 s(  0.15%)p99.99( 99.61%)d 1.54(  0.23%)
                                    0.0000 -0.0380 -0.0087 -0.0006  0.0003
                                    0.0002  0.7221 -0.0075 -0.0076  0.5234
                                   -0.0065 -0.0091  0.4477 -0.0051 -0.0026
                                    0.0192 -0.0281 -0.0044 -0.0243 -0.0238
              ( 25.05%)  -0.5005* O 44 s(  0.23%)p99.99( 99.39%)d 1.71(  0.39%)
                                    0.0000 -0.0475  0.0020  0.0001  0.0000
                                    0.0000  0.7032  0.0002  0.0009  0.6072
                                   -0.0014  0.0003  0.3614  0.0018  0.0008
                                   -0.0247  0.0334  0.0131  0.0334  0.0293
910. (0.18514) BD*( 2) C  4- O 44
              ( 74.32%)   0.8621* C  4 s(  0.00%)p 1.00( 99.77%)d 0.00(  0.22%)
                                    0.0000 -0.0059 -0.0009 -0.0006  0.0001
                                    0.0000 -0.6809  0.0046  0.0083  0.4395
                                   -0.0023 -0.0055  0.5837 -0.0060 -0.0074
                                   -0.0259  0.0178  0.0042 -0.0091 -0.0338
              ( 25.68%)  -0.5068* O 44 s(  0.00%)p 1.00( 99.61%)d 0.00(  0.39%)
                                    0.0000 -0.0044  0.0003  0.0000  0.0000
                                    0.0000 -0.6818  0.0007 -0.0008  0.4461
                                   -0.0006  0.0004  0.5764  0.0002  0.0008
                                    0.0335 -0.0253 -0.0052  0.0135  0.0441
911. (0.01434) BD*( 3) C  4- O 44
              ( 68.08%)   0.8251* C  4 s( 39.05%)p 1.56( 60.89%)d 0.00(  0.06%)
                                    0.0000  0.6101  0.1354 -0.0010 -0.0005
                                   -0.0005 -0.0699  0.0073 -0.0040  0.5817
                                   -0.0264  0.0181 -0.5131  0.0288 -0.0195
                                   -0.0036  0.0024 -0.0208 -0.0115  0.0037
              ( 31.92%)  -0.5649* O 44 s( 42.47%)p 1.34( 56.76%)d 0.02(  0.77%)
                                    0.0001  0.6512 -0.0237 -0.0025  0.0001
                                    0.0000  0.1628 -0.0049 -0.0009 -0.4722
                                    0.0214  0.0045  0.5632 -0.0218 -0.0046
                                   -0.0178  0.0184 -0.0734 -0.0320  0.0244
912. (0.34326) BD*( 1) C  4-Ru 51
              ( 33.60%)   0.5796* C  4 s( 62.06%)p 0.61( 37.93%)d 0.00(  0.01%)
                                   -0.0001 -0.7871  0.0334 -0.0003 -0.0001
                                   -0.0003 -0.0851  0.0001  0.0007  0.4299
                                    0.0295  0.0056 -0.4310 -0.0241 -0.0045
                                    0.0017  0.0006  0.0085  0.0049 -0.0011
              ( 66.40%)  -0.8149*Ru 51 s( 35.74%)p 0.00(  0.09%)d 1.80( 64.17%)
                                    0.0000  0.0000  0.0001  0.0009 -0.5974
                                   -0.0220  0.0084  0.0018 -0.0004 -0.0001
                                    0.0009 -0.0003  0.0002  0.0000  0.0001
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0003  0.0181  0.0111  0.0009 -0.0001
                                    0.0000  0.0000  0.0000  0.0007  0.0045
                                   -0.0058  0.0128  0.0003  0.0000  0.0000
                                    0.0000 -0.0007  0.0080  0.0142 -0.0015
                                   -0.0005  0.0000  0.0000  0.1203  0.0023
                                    0.0003 -0.0001  0.0000  0.0000 -0.1945
                                   -0.0122  0.0052 -0.0010  0.0000  0.0000
                                    0.6690  0.0320 -0.0033  0.0023  0.0001
                                    0.0000  0.2836  0.0128 -0.0039  0.0011
                                    0.0000  0.0000 -0.2447 -0.0116 -0.0007
                                   -0.0009  0.0000
913. (0.32707) BD*( 1) C 10-Ru 51
              ( 31.56%)   0.5618* C 10 s( 63.04%)p 0.59( 36.95%)d 0.00(  0.01%)
                                   -0.0001 -0.7931  0.0385 -0.0016 -0.0002
                                   -0.0003 -0.4185  0.0230 -0.0046  0.2943
                                   -0.0168  0.0038  0.3260 -0.0237  0.0052
                                    0.0048  0.0059 -0.0037 -0.0024  0.0000
              ( 68.44%)  -0.8273*Ru 51 s( 37.53%)p 0.00(  0.07%)d 1.66( 62.39%)
                                    0.0000  0.0000  0.0000  0.0009 -0.6122
                                   -0.0224  0.0047  0.0016  0.0001 -0.0008
                                    0.0001 -0.0002  0.0001  0.0000  0.0000
                                    0.0000  0.0000  0.0000  0.0000  0.0000
                                   -0.0004  0.0082  0.0173 -0.0041 -0.0006
                                    0.0000  0.0000  0.0000  0.0006  0.0044
                                    0.0012  0.0138  0.0000  0.0000  0.0000
                                    0.0000  0.0003  0.0080 -0.0064  0.0045
                                    0.0003  0.0000  0.0000  0.3840  0.0243
                                   -0.0036  0.0008  0.0001  0.0000  0.5124
                                    0.0197  0.0002  0.0013  0.0001  0.0000
                                   -0.2859 -0.0033  0.0033 -0.0012  0.0000
                                    0.0000 -0.3499 -0.0208  0.0007 -0.0006
                                   -0.0001  0.0000  0.0908 -0.0024 -0.0023
                                    0.0002  0.0000
914. (0.20527) BD*( 1) C 10- O 48
              ( 74.74%)   0.8645* C 10 s(  0.38%)p99.99( 99.39%)d 0.60(  0.23%)
                                    0.0000  0.0606  0.0123  0.0005 -0.0001
                                    0.0000  0.4815  0.0025 -0.0084 -0.1110
                                   -0.0062  0.0033  0.8655  0.0198 -0.0113
                                    0.0163 -0.0160  0.0188 -0.0140  0.0351
              ( 25.26%)  -0.5026* O 48 s(  0.33%)p99.99( 99.26%)d 1.21(  0.40%)
                                    0.0000  0.0578 -0.0021 -0.0002  0.0000
                                    0.0000  0.5713 -0.0022  0.0000 -0.1759
                                    0.0041  0.0001  0.7970 -0.0018  0.0012
                                   -0.0269  0.0141 -0.0170  0.0199 -0.0493
915. (0.23397) BD*( 2) C 10- O 48
              ( 74.91%)   0.8655* C 10 s(  0.70%)p99.99( 99.07%)d 0.33(  0.23%)
                                    0.0000 -0.0816 -0.0189 -0.0010  0.0004
                                    0.0001  0.5579  0.0002 -0.0045  0.7990
                                    0.0041 -0.0139 -0.2018 -0.0072  0.0010
                                   -0.0142  0.0175  0.0159 -0.0387 -0.0067
              ( 25.09%)  -0.5009* O 48 s(  0.72%)p99.99( 98.88%)d 0.56(  0.40%)
                                    0.0000 -0.0846  0.0035  0.0004  0.0000
                                    0.0000  0.4271  0.0052  0.0008  0.8921
                                   -0.0023  0.0002 -0.1030 -0.0006 -0.0007
                                    0.0285 -0.0165 -0.0286  0.0449  0.0097
916. (0.01837) BD*( 3) C 10- O 48
              ( 68.76%)   0.8292* C 10 s( 37.37%)p 1.67( 62.57%)d 0.00(  0.06%)
                                   -0.0001  0.5953  0.1388 -0.0020 -0.0008
                                   -0.0007 -0.5205 -0.0290 -0.0203  0.5058
                                    0.0175  0.0135  0.3109  0.0139  0.0172
                                   -0.0182 -0.0111  0.0115  0.0002 -0.0062
              ( 31.24%)  -0.5589* O 48 s( 42.68%)p 1.33( 56.56%)d 0.02(  0.76%)
                                    0.0001  0.6528 -0.0252 -0.0027  0.0001
                                    0.0000  0.5255 -0.0186 -0.0041 -0.2442
                                    0.0150  0.0032 -0.4785  0.0155  0.0030
                                   -0.0470 -0.0592  0.0376  0.0222 -0.0018
917. (0.01267) BD*( 1) C 21- C 23
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              ( 50.25%)   0.7089* C 21 s( 35.54%)p 1.81( 64.36%)d 0.00(  0.09%)
                                        0.0000  0.5961  0.0058  0.0039  0.0001
                                       -0.0001  0.5200 -0.0014 -0.0047 -0.5375
                                        0.0118  0.0038  0.2891 -0.0236  0.0001
                                       -0.0246  0.0098 -0.0111  0.0003 -0.0101
              ( 49.75%)  -0.7053* C 23 s( 35.95%)p 1.78( 63.96%)d 0.00(  0.09%)
                                        0.0000  0.5994  0.0131  0.0032  0.0001
                                       -0.0001 -0.5311  0.0167 -0.0021  0.5440
                                       -0.0066 -0.0002 -0.2472 -0.0144  0.0043
                                       -0.0233  0.0110 -0.0139 -0.0009 -0.0072
  918. (0.28104) BD*( 2) C 21- C 23
              ( 51.95%)   0.7207* C 21 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                        0.0000 -0.0017  0.0009 -0.0002  0.0000
                                       -0.0001  0.5864  0.0074  0.0052  0.7410
                                        0.0099  0.0071  0.3262  0.0041  0.0028
                                        0.0051  0.0036 -0.0064  0.0184 -0.0015
              ( 48.05%)  -0.6932* C 23 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.04%)
                                        0.0000 -0.0022  0.0010 -0.0002 -0.0001
                                       -0.0001  0.5934  0.0061  0.0056  0.7327
                                        0.0072  0.0069  0.3323  0.0039  0.0035
                                        0.0024 -0.0104 -0.0076 -0.0102 -0.0087
  919. (0.01456) BD*( 1) C 21- H 37
              ( 38.58%)   0.6211* C 21 s( 29.42%)p 2.40( 70.50%)d 0.00(  0.08%)
                                       -0.0003  0.5423 -0.0086 -0.0070 -0.0001
                                        0.0001 -0.6184 -0.0100  0.0007  0.2710
                                        0.0036 -0.0001  0.4990  0.0081 -0.0015
                                       -0.0105 -0.0211  0.0097  0.0108  0.0005
              ( 61.42%)  -0.7837* H 37 s( 99.96%)p 0.00(  0.04%)
                                        0.9998  0.0021  0.0002  0.0138 -0.0065
                                       -0.0116
  920. (0.01533) BD*( 1) C 23- H 38
              ( 38.79%)   0.6228* C 23 s( 29.60%)p 2.38( 70.33%)d 0.00(  0.07%)
                                        0.0004 -0.5440  0.0033  0.0092  0.0002
                                       -0.0002  0.0598 -0.0002  0.0037  0.3034
                                        0.0027 -0.0057 -0.7794 -0.0048  0.0061
                                       -0.0005  0.0028  0.0158  0.0029 -0.0202
              ( 61.21%)  -0.7824* H 38 s( 99.94%)p 0.00(  0.06%)
                                       -0.9997 -0.0021 -0.0001 -0.0031 -0.0078
                                        0.0230
  921. (0.03584) BD*( 1) C 20- N 50
              ( 59.31%)   0.7701* C 20 s( 29.92%)p 2.34( 70.01%)d 0.00(  0.07%)
                                        0.0001 -0.5466 -0.0197  0.0008 -0.0004
                                       -0.0002 -0.0565 -0.0065 -0.0006 -0.3186
                                       -0.0004  0.0001  0.7716  0.0098  0.0013
                                       -0.0001  0.0029  0.0163  0.0031 -0.0207
              ( 40.69%)  -0.6379* N 50 s( 33.94%)p 1.94( 65.88%)d 0.01(  0.18%)
                                        0.0001 -0.5824 -0.0135  0.0005 -0.0007
                                        0.0002  0.0647 -0.0066 -0.0015  0.3034
                                        0.0105  0.0019 -0.7498 -0.0143 -0.0012
                                        0.0003  0.0153  0.0204  0.0003 -0.0332
  922. (0.49866) BD*( 2) C 20- N 50
              ( 65.90%)   0.8118* C 20 s(  0.00%)p 1.00( 99.92%)d 0.00(  0.08%)
                                        0.0000  0.0036  0.0010  0.0002 -0.0001
                                        0.0000  0.5978  0.0243 -0.0015  0.7221
                                        0.0289 -0.0023  0.3445  0.0153 -0.0007
                                        0.0054 -0.0155 -0.0133 -0.0130 -0.0145
              ( 34.10%)  -0.5839* N 50 s(  0.00%)p 1.00( 99.91%)d 0.00(  0.09%)
                                        0.0000  0.0014  0.0000  0.0007 -0.0001
                                        0.0000  0.5824  0.0193 -0.0009  0.7341
                                        0.0243 -0.0013  0.3460  0.0146 -0.0010
                                       -0.0127  0.0054  0.0179 -0.0159  0.0135
  923. (0.03162) BD*( 1) C 20- C 23
              ( 49.73%)   0.7052* C 20 s( 35.44%)p 1.82( 64.50%)d 0.00(  0.07%)
                                        0.0002 -0.5953  0.0001  0.0024 -0.0001
                                        0.0000  0.5887 -0.0155  0.0013 -0.2537
                                        0.0120 -0.0001 -0.4833 -0.0012 -0.0020
                                        0.0103  0.0190 -0.0094 -0.0100  0.0006
              ( 50.27%)  -0.7090* C 23 s( 34.40%)p 1.90( 65.50%)d 0.00(  0.09%)
                                        0.0000 -0.5865  0.0072 -0.0068 -0.0002
                                        0.0002 -0.6007  0.0114  0.0022  0.2720
                                       -0.0080 -0.0002  0.4690 -0.0011 -0.0037
                                        0.0124  0.0236 -0.0089 -0.0113 -0.0032
  924. (0.03005) BD*( 1) C 20- C 22
              ( 49.07%)   0.7005* C 20 s( 34.65%)p 1.88( 65.30%)d 0.00(  0.05%)
                                        0.0003 -0.5885  0.0130 -0.0016  0.0004
                                        0.0000 -0.5395  0.0151  0.0027  0.5573
                                       -0.0130 -0.0011 -0.2257  0.0004 -0.0021
                                        0.0174 -0.0060  0.0055  0.0007  0.0098
              ( 50.93%)  -0.7137* C 22 s( 30.47%)p 2.28( 69.46%)d 0.00(  0.07%)
                                        0.0002 -0.5519  0.0082 -0.0013  0.0002
                                       -0.0003  0.5678 -0.0083  0.0016 -0.5855
                                        0.0102 -0.0006  0.1708 -0.0074 -0.0018
                                        0.0216 -0.0073  0.0074  0.0006  0.0110
  925. (0.02958) BD*( 1) C 22- C 25
              ( 49.08%)   0.7006* C 22 s( 34.61%)p 1.89( 65.32%)d 0.00(  0.07%)
                                        0.0003 -0.5883 -0.0063  0.0002 -0.0003
                                        0.0000 -0.0040  0.0057 -0.0001  0.3357
                                       -0.0088  0.0010 -0.7351  0.0040 -0.0027
                                        0.0008  0.0009  0.0163  0.0033 -0.0194
              ( 50.92%)  -0.7136* C 25 s( 35.21%)p 1.84( 64.71%)d 0.00(  0.08%)
                                        0.0000 -0.5933  0.0063 -0.0078 -0.0002
                                        0.0002  0.0447 -0.0063  0.0003 -0.3525
                                        0.0108  0.0013  0.7215 -0.0094 -0.0030
                                        0.0024 -0.0002  0.0188  0.0040 -0.0208
  926. (0.27531) BD*( 1) C 16-Ru 52
              ( 40.28%)   0.6347* C 16 s( 27.83%)p 2.59( 72.16%)d 0.00(  0.01%)
                                       -0.0001  0.5265 -0.0324  0.0024 -0.0006
                                       -0.0002 -0.0237  0.0060  0.0018  0.3735
                                       -0.0375  0.0010 -0.7602  0.0477 -0.0024
                                       -0.0008  0.0009 -0.0065 -0.0024  0.0026
              ( 59.72%)  -0.7728*Ru 52 s( 27.00%)p 0.00(  0.05%)d 2.70( 72.94%)
                                        0.0000  0.0000 -0.0001  0.0007  0.5194
                                        0.0130 -0.0091  0.0005  0.0009 -0.0011
                                        0.0015 -0.0005  0.0001  0.0000  0.0000
                                        0.0000  0.0001 -0.0001  0.0000  0.0000
                                       -0.0004  0.0044  0.0046 -0.0002  0.0000
                                        0.0000  0.0000  0.0000  0.0006  0.0062
                                       -0.0091  0.0100 -0.0002  0.0000  0.0000
                                        0.0000 -0.0012 -0.0134  0.0086 -0.0038
                                        0.0003  0.0000  0.0000 -0.0615  0.0116
                                       -0.0024  0.0001  0.0000  0.0000  0.0838
                                        0.0079 -0.0021  0.0003  0.0000 -0.0001
                                       -0.7381  0.0062 -0.0005 -0.0016  0.0000
                                        0.0000 -0.3002  0.0017  0.0032 -0.0006
                                        0.0000  0.0000  0.2888 -0.0042  0.0040
                                        0.0010  0.0000
```

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927. (0.03384) BD*( 1) C 16- C 22
              ( 53.59%)   0.7320* C 16 s( 35.00%)p 1.85( 64.90%)d 0.00(  0.10%)
                                      -0.0001  0.5915  0.0126  0.0014  0.0005
                                       0.0004 -0.5379 -0.0145 -0.0041  0.2456
                                       0.0078  0.0011  0.5467  0.0109  0.0032
                                      -0.0103 -0.0258  0.0067  0.0083  0.0119
              ( 46.41%)  -0.6813* C 22 s( 34.87%)p 1.87( 65.07%)d 0.00(  0.06%)
                                      -0.0001  0.5905  0.0028 -0.0024  0.0000
                                      -0.0002  0.5253 -0.0040 -0.0035 -0.2142
                                       0.0037 -0.0004 -0.5734 -0.0020  0.0062
                                      -0.0088 -0.0198  0.0058  0.0070  0.0085
928. (0.02097) BD*( 1) C 16- C 18
              ( 51.97%)   0.7209* C 16 s( 37.20%)p 1.69( 62.70%)d 0.00(  0.09%)
                                       0.0001 -0.6090 -0.0344  0.0021 -0.0002
                                       0.0000 -0.5386 -0.0193 -0.0054  0.5660
                                       0.0158  0.0048 -0.1260  0.0088  0.0024
                                       0.0240 -0.0091  0.0127  0.0035  0.0096
              ( 48.03%)  -0.6931* C 18 s( 36.77%)p 1.72( 63.14%)d 0.00(  0.09%)
                                      -0.0001 -0.6063 -0.0081 -0.0016  0.0000
                                       0.0004  0.5122 -0.0016 -0.0040 -0.5735
                                       0.0089  0.0039  0.1992 -0.0181  0.0003
                                       0.0261 -0.0057  0.0076  0.0018  0.0125
929. (0.01536) BD*( 1) C 24- C 26
              ( 50.20%)   0.7085* C 24 s( 35.31%)p 1.83( 64.60%)d 0.00(  0.09%)
                                       0.0000  0.5941  0.0077  0.0033  0.0000
                                       0.0001 -0.5059  0.0016  0.0031  0.2134
                                       0.0093 -0.0026  0.5864 -0.0244 -0.0001
                                      -0.0107 -0.0238  0.0106  0.0087  0.0072
              ( 49.80%)  -0.7057* C 26 s( 35.27%)p 1.83( 64.64%)d 0.00(  0.09%)
                                       0.0000  0.5938  0.0050  0.0041  0.0001
                                      -0.0001  0.5282 -0.0189 -0.0003 -0.2507
                                       0.0180 -0.0019 -0.5513 -0.0014  0.0047
                                      -0.0098 -0.0235  0.0092  0.0083  0.0091
930. (0.01452) BD*( 1) C 24- H 36
              ( 39.09%)   0.6252* C 24 s( 28.62%)p 2.49( 71.30%)d 0.00(  0.08%)
                                       0.0004 -0.5349  0.0065  0.0085 -0.0001
                                       0.0001 -0.5664 -0.0068  0.0028  0.6034
                                       0.0084 -0.0018 -0.1670 -0.0037 -0.0018
                                       0.0230 -0.0069  0.0064  0.0015  0.0134
              ( 60.91%)  -0.7805* H 36 s( 99.96%)p 0.00(  0.04%)
                                      -0.9998 -0.0021  0.0000  0.0131 -0.0132
                                       0.0035
931. (0.02232) BD*( 1) C 18- C 24
              ( 50.12%)   0.7079* C 18 s( 35.03%)p 1.85( 64.87%)d 0.00(  0.10%)
                                      -0.0001  0.5918  0.0077  0.0045  0.0002
                                       0.0000  0.0242 -0.0163  0.0043 -0.3525
                                       0.0149 -0.0049  0.7234 -0.0003  0.0025
                                      -0.0013 -0.0008 -0.0205 -0.0043  0.0234
              ( 49.88%)  -0.7063* C 24 s( 36.03%)p 1.77( 63.89%)d 0.00(  0.08%)
                                       0.0000  0.6002  0.0018  0.0056 -0.0001
                                       0.0001 -0.0060 -0.0143  0.0012  0.3240
                                       0.0039 -0.0033 -0.7302  0.0210  0.0043
                                      -0.0019  0.0017 -0.0194 -0.0044  0.0203
932. (0.31818) BD*( 2) C 18- C 24
              ( 48.86%)   0.6990* C 18 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                       0.0000 -0.0001  0.0000 -0.0001  0.0000
                                       0.0000 -0.6509 -0.0046 -0.0057 -0.6906
                                      -0.0069 -0.0063 -0.3146 -0.0018 -0.0030
                                       0.0052 -0.0081 -0.0110  0.0039 -0.0084
              ( 51.14%)  -0.7151* C 24 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                       0.0000 -0.0020 -0.0005  0.0001  0.0000
                                       0.0000 -0.6496 -0.0079 -0.0058 -0.6960
                                      -0.0088 -0.0061 -0.3051 -0.0037 -0.0026
                                      -0.0027  0.0095  0.0046  0.0117  0.0062
933. (0.01892) BD*( 1) C 18- H 32
              ( 39.07%)   0.6250* C 18 s( 28.15%)p 2.55( 71.78%)d 0.00(  0.07%)
                                       0.0004 -0.5304  0.0149  0.0061  0.0001
                                      -0.0003 -0.5588 -0.0073  0.0037  0.2625
                                       0.0040  0.0006  0.5800  0.0078 -0.0066
                                       0.0088  0.0206 -0.0097 -0.0077 -0.0057
              ( 60.93%)  -0.7806* H 32 s( 99.92%)p 0.00(  0.08%)
                                      -0.9996 -0.0012 -0.0025  0.0196 -0.0085
                                      -0.0187
934. (0.00644) BD*( 1) H 43- O 45
              ( 74.33%)   0.8621* H 43 s( 99.99%)p 0.00(  0.01%)
                                      -0.9999 -0.0036 -0.0005 -0.0006 -0.0013
                                      -0.0093
              ( 25.67%)  -0.5067* O 45 s( 22.37%)p 3.46( 77.38%)d 0.01(  0.25%)
                                       0.0000 -0.4725  0.0212  0.0037 -0.0002
                                       0.0000  0.7970  0.0362  0.0010 -0.1547
                                      -0.0063  0.0000  0.3355  0.0268  0.0011
                                       0.0154 -0.0243  0.0057 -0.0349  0.0195


NHO DIRECTIONALITY AND BOND BENDING (deviations from line of nuclear centers)

       [Thresholds for printing:  angular deviation  >  1.0 degree]
                                  p- or d-character  > 25.0%
                                  orbital occupancy  >  0.10e

                    Line of Centers        Hybrid 1              Hybrid 2
                    ---------------  -------------------  -------------------
          NBO         Theta    Phi    Theta    Phi    Dev    Theta    Phi    Dev
==========================================================================================
  2. BD ( 2) C 1- C 2    66.3  159.3    46.8  273.1  89.6     46.8  274.0  89.7
  3. BD ( 1) C 1- C 3    69.3   23.3    70.5   22.5   1.4      --     --     --
  5. BD ( 1) C 2- H27   106.1  200.7   108.0  201.1   1.9      --     --     --
  6. BD ( 1) C 2- N49    42.9   91.6    43.0   88.8   2.0    136.9  268.0   2.5
  8. BD ( 2) C 3- C 5    43.1   91.8    47.2  -87.5  90.2     46.7  272.7  90.2
 10. BD ( 1) C 4- O44   134.9  102.5   117.0  215.5  85.7    111.0  221.0  86.4
 11. BD ( 2) C 4- O44   134.9  102.5    54.6  147.0  89.8     54.2  147.1  89.8
 12. BD ( 3) C 4- O44   134.9  102.5   131.1   96.6   5.8     41.5  289.1   5.7
 13. BD ( 1) C 4-Ru51    44.1  281.9    45.8  280.3   2.1    137.6  104.0   2.2
 14. BD ( 1) C 5- C 7    68.2  160.6     --     --    --     110.5  342.1   2.0
 16. BD ( 1) C 6- O46   111.7  326.0    32.9  359.0  83.5     22.9   16.8  83.5
 17. BD ( 2) C 6- O46   111.7  326.0   124.1    0.0  32.3    106.1   65.2  87.7
 18. BD ( 3) C 6- O46   111.7  326.0   119.8  318.7  10.5     77.8  153.1  11.6
 19. BD ( 1) C 6-Ru52    66.3  151.1    69.2  147.4   4.5    116.0  333.8   3.3
 20. BD ( 1) C 7- C 9    44.9  100.0    44.1   96.0   2.9    134.1  283.6   2.7
 22. BD ( 2) C 7- N49   110.9  204.7    46.1  273.0  89.9     46.8  -85.9  89.7
 23. BD ( 1) C 8- O47   117.4  230.6   134.4  117.2  85.9    129.8  109.2  86.5
 24. BD ( 2) C 8- O47   117.4  230.6   126.3  341.0  88.7    124.9  -16.4  88.8
 25. BD ( 3) C 8- O47   117.4  230.6   112.3  233.3   5.7     57.6   47.4   5.7
 26. BD ( 1) C 8-Ru52    62.6   49.5    64.1   51.0   2.0    119.0  228.1   2.1
 27. BD ( 1) C 9- C11    76.4  165.3     --     --    --     105.8  342.8   3.3
 28. BD ( 1) C 9- C13    62.7   29.6    64.3   28.2   2.0    118.5  210.3   1.4
```

29.	BD (2) C 9- C13	62.7	29.6	-44.9	89.5	89.4	45.1	267.7	89.5
30.	BD (1) C10- O48	58.5	144.3	-28.9	166.7	85.6	37.2	343.0	85.8
31.	BD (2) C10- O48	58.5	144.3	-77.7	54.7	83.9	84.3	244.5	84.4
32.	BD (3) C10- O48	58.5	144.3	66.4	136.7	10.4	129.6	335.4	12.1
33.	BD (1) C10-Ru51	121.5	330.9	122.2	324.9	5.1	60.0	155.1	4.0
34.	BD (1) C11- C15	46.8	100.4	47.8	107.1	5.0	--	--	--
35.	BD (2) C11- C15	46.8	100.4	43.7	269.5	90.0	44.1	268.9	89.7
36.	BD (1) C11-Ru51	116.2	219.6	116.8	209.2	9.3	64.0	49.2	8.6
37.	BD (1) C12- C14	56.0	155.9	55.4	157.1	1.1	--	--	--
38.	BD (2) C12- C14	56.0	155.9	-70.0	232.0	89.8	60.4	0.0	67.6
39.	BD (1) C12- H29	158.8	66.5	159.7	67.9	1.1	--	--	--
40.	BD (1) C12- N50	70.7	314.6	69.0	314.1	1.8	112.0	133.2	3.0
43.	BD (1) C14- C21	20.9	255.9	20.6	251.6	1.5	--	--	--
47.	BD (1) C16- C18	77.2	312.3	81.9	313.8	5.0	--	--	--
48.	BD (1) C16- C22	44.7	157.5	47.5	155.4	3.1	--	--	--
49.	BD (1) C16-Ru52	146.3	94.8	154.7	92.7	8.5	41.1	276.2	7.4
51.	BD (2) C17- C19	76.9	164.1	-44.7	87.6	90.0	44.5	267.8	90.0
54.	BD (2) C18- C24	25.1	272.9	64.2	0.0	65.6	72.3	47.0	89.7
57.	BD (1) C20- C22	76.0	313.9	73.2	313.8	2.7	101.4	134.3	2.7
58.	BD (1) C20- C23	53.5	156.2	52.0	157.2	1.7	--	--	--
59.	BD (1) C20- N50	157.7	76.9	--	--	--	22.7	259.6	1.1
60.	BD (2) C20- N50	157.7	76.9	69.8	50.4	90.0	59.0	0.0	66.2
62.	BD (2) C21- C23	70.5	314.2	109.0	231.7	89.6	109.5	231.0	89.6
64.	BD (1) C22- C25	25.2	273.8	24.1	269.7	2.0	154.2	96.5	1.3
69.	BD (2) C25- C26	78.1	313.4	107.6	227.5	89.8	107.6	227.1	89.8
147.	LP (1) C22	--	--	63.1	0.0	--	--	--	--
148.	LP (1) O44	--	--	45.0	282.7	--	--	--	--
149.	LP (1) O45	--	--	136.3	339.2	--	--	--	--
150.	LP (2) O45	--	--	7.9	348.8	--	--	--	--
151.	LP (3) O45	--	--	102.0	0.0	--	--	--	--
152.	LP (1) O46	--	--	111.6	325.9	--	--	--	--
153.	LP (1) O47	--	--	50.7	0.0	--	--	--	--
154.	LP (1) O48	--	--	121.5	324.2	--	--	--	--
155.	LP (1) N49	--	--	112.6	340.9	--	--	--	--
156.	LP (1) N50	--	--	125.9	337.2	--	--	--	--
157.	LP (1)Ru51	--	--	8.9	0.0	--	--	--	--
158.	LP (2)Ru51	--	--	56.2	357.2	--	--	--	--
159.	LP (3)Ru51	--	--	80.5	312.5	--	--	--	--
160.	LP (1)Ru52	--	--	65.1	327.0	--	--	--	--
161.	LP (2)Ru52	--	--	10.6	0.0	--	--	--	--
162.	LP (3)Ru52	--	--	86.0	0.0	--	--	--	--
163.	LP (1)Cl53	--	--	32.8	359.6	--	--	--	--
164.	LP (2)Cl53	--	--	120.8	342.9	--	--	--	--
165.	LP (3)Cl53	--	--	33.4	315.2	--	--	--	--
166.	LP (4)Cl53	--	--	71.1	0.0	--	--	--	--
167.	LP*(1) C16	--	--	63.2	0.0	--	--	--	--
864.	BD*(2) C12- C14	56.0	155.9	-70.0	232.0	89.8	60.4	0.0	67.6
870.	BD*(2) C25- C26	78.1	313.4	107.6	227.5	89.8	107.6	227.1	89.8
874.	BD*(2) C 3- C 5	43.1	91.8	47.2	-87.5	90.2	46.7	272.7	90.2
878.	BD*(1) C 8- O47	117.4	230.6	134.4	117.2	85.9	129.8	109.2	86.5
879.	BD*(2) C 8- O47	117.4	230.6	126.3	341.0	88.7	124.9	-16.4	88.8
881.	BD*(1) C 8-Ru52	62.6	49.5	64.1	51.0	2.0	119.0	228.1	2.1
882.	BD*(1) C 6-Ru52	66.3	151.1	69.2	147.4	4.5	116.0	333.8	3.3
883.	BD*(1) C 6- O46	111.7	326.0	32.9	359.0	83.5	22.9	16.8	83.5
884.	BD*(2) C 6- O46	111.7	326.0	124.1	0.0	32.3	106.1	65.2	87.7
888.	BD*(2) C 1- C 2	66.3	159.3	46.8	273.1	89.6	46.8	274.0	89.7
893.	BD*(2) C 7- N49	110.9	204.7	46.1	273.0	89.9	46.8	-85.9	89.7
896.	BD*(2) C 9- C13	62.7	29.6	-44.9	89.5	89.4	45.1	267.7	89.5
901.	BD*(2) C11- C15	46.8	100.4	43.7	269.5	90.0	44.1	268.9	89.7
902.	BD*(1) C11-Ru51	116.2	219.6	116.8	209.2	9.3	64.0	49.2	8.6
904.	BD*(2) C17- C19	76.9	164.1	-44.7	87.6	90.0	44.5	267.8	90.0
909.	BD*(1) C 4- O44	134.9	102.5	117.0	215.5	85.7	111.0	221.0	86.4
910.	BD*(2) C 4- O44	134.9	102.5	54.6	147.0	89.8	54.2	147.1	89.8
912.	BD*(1) C 4-Ru51	44.1	281.9	45.8	280.3	2.1	137.6	104.0	2.2
913.	BD*(1) C10-Ru51	121.5	330.9	122.2	324.9	5.1	60.0	155.1	4.0
914.	BD*(1) C10- O48	58.5	144.3	-28.9	166.7	85.6	37.2	343.0	85.8
915.	BD*(2) C10- O48	58.5	144.3	-77.7	54.7	83.9	84.3	244.5	84.4
918.	BD*(2) C21- C23	70.5	314.2	109.0	231.7	89.6	109.5	231.0	89.6
922.	BD*(2) C20- N50	157.7	76.9	69.8	50.4	90.0	59.0	0.0	66.2
926.	BD*(1) C16-Ru52	146.3	94.8	154.7	92.7	8.5	41.1	276.2	7.4
932.	BD*(2) C18- C24	25.1	272.9	64.2	0.0	65.6	72.3	47.0	89.7

3-Center, 4-Electron A:-B-:C Hyperbonds (A-B :C <=> A: B-C)
[threshold for detection: 33.3%]

				NBOs		3-center hybrids		
Hyperbond A:-B-:C	%A-B/%B-C	OCC.	BD(A-B)	LP(C)	h(A)	h(B)	h(C)
1. C 6:-Ru 52-: N 50	65.5/34.5	3.9159	19	156	37	38	228
2. C 10:-Ru 51-: N 49	64.9/35.1	3.9129	33	155	65	66	227
3. C 26:- C 25-: C 22	56.7/43.3	3.0616	69	147	137	138	219

*** sorry: cannot construct NLMOMO matrix.
*** AOMO matrix not available

CMO: NBO Analysis of Canonical Molecular Orbitals

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.50 kcal/mol
(Intermolecular threshold: 0.05 kcal/mol)

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1- C 2	199. RY*(2) C 3	0.97	2.37	0.043
1. BD (1) C 1- C 2	718. RY*(1) N49	1.85	2.58	0.062
1. BD (1) C 1- C 2	748. RY*(1)Ru51	0.62	18.72	0.096
1. BD (1) C 1- C 2	755. RY*(8)Ru51	0.61	6.80	0.058
1. BD (1) C 1- C 2	759. RY*(12)Ru51	0.54	15.40	0.082
1. BD (1) C 1- C 2	767. RY*(20)Ru51	0.56	17.86	0.089
1. BD (1) C 1- C 2	776. RY*(29)Ru51	0.68	78.09	0.206
1. BD (1) C 1- C 2	777. RY*(30)Ru51	0.57	26.37	0.110
1. BD (1) C 1- C 2	780. RY*(33)Ru51	0.59	324.99	0.391
1. BD (1) C 1- C 2	875. BD*(1) C 3- H41	2.41	1.03	0.045
1. BD (1) C 1- C 2	886. BD*(1) C 1- C 3	0.72	1.10	0.025
1. BD (1) C 1- C 2	890. BD*(1) C 2- N49	0.55	1.10	0.022
2. BD (2) C 1- C 2	200. RY*(3) C 3	0.94	0.78	0.027
2. BD (2) C 1- C 2	719. RY*(2) N49	0.85	1.10	0.030
2. BD (2) C 1- C 2	874. BD*(2) C 3- C 5	16.57	0.23	0.056
2. BD (2) C 1- C 2	888. BD*(2) C 1- C 2	0.60	0.23	0.011
2. BD (2) C 1- C 2	893. BD*(2) C 7- N49	10.69	0.21	0.044

3. BD (1) C 1- C 3	230. RY*(3) C 5	0.98	2.31	0.043
3. BD (1) C 1- C 3	873. BD*(1) C 3- C 5	0.81	1.12	0.027
3. BD (1) C 1- C 3	877. BD*(1) C 5- H28	2.48	1.03	0.045
3. BD (1) C 1- C 3	887. BD*(1) C 1- C 2	0.76	1.12	0.026
3. BD (1) C 1- C 3	891. BD*(1) C 2- H27	2.40	1.03	0.044
4. BD (1) C 1- H42	183. RY*(1) C 2	0.68	1.99	0.033
4. BD (1) C 1- H42	198. RY*(1) C 3	0.85	2.22	0.039
4. BD (1) C 1- H42	873. BD*(1) C 3- C 5	3.39	0.95	0.051
4. BD (1) C 1- H42	890. BD*(1) C 2- N49	5.27	0.92	0.062
5. BD (1) C 2- H27	168. RY*(1) C 1	0.88	2.14	0.039
5. BD (1) C 2- H27	718. RY*(1) N49	2.04	2.39	0.063
5. BD (1) C 2- H27	748. RY*(1)Ru51	0.79	18.54	0.109
5. BD (1) C 2- H27	755. RY*(8)Ru51	0.91	6.62	0.070
5. BD (1) C 2- H27	757. RY*(10)Ru51	0.78	21.72	0.117
5. BD (1) C 2- H27	759. RY*(12)Ru51	0.80	15.22	0.099
5. BD (1) C 2- H27	764. RY*(17)Ru51	0.62	11.01	0.075
5. BD (1) C 2- H27	767. RY*(20)Ru51	0.78	17.68	0.106
5. BD (1) C 2- H27	776. RY*(29)Ru51	0.69	77.91	0.209
5. BD (1) C 2- H27	777. RY*(30)Ru51	0.54	26.19	0.107
5. BD (1) C 2- H27	780. RY*(33)Ru51	0.66	324.81	0.416
5. BD (1) C 2- H27	785. RY*(38)Ru51	0.50	596.64	0.493
5. BD (1) C 2- H27	886. BD*(1) C 1- C 3	3.28	0.92	0.049
5. BD (1) C 2- H27	892. BD*(1) C 7- N49	6.93	0.90	0.070
6. BD (1) C 2- N49	170. RY*(3) C 1	0.80	2.62	0.041
6. BD (1) C 2- N49	188. RY*(6) C 2	1.11	4.43	0.063
6. BD (1) C 2- N49	189. RY*(7) C 2	0.62	5.62	0.053
6. BD (1) C 2- N49	196. RY*(14) C 2	0.63	40.77	0.144
6. BD (1) C 2- N49	197. RY*(15) C 2	0.89	26.93	0.139
6. BD (1) C 2- N49	219. RY*(7) C 4	0.58	7.40	0.059
6. BD (1) C 2- N49	258. RY*(1) C 7	0.75	2.32	0.037
6. BD (1) C 2- N49	260. RY*(3) C 7	1.93	2.74	0.065
6. BD (1) C 2- N49	293. RY*(6) C 9	0.70	4.66	0.051
6. BD (1) C 2- N49	720. RY*(3) N49	0.53	2.89	0.035
6. BD (1) C 2- N49	721. RY*(4) N49	1.36	5.32	0.076
6. BD (1) C 2- N49	748. RY*(1)Ru51	2.15	18.83	0.180
6. BD (1) C 2- N49	750. RY*(3)Ru51	1.02	9.03	0.086
6. BD (1) C 2- N49	754. RY*(7)Ru51	0.53	4.97	0.046
6. BD (1) C 2- N49	755. RY*(8)Ru51	2.75	6.91	0.124
6. BD (1) C 2- N49	757. RY*(10)Ru51	2.48	22.02	0.209
6. BD (1) C 2- N49	759. RY*(12)Ru51	2.95	15.51	0.192
6. BD (1) C 2- N49	760. RY*(13)Ru51	1.50	5.55	0.082
6. BD (1) C 2- N49	761. RY*(14)Ru51	1.00	8.30	0.082
6. BD (1) C 2- N49	762. RY*(15)Ru51	1.58	14.99	0.138
6. BD (1) C 2- N49	763. RY*(16)Ru51	0.70	13.57	0.087
6. BD (1) C 2- N49	764. RY*(17)Ru51	1.89	11.31	0.131
6. BD (1) C 2- N49	767. RY*(20)Ru51	2.41	17.98	0.186
6. BD (1) C 2- N49	772. RY*(25)Ru51	1.32	9406.82	3.159
6. BD (1) C 2- N49	773. RY*(26)Ru51	0.74	37514.38	4.712
6. BD (1) C 2- N49	776. RY*(29)Ru51	2.27	78.20	0.377
6. BD (1) C 2- N49	777. RY*(30)Ru51	1.69	26.49	0.189
6. BD (1) C 2- N49	780. RY*(33)Ru51	2.17	325.10	0.752
6. BD (1) C 2- N49	785. RY*(38)Ru51	1.74	596.94	0.914
6. BD (1) C 2- N49	789. RY*(42)Ru51	1.24	533.54	0.730
6. BD (1) C 2- N49	887. BD*(1) C 1- C 2	0.77	1.24	0.028
6. BD (1) C 2- N49	889. BD*(1) C 1- H42	1.64	1.15	0.039
6. BD (1) C 2- N49	892. BD*(1) C 7- N49	0.63	1.19	0.025
6. BD (1) C 2- N49	894. BD*(1) C 7- C 9	2.68	1.19	0.051
6. BD (1) C 2- N49	913. BD*(1) C10-Ru51	4.82	0.88	0.063
7. BD (1) C 3- C 5	170. RY*(3) C 1	0.86	2.51	0.042
7. BD (1) C 3- C 5	258. RY*(1) C 7	0.67	2.21	0.035
7. BD (1) C 3- C 5	876. BD*(1) C 5- C 7	1.07	1.12	0.031
7. BD (1) C 3- C 5	886. BD*(1) C 1- C 3	0.77	1.11	0.026
7. BD (1) C 3- C 5	889. BD*(1) C 1- H42	2.44	1.04	0.045
7. BD (1) C 3- C 5	894. BD*(1) C 7- C 9	3.59	1.08	0.056
8. BD (2) C 3- C 5	169. RY*(2) C 1	1.10	0.79	0.029
8. BD (2) C 3- C 5	263. RY*(6) C 7	0.63	2.07	0.035
8. BD (2) C 3- C 5	888. BD*(2) C 1- C 2	12.35	0.23	0.048
8. BD (2) C 3- C 5	893. BD*(2) C 7- N49	22.41	0.21	0.064
9. BD (1) C 3- H41	168. RY*(1) C 1	0.87	2.15	0.039
9. BD (1) C 3- H41	228. RY*(1) C 5	0.91	2.02	0.039
9. BD (1) C 3- H41	876. BD*(1) C 5- C 7	3.87	0.95	0.054
9. BD (1) C 3- H41	887. BD*(1) C 1- C 2	3.37	0.96	0.051
12. BD (3) C 4- O44	188. RY*(6) C 2	3.44	4.73	0.114
12. BD (3) C 4- O44	189. RY*(7) C 2	0.57	5.93	0.052
12. BD (3) C 4- O44	213. RY*(1) C 4	13.96	3.33	0.193
12. BD (3) C 4- O44	214. RY*(2) C 4	0.96	2.55	0.044
12. BD (3) C 4- O44	215. RY*(3) C 4	1.04	2.67	0.047
12. BD (3) C 4- O44	219. RY*(7) C 4	8.20	7.70	0.225
12. BD (3) C 4- O44	220. RY*(8) C 4	2.15	5.15	0.094
12. BD (3) C 4- O44	221. RY*(9) C 4	0.71	4.02	0.048
12. BD (3) C 4- O44	224. RY*(12) C 4	0.64	4.44	0.048
12. BD (3) C 4- O44	227. RY*(15) C 4	0.59	27.69	0.114
12. BD (3) C 4- O44	264. RY*(7) C 7	1.54	5.11	0.079
12. BD (3) C 4- O44	288. RY*(1) C 9	0.64	2.52	0.036
12. BD (3) C 4- O44	293. RY*(6) C 9	1.64	4.97	0.081
12. BD (3) C 4- O44	303. RY*(1) C10	2.87	3.15	0.085
12. BD (3) C 4- O44	309. RY*(7) C10	1.22	7.76	0.087
12. BD (3) C 4- O44	310. RY*(8) C10	0.88	5.06	0.060
12. BD (3) C 4- O44	315. RY*(13) C10	0.65	3.87	0.045
12. BD (3) C 4- O44	318. RY*(1) C11	1.15	2.32	0.046
12. BD (3) C 4- O44	319. RY*(2) C11	0.82	1.82	0.034
12. BD (3) C 4- O44	321. RY*(4) C11	0.87	3.34	0.048
12. BD (3) C 4- O44	326. RY*(9) C11	0.56	15.06	0.082
12. BD (3) C 4- O44	329. RY*(12) C11	0.93	4.22	0.056
12. BD (3) C 4- O44	330. RY*(13) C11	0.71	4.56	0.051
12. BD (3) C 4- O44	383. RY*(6) C15	3.69	4.55	0.116
12. BD (3) C 4- O44	384. RY*(7) C15	0.76	9.26	0.075
12. BD (3) C 4- O44	595. RY*(3) H34	0.67	2.51	0.037
12. BD (3) C 4- O44	630. RY*(3) H41	0.62	2.31	0.034
12. BD (3) C 4- O44	645. RY*(3) O44	1.48	2.84	0.058
12. BD (3) C 4- O44	646. RY*(4) O44	3.28	1.80	0.069
12. BD (3) C 4- O44	647. RY*(5) O44	0.61	3.48	0.041
12. BD (3) C 4- O44	705. RY*(3) O48	0.69	3.07	0.041
12. BD (3) C 4- O44	706. RY*(4) O48	1.76	1.79	0.050
12. BD (3) C 4- O44	707. RY*(5) O48	0.79	3.17	0.045
12. BD (3) C 4- O44	718. RY*(1) N49	1.35	2.99	0.057
12. BD (3) C 4- O44	721. RY*(4) N49	0.51	5.63	0.048
12. BD (3) C 4- O44	726. RY*(9) N49	0.68	5.59	0.055
12. BD (3) C 4- O44	748. RY*(1)Ru51	20.43	19.13	0.559
12. BD (3) C 4- O44	749. RY*(2)Ru51	0.56	1.97	0.030
12. BD (3) C 4- O44	750. RY*(3)Ru51	17.43	9.33	0.360
12. BD (3) C 4- O44	752. RY*(5)Ru51	13.70	5.24	0.239
12. BD (3) C 4- O44	754. RY*(7)Ru51	1.75	5.28	0.086
12. BD (3) C 4- O44	755. RY*(8)Ru51	13.53	7.22	0.279
12. BD (3) C 4- O44	757. RY*(10)Ru51	10.46	22.32	0.432
12. BD (3) C 4- O44	759. RY*(12)Ru51	7.50	15.81	0.308

12. BD (3) C 4- O44	760. RY*(13)Ru51	6.70	5.86	0.177
12. BD (3) C 4- O44	761. RY*(14)Ru51	2.82	8.61	0.139
12. BD (3) C 4- O44	762. RY*(15)Ru51	10.59	15.30	0.360
12. BD (3) C 4- O44	763. RY*(16)Ru51	11.69	13.88	0.360
12. BD (3) C 4- O44	764. RY*(17)Ru51	9.02	11.61	0.289
12. BD (3) C 4- O44	765. RY*(18)Ru51	3.65	7.78	0.151
12. BD (3) C 4- O44	766. RY*(19)Ru51	4.85	7.92	0.175
12. BD (3) C 4- O44	767. RY*(20)Ru51	15.46	18.28	0.475
12. BD (3) C 4- O44	768. RY*(21)Ru51	2.26	17.93	0.180
12. BD (3) C 4- O44	769. RY*(22)Ru51	0.76	9.99	0.078
12. BD (3) C 4- O44	770. RY*(23)Ru51	7.07	17.23	0.312
12. BD (3) C 4- O44	772. RY*(25)Ru51	9.00	9407.13	8.222
12. BD (3) C 4- O44	773. RY*(26)Ru51	5.09	37514.68	12.355
12. BD (3) C 4- O44	774. RY*(27)Ru51	0.81	50.29	0.180
12. BD (3) C 4- O44	775. RY*(28)Ru51	0.50	187.15	0.274
12. BD (3) C 4- O44	776. RY*(29)Ru51	15.62	78.50	0.990
12. BD (3) C 4- O44	777. RY*(30)Ru51	12.72	26.79	0.522
12. BD (3) C 4- O44	780. RY*(33)Ru51	15.33	325.40	1.996
12. BD (3) C 4- O44	785. RY*(38)Ru51	12.19	597.24	2.412
12. BD (3) C 4- O44	788. RY*(41)Ru51	3.05	90.01	0.468
12. BD (3) C 4- O44	789. RY*(42)Ru51	8.62	533.84	1.917
12. BD (3) C 4- O44	792. RY*(45)Ru51	0.72	52.03	0.173
12. BD (3) C 4- O44	793. RY*(46)Ru51	0.58	187.11	0.294
13. BD (1) C 4-Ru51	213. RY*(1) C 4	1.80	2.79	0.064
13. BD (1) C 4-Ru51	219. RY*(7) C 4	1.43	7.15	0.092
13. BD (1) C 4-Ru51	304. RY*(2) C10	1.90	1.44	0.048
13. BD (1) C 4-Ru51	305. RY*(3) C10	2.92	3.14	0.087
13. BD (1) C 4-Ru51	317. RY*(15) C10	0.64	25.95	0.117
13. BD (1) C 4-Ru51	318. RY*(1) C11	1.60	1.77	0.048
13. BD (1) C 4-Ru51	645. RY*(3) O44	1.67	2.29	0.056
13. BD (1) C 4-Ru51	706. RY*(4) O48	0.84	1.25	0.030
13. BD (1) C 4-Ru51	718. RY*(1) N49	4.87	2.44	0.099
13. BD (1) C 4-Ru51	748. RY*(1)Ru51	0.62	18.59	0.097
13. BD (1) C 4-Ru51	750. RY*(3)Ru51	0.76	8.79	0.074
13. BD (1) C 4-Ru51	754. RY*(7)Ru51	1.19	4.73	0.068
13. BD (1) C 4-Ru51	756. RY*(9)Ru51	0.79	3.14	0.045
13. BD (1) C 4-Ru51	757. RY*(10)Ru51	0.58	21.77	0.102
13. BD (1) C 4-Ru51	759. RY*(12)Ru51	1.42	15.27	0.134
13. BD (1) C 4-Ru51	764. RY*(17)Ru51	0.52	11.06	0.069
13. BD (1) C 4-Ru51	767. RY*(20)Ru51	0.73	17.73	0.103
13. BD (1) C 4-Ru51	768. RY*(21)Ru51	0.60	17.38	0.093
13. BD (1) C 4-Ru51	777. RY*(30)Ru51	0.66	26.24	0.120
13. BD (1) C 4-Ru51	890. BD*(1) C 2- N49	0.61	0.97	0.022
13. BD (1) C 4-Ru51	892. BD*(1) C 7- N49	0.75	0.95	0.024
13. BD (1) C 4-Ru51	897. BD*(1) C 9- C11	0.56	1.02	0.022
13. BD (1) C 4-Ru51	900. BD*(1) C11- C15	0.73	1.03	0.025
13. BD (1) C 4-Ru51	901. BD*(2) C11- C15	0.51	0.55	0.016
13. BD (1) C 4-Ru51	902. BD*(1) C11-Ru51	17.21	0.55	0.092
13. BD (1) C 4-Ru51	911. BD*(3) C 4- O44	0.75	1.12	0.026
13. BD (1) C 4-Ru51	912. BD*(1) C 4-Ru51	2.04	0.60	0.033
13. BD (1) C 4-Ru51	913. BD*(1) C10-Ru51	15.87	0.64	0.096
13. BD (1) C 4-Ru51	914. BD*(1) C10- O48	1.73	0.52	0.028
13. BD (1) C 4-Ru51	915. BD*(2) C10- O48	1.25	0.52	0.024
13. BD (1) C 4-Ru51	916. BD*(3) C10- O48	1.66	1.12	0.039
14. BD (1) C 5- C 7	199. RY*(2) C 3	1.52	2.36	0.054
14. BD (1) C 5- C 7	290. RY*(3) C 9	0.79	2.46	0.040
14. BD (1) C 5- C 7	718. RY*(1) N49	0.72	2.57	0.039
14. BD (1) C 5- C 7	873. BD*(1) C 3- C 5	0.92	1.11	0.029
14. BD (1) C 5- C 7	875. BD*(1) C 3- H41	2.31	1.02	0.043
14. BD (1) C 5- C 7	892. BD*(1) C 7- N49	0.51	1.07	0.021
14. BD (1) C 5- C 7	894. BD*(1) C 7- C 9	1.10	1.07	0.031
14. BD (1) C 5- C 7	897. BD*(1) C 9- C11	2.18	1.14	0.045
15. BD (1) C 5- H28	198. RY*(1) C 3	0.91	2.22	0.040
15. BD (1) C 5- H28	258. RY*(1) C 7	1.00	2.04	0.041
15. BD (1) C 5- H28	886. BD*(1) C 1- C 3	3.52	0.93	0.051
15. BD (1) C 5- H28	892. BD*(1) C 7- N49	5.65	0.91	0.064
20. BD (1) C 7- C 9	228. RY*(1) C 5	0.78	2.13	0.037
20. BD (1) C 7- C 9	318. RY*(1) C11	0.98	1.84	0.038
20. BD (1) C 7- C 9	348. RY*(1) C13	0.85	2.14	0.038
20. BD (1) C 7- C 9	354. RY*(7) C13	0.56	7.85	0.060
20. BD (1) C 7- C 9	718. RY*(1) N49	0.89	2.52	0.043
20. BD (1) C 7- C 9	754. RY*(7)Ru51	0.70	4.80	0.052
20. BD (1) C 7- C 9	873. BD*(1) C 3- C 5	1.99	1.06	0.041
20. BD (1) C 7- C 9	876. BD*(1) C 5- C 7	0.99	1.06	0.029
20. BD (1) C 7- C 9	890. BD*(1) C 2- N49	4.72	1.04	0.062
20. BD (1) C 7- C 9	895. BD*(1) C 9- C13	0.86	1.08	0.027
20. BD (1) C 7- C 9	897. BD*(1) C 9- C11	1.04	1.09	0.030
20. BD (1) C 7- C 9	898. BD*(1) C13- C17	2.11	1.09	0.043
20. BD (1) C 7- C 9	900. BD*(1) C11- C15	2.57	1.11	0.048
21. BD (1) C 7- N49	185. RY*(3) C 2	2.44	2.55	0.071
21. BD (1) C 7- N49	233. RY*(6) C 5	0.58	7.03	0.057
21. BD (1) C 7- N49	235. RY*(8) C 5	0.51	3.93	0.040
21. BD (1) C 7- N49	265. RY*(8) C 7	0.69	12.36	0.083
21. BD (1) C 7- N49	268. RY*(11) C 7	0.52	6.27	0.051
21. BD (1) C 7- N49	271. RY*(14) C 7	0.76	42.72	0.161
21. BD (1) C 7- N49	272. RY*(15) C 7	1.01	24.65	0.141
21. BD (1) C 7- N49	288. RY*(1) C 9	0.57	2.20	0.032
21. BD (1) C 7- N49	291. RY*(4) C 9	0.56	1.92	0.029
21. BD (1) C 7- N49	720. RY*(3) N49	0.95	2.87	0.047
21. BD (1) C 7- N49	748. RY*(1)Ru51	0.54	18.81	0.090
21. BD (1) C 7- N49	749. RY*(2)Ru51	0.78	1.65	0.032
21. BD (1) C 7- N49	750. RY*(3)Ru51	1.05	9.01	0.087
21. BD (1) C 7- N49	754. RY*(7)Ru51	0.99	4.96	0.063
21. BD (1) C 7- N49	755. RY*(8)Ru51	0.56	6.90	0.056
21. BD (1) C 7- N49	757. RY*(10)Ru51	0.60	22.00	0.103
21. BD (1) C 7- N49	759. RY*(12)Ru51	1.21	15.50	0.123
21. BD (1) C 7- N49	762. RY*(15)Ru51	0.79	14.98	0.097
21. BD (1) C 7- N49	764. RY*(17)Ru51	0.52	11.29	0.069
21. BD (1) C 7- N49	767. RY*(20)Ru51	0.72	17.96	0.102
21. BD (1) C 7- N49	776. RY*(29)Ru51	0.73	78.18	0.215
21. BD (1) C 7- N49	777. RY*(30)Ru51	0.63	26.47	0.116
21. BD (1) C 7- N49	780. RY*(33)Ru51	0.70	325.08	0.427
21. BD (1) C 7- N49	785. RY*(38)Ru51	0.54	596.92	0.508
21. BD (1) C 7- N49	876. BD*(1) C 5- C 7	0.99	1.22	0.031
21. BD (1) C 7- N49	877. BD*(1) C 5- H28	1.67	1.13	0.039
21. BD (1) C 7- N49	891. BD*(1) C 2- H27	1.81	1.13	0.040
21. BD (1) C 7- N49	894. BD*(1) C 7- C 9	0.64	1.17	0.024
21. BD (1) C 7- N49	895. BD*(1) C 9- C13	2.30	1.24	0.048
21. BD (1) C 7- N49	913. BD*(1) C10-Ru51	5.43	0.87	0.067
22. BD (2) C 7- N49	184. RY*(2) C 2	2.86	0.94	0.050
22. BD (2) C 7- N49	229. RY*(2) C 5	0.97	0.76	0.026
22. BD (2) C 7- N49	289. RY*(2) C 9	0.67	0.85	0.023
22. BD (2) C 7- N49	874. BD*(2) C 3- C 5	7.48	0.27	0.041
22. BD (2) C 7- N49	888. BD*(2) C 1- C 2	20.33	0.28	0.067
22. BD (2) C 7- N49	896. BD*(2) C 9- C13	7.39	0.30	0.044
22. BD (2) C 7- N49	912. BD*(1) C 4-Ru51	0.55	0.37	0.013

27. BD (1) C 9- C11	258. RY*(1) C 7	0.90	2.16	0.040
27. BD (1) C 9- C11	290. RY*(3) C 9	0.64	2.42	0.035
27. BD (1) C 9- C11	293. RY*(6) C 9	0.82	4.50	0.055
27. BD (1) C 9- C11	296. RY*(9) C 9	0.93	14.34	0.104
27. BD (1) C 9- C11	301. RY*(14) C 9	0.85	42.23	0.171
27. BD (1) C 9- C11	302. RY*(15) C 9	1.00	26.36	0.146
27. BD (1) C 9- C11	318. RY*(1) C11	0.89	1.85	0.036
27. BD (1) C 9- C11	350. RY*(3) C13	0.73	2.34	0.037
27. BD (1) C 9- C11	351. RY*(4) C13	1.00	2.15	0.042
27. BD (1) C 9- C11	354. RY*(7) C13	0.53	7.85	0.058
27. BD (1) C 9- C11	355. RY*(8) C13	0.57	3.41	0.040
27. BD (1) C 9- C11	378. RY*(1) C15	0.65	2.26	0.034
27. BD (1) C 9- C11	380. RY*(3) C15	1.67	2.36	0.057
27. BD (1) C 9- C11	748. RY*(1)Ru51	0.94	18.66	0.119
27. BD (1) C 9- C11	749. RY*(2)Ru51	0.91	1.50	0.033
27. BD (1) C 9- C11	750. RY*(3)Ru51	1.47	8.86	0.102
27. BD (1) C 9- C11	754. RY*(7)Ru51	1.28	4.81	0.070
27. BD (1) C 9- C11	755. RY*(8)Ru51	0.80	6.75	0.066
27. BD (1) C 9- C11	757. RY*(10)Ru51	1.29	21.85	0.151
27. BD (1) C 9- C11	759. RY*(12)Ru51	1.09	15.34	0.116
27. BD (1) C 9- C11	760. RY*(13)Ru51	0.57	5.38	0.050
27. BD (1) C 9- C11	761. RY*(14)Ru51	0.85	8.14	0.075
27. BD (1) C 9- C11	762. RY*(15)Ru51	0.85	14.83	0.101
27. BD (1) C 9- C11	763. RY*(16)Ru51	0.66	13.40	0.085
27. BD (1) C 9- C11	764. RY*(17)Ru51	0.61	11.14	0.074
27. BD (1) C 9- C11	767. RY*(20)Ru51	1.34	17.81	0.139
27. BD (1) C 9- C11	772. RY*(25)Ru51	0.58	9406.65	2.106
27. BD (1) C 9- C11	776. RY*(29)Ru51	1.09	78.03	0.262
27. BD (1) C 9- C11	777. RY*(30)Ru51	0.91	26.32	0.139
27. BD (1) C 9- C11	780. RY*(33)Ru51	1.04	324.93	0.524
27. BD (1) C 9- C11	781. RY*(34)Ru51	0.52	50.79	0.145
27. BD (1) C 9- C11	785. RY*(38)Ru51	0.80	596.77	0.621
27. BD (1) C 9- C11	789. RY*(42)Ru51	0.55	533.37	0.485
27. BD (1) C 9- C11	876. BD*(1) C 5- C 7	3.48	1.07	0.054
27. BD (1) C 9- C11	894. BD*(1) C 7- C 9	1.05	1.02	0.029
27. BD (1) C 9- C11	895. BD*(1) C 9- C13	2.12	1.09	0.043
27. BD (1) C 9- C11	899. BD*(1) C13- H30	2.30	1.00	0.043
27. BD (1) C 9- C11	900. BD*(1) C11- C15	0.55	1.11	0.022
27. BD (1) C 9- C11	908. BD*(1) C15- H33	2.91	1.01	0.048
28. BD (1) C 9- C13	260. RY*(3) C 7	1.18	2.59	0.050
28. BD (1) C 9- C13	320. RY*(3) C11	0.66	1.64	0.029
28. BD (1) C 9- C13	410. RY*(3) C17	1.70	2.53	0.059
28. BD (1) C 9- C13	892. BD*(1) C 7- N49	2.80	1.04	0.048
28. BD (1) C 9- C13	894. BD*(1) C 7- C 9	0.96	1.04	0.028
28. BD (1) C 9- C13	897. BD*(1) C 9- C11	2.18	1.11	0.044
28. BD (1) C 9- C13	898. BD*(1) C13- C17	1.01	1.11	0.030
28. BD (1) C 9- C13	902. BD*(1) C11-Ru51	3.18	0.64	0.043
28. BD (1) C 9- C13	905. BD*(1) C17- H34	2.31	1.02	0.043
29. BD (2) C 9- C13	262. RY*(5) C 7	0.52	2.00	0.032
29. BD (2) C 9- C13	289. RY*(2) C 9	0.81	0.77	0.025
29. BD (2) C 9- C13	319. RY*(2) C11	0.84	0.97	0.028
29. BD (2) C 9- C13	409. RY*(2) C17	1.07	0.71	0.027
29. BD (2) C 9- C13	893. BD*(2) C 7- N49	23.93	0.18	0.060
29. BD (2) C 9- C13	896. BD*(2) C 9- C13	0.51	0.23	0.010
29. BD (2) C 9- C13	901. BD*(2) C11- C15	15.34	0.24	0.055
29. BD (2) C 9- C13	904. BD*(2) C17- C19	14.31	0.22	0.051
32. BD (3) C10- O48	188. RY*(6) C 2	3.09	4.72	0.108
32. BD (3) C10- O48	213. RY*(1) C 4	3.88	3.33	0.102
32. BD (3) C10- O48	219. RY*(7) C 4	4.29	7.69	0.162
32. BD (3) C10- O48	264. RY*(7) C 7	1.16	5.11	0.069
32. BD (3) C10- O48	288. RY*(1) C 9	0.70	2.51	0.037
32. BD (3) C10- O48	293. RY*(6) C 9	1.10	4.96	0.066
32. BD (3) C10- O48	303. RY*(1) C10	12.59	3.15	0.178
32. BD (3) C10- O48	305. RY*(3) C10	2.34	3.68	0.083
32. BD (3) C10- O48	309. RY*(7) C10	5.49	7.75	0.184
32. BD (3) C10- O48	310. RY*(8) C10	2.16	5.05	0.093
32. BD (3) C10- O48	316. RY*(14) C10	0.62	46.62	0.151
32. BD (3) C10- O48	317. RY*(15) C10	0.65	26.49	0.117
32. BD (3) C10- O48	318. RY*(1) C11	1.22	2.31	0.047
32. BD (3) C10- O48	319. RY*(2) C11	0.95	1.82	0.037
32. BD (3) C10- O48	321. RY*(4) C11	0.58	3.33	0.039
32. BD (3) C10- O48	329. RY*(12) C11	0.99	4.22	0.058
32. BD (3) C10- O48	330. RY*(13) C11	0.63	4.55	0.048
32. BD (3) C10- O48	380. RY*(3) C15	0.57	2.82	0.036
32. BD (3) C10- O48	383. RY*(6) C15	4.00	4.54	0.120
32. BD (3) C10- O48	384. RY*(7) C15	0.76	9.25	0.075
32. BD (3) C10- O48	595. RY*(3) H34	0.68	2.50	0.037
32. BD (3) C10- O48	630. RY*(3) H41	0.55	2.30	0.032
32. BD (3) C10- O48	646. RY*(4) O44	2.41	1.79	0.059
32. BD (3) C10- O48	647. RY*(5) O44	1.09	3.47	0.055
32. BD (3) C10- O48	705. RY*(3) O48	2.17	3.06	0.073
32. BD (3) C10- O48	706. RY*(4) O48	2.02	1.79	0.054
32. BD (3) C10- O48	718. RY*(1) N49	0.80	2.98	0.044
32. BD (3) C10- O48	726. RY*(9) N49	0.57	5.58	0.050
32. BD (3) C10- O48	748. RY*(1)Ru51	19.28	19.13	0.542
32. BD (3) C10- O48	750. RY*(3)Ru51	18.86	9.32	0.374
32. BD (3) C10- O48	751. RY*(4)Ru51	1.21	2.32	0.047
32. BD (3) C10- O48	752. RY*(5)Ru51	13.08	5.23	0.234
32. BD (3) C10- O48	753. RY*(6)Ru51	4.51	4.18	0.123
32. BD (3) C10- O48	755. RY*(8)Ru51	11.40	7.21	0.256
32. BD (3) C10- O48	757. RY*(10)Ru51	15.56	22.31	0.526
32. BD (3) C10- O48	759. RY*(12)Ru51	4.98	15.81	0.251
32. BD (3) C10- O48	760. RY*(13)Ru51	5.69	5.85	0.163
32. BD (3) C10- O48	761. RY*(14)Ru51	1.76	8.60	0.110
32. BD (3) C10- O48	762. RY*(15)Ru51	9.84	15.29	0.347
32. BD (3) C10- O48	763. RY*(16)Ru51	6.73	13.87	0.273
32. BD (3) C10- O48	764. RY*(17)Ru51	10.77	11.60	0.316
32. BD (3) C10- O48	765. RY*(18)Ru51	3.46	7.77	0.147
32. BD (3) C10- O48	766. RY*(19)Ru51	6.63	7.91	0.205
32. BD (3) C10- O48	767. RY*(20)Ru51	16.23	18.27	0.487
32. BD (3) C10- O48	768. RY*(21)Ru51	5.66	17.92	0.285
32. BD (3) C10- O48	770. RY*(23)Ru51	7.09	17.22	0.312
32. BD (3) C10- O48	772. RY*(25)Ru51	9.50	9407.12	8.451
32. BD (3) C10- O48	773. RY*(26)Ru51	5.31	37514.67	12.616
32. BD (3) C10- O48	776. RY*(29)Ru51	16.35	78.50	1.012
32. BD (3) C10- O48	777. RY*(30)Ru51	12.36	26.78	0.514
32. BD (3) C10- O48	780. RY*(33)Ru51	15.74	325.39	2.023
32. BD (3) C10- O48	781. RY*(34)Ru51	0.72	51.25	0.172
32. BD (3) C10- O48	785. RY*(38)Ru51	12.72	597.23	2.464
32. BD (3) C10- O48	788. RY*(41)Ru51	3.15	90.00	0.476
32. BD (3) C10- O48	789. RY*(42)Ru51	9.08	533.83	1.967
33. BD (1) C10-Ru51	215. RY*(3) C 4	1.55	2.13	0.052
33. BD (1) C10-Ru51	288. RY*(1) C 9	0.51	1.98	0.029
33. BD (1) C10-Ru51	303. RY*(1) C10	1.17	2.61	0.050
33. BD (1) C10-Ru51	309. RY*(7) C10	0.59	7.21	0.060
33. BD (1) C10-Ru51	318. RY*(1) C11	2.11	1.77	0.055

33. BD (1) C10-Ru51	588. RY*(1) H33	0.55	1.91	0.029
33. BD (1) C10-Ru51	705. RY*(3) O48	2.20	2.53	0.068
33. BD (1) C10-Ru51	715. RY*(13) O48	0.51	70.42	0.173
33. BD (1) C10-Ru51	721. RY*(4) N49	0.67	5.09	0.053
33. BD (1) C10-Ru51	897. BD*(1) C 9- C11	1.96	1.03	0.040
33. BD (1) C10-Ru51	902. BD*(1) C11-Ru51	12.74	0.56	0.079
33. BD (1) C10-Ru51	910. BD*(2) C 4- O44	2.04	0.52	0.030
33. BD (1) C10-Ru51	911. BD*(3) C 4- O44	1.50	1.13	0.037
33. BD (1) C10-Ru51	912. BD*(1) C 4-Ru51	12.20	0.61	0.083
33. BD (1) C10-Ru51	913. BD*(1) C10-Ru51	0.99	0.65	0.024
33. BD (1) C10-Ru51	916. BD*(3) C10- O48	0.65	1.13	0.024
34. BD (1) C11- C15	188. RY*(6) C 2	0.70	4.27	0.049
34. BD (1) C11- C15	213. RY*(1) C 4	1.27	2.87	0.054
34. BD (1) C11- C15	219. RY*(7) C 4	1.52	7.24	0.094
34. BD (1) C11- C15	264. RY*(7) C 7	0.85	4.65	0.056
34. BD (1) C11- C15	288. RY*(1) C 9	1.97	2.05	0.057
34. BD (1) C11- C15	290. RY*(3) C 9	1.35	2.42	0.051
34. BD (1) C11- C15	303. RY*(1) C10	1.08	2.69	0.048
34. BD (1) C11- C15	318. RY*(1) C11	1.05	1.85	0.040
34. BD (1) C11- C15	320. RY*(3) C11	0.70	1.63	0.030
34. BD (1) C11- C15	321. RY*(4) C11	2.65	2.87	0.078
34. BD (1) C11- C15	326. RY*(9) C11	0.86	14.60	0.100
34. BD (1) C11- C15	380. RY*(3) C15	0.73	2.37	0.037
34. BD (1) C11- C15	381. RY*(4) C15	0.66	1.64	0.030
34. BD (1) C11- C15	383. RY*(6) C15	2.37	4.08	0.088
34. BD (1) C11- C15	384. RY*(7) C15	0.75	8.80	0.073
34. BD (1) C11- C15	391. RY*(14) C15	0.68	27.48	0.123
34. BD (1) C11- C15	392. RY*(15) C15	0.62	40.82	0.142
34. BD (1) C11- C15	440. RY*(3) C19	1.35	2.49	0.052
34. BD (1) C11- C15	441. RY*(4) C19	0.53	1.99	0.029
34. BD (1) C11- C15	588. RY*(1) H33	0.60	1.99	0.031
34. BD (1) C11- C15	589. RY*(2) H33	0.56	2.53	0.034
34. BD (1) C11- C15	592. RY*(5) H33	0.69	4.73	0.051
34. BD (1) C11- C15	646. RY*(4) O44	0.83	1.33	0.030
34. BD (1) C11- C15	706. RY*(4) O48	0.57	1.33	0.025
34. BD (1) C11- C15	748. RY*(1)Ru51	5.25	18.67	0.280
34. BD (1) C11- C15	750. RY*(3)Ru51	5.23	8.87	0.193
34. BD (1) C11- C15	752. RY*(5)Ru51	4.92	4.77	0.137
34. BD (1) C11- C15	753. RY*(6)Ru51	1.43	3.72	0.065
34. BD (1) C11- C15	754. RY*(7)Ru51	1.42	4.81	0.074
34. BD (1) C11- C15	755. RY*(8)Ru51	1.90	6.75	0.102
34. BD (1) C11- C15	757. RY*(10)Ru51	4.06	21.86	0.267
34. BD (1) C11- C15	758. RY*(11)Ru51	1.66	7.45	0.100
34. BD (1) C11- C15	759. RY*(12)Ru51	3.41	15.35	0.205
34. BD (1) C11- C15	760. RY*(13)Ru51	2.13	5.39	0.096
34. BD (1) C11- C15	761. RY*(14)Ru51	0.81	8.14	0.073
34. BD (1) C11- C15	762. RY*(15)Ru51	3.37	14.83	0.201
34. BD (1) C11- C15	763. RY*(16)Ru51	3.38	13.41	0.191
34. BD (1) C11- C15	764. RY*(17)Ru51	2.22	11.15	0.141
34. BD (1) C11- C15	766. RY*(19)Ru51	1.80	7.46	0.104
34. BD (1) C11- C15	767. RY*(20)Ru51	4.70	17.82	0.260
34. BD (1) C11- C15	768. RY*(21)Ru51	3.05	17.47	0.207
34. BD (1) C11- C15	770. RY*(23)Ru51	0.83	16.77	0.106
34. BD (1) C11- C15	772. RY*(25)Ru51	2.63	9406.66	4.464
34. BD (1) C11- C15	773. RY*(26)Ru51	1.53	37514.22	6.790
34. BD (1) C11- C15	776. RY*(29)Ru51	4.52	78.04	0.533
34. BD (1) C11- C15	777. RY*(30)Ru51	3.68	26.33	0.279
34. BD (1) C11- C15	780. RY*(33)Ru51	4.51	324.94	1.086
34. BD (1) C11- C15	785. RY*(38)Ru51	3.58	596.78	1.311
34. BD (1) C11- C15	788. RY*(41)Ru51	0.95	89.55	0.261
34. BD (1) C11- C15	789. RY*(42)Ru51	2.52	533.38	1.040
34. BD (1) C11- C15	894. BD*(1) C 7- C 9	3.68	1.03	0.055
34. BD (1) C11- C15	897. BD*(1) C 9- C11	0.68	1.11	0.025
34. BD (1) C11- C15	906. BD*(1) C19- H35	2.20	1.01	0.042
34. BD (1) C11- C15	907. BD*(1) C15- C19	1.11	1.09	0.031
34. BD (1) C11- C15	908. BD*(1) C15- H33	0.72	1.02	0.024
35. BD (2) C11- C15	289. RY*(2) C 9	1.84	0.76	0.037
35. BD (2) C11- C15	319. RY*(2) C11	0.56	0.96	0.023
35. BD (2) C11- C15	439. RY*(2) C19	1.42	0.73	0.032
35. BD (2) C11- C15	896. BD*(2) C 9- C13	14.86	0.22	0.051
35. BD (2) C11- C15	904. BD*(2) C17- C19	18.02	0.21	0.056
35. BD (2) C11- C15	912. BD*(1) C 4-Ru51	1.03	0.28	0.015
36. BD (1) C11-Ru51	288. RY*(1) C 9	0.80	1.80	0.035
36. BD (1) C11-Ru51	304. RY*(2) C10	0.82	1.27	0.030
36. BD (1) C11-Ru51	305. RY*(3) C10	2.81	2.97	0.085
36. BD (1) C11-Ru51	378. RY*(1) C15	0.83	2.01	0.038
36. BD (1) C11-Ru51	380. RY*(3) C15	0.52	2.12	0.031
36. BD (1) C11-Ru51	718. RY*(1) N49	3.62	2.28	0.084
36. BD (1) C11-Ru51	876. BD*(1) C 5- C 7	0.69	0.82	0.022
36. BD (1) C11-Ru51	890. BD*(1) C 2- N49	1.65	0.80	0.033
36. BD (1) C11-Ru51	894. BD*(1) C 7- C 9	0.61	0.78	0.020
36. BD (1) C11-Ru51	895. BD*(1) C 9- C13	6.53	0.84	0.068
36. BD (1) C11-Ru51	902. BD*(1) C11-Ru51	2.42	0.38	0.028
36. BD (1) C11-Ru51	907. BD*(1) C15- C19	5.66	0.84	0.064
36. BD (1) C11-Ru51	908. BD*(1) C15- H33	0.91	0.76	0.024
36. BD (1) C11-Ru51	909. BD*(1) C 4- O44	2.09	0.35	0.025
36. BD (1) C11-Ru51	911. BD*(3) C 4- O44	0.54	0.95	0.021
36. BD (1) C11-Ru51	912. BD*(1) C 4-Ru51	15.38	0.43	0.077
36. BD (1) C11-Ru51	913. BD*(1) C10-Ru51	16.14	0.47	0.082
36. BD (1) C11-Ru51	914. BD*(1) C10- O48	0.63	0.35	0.013
36. BD (1) C11-Ru51	915. BD*(2) C10- O48	1.85	0.35	0.023
36. BD (1) C11-Ru51	916. BD*(3) C10- O48	1.53	0.95	0.035
41. BD (1) C13- C17	288. RY*(1) C 9	0.69	2.07	0.034
41. BD (1) C13- C17	440. RY*(3) C19	1.04	2.51	0.046
41. BD (1) C13- C17	894. BD*(1) C 7- C 9	3.42	1.05	0.054
41. BD (1) C13- C17	895. BD*(1) C 9- C13	1.27	1.11	0.034
41. BD (1) C13- C17	903. BD*(1) C17- C19	0.87	1.10	0.028
41. BD (1) C13- C17	906. BD*(1) C19- H35	2.33	1.03	0.044
42. BD (1) C13- H30	288. RY*(1) C 9	1.11	1.91	0.041
42. BD (1) C13- H30	408. RY*(1) C17	0.96	2.18	0.041
42. BD (1) C13- H30	897. BD*(1) C 9- C11	5.02	0.96	0.062
42. BD (1) C13- H30	903. BD*(1) C17- C19	3.56	0.94	0.052
45. BD (1) C15- C19	318. RY*(1) C11	1.05	1.86	0.040
45. BD (1) C15- C19	410. RY*(3) C17	0.99	2.53	0.045
45. BD (1) C15- C19	748. RY*(1)Ru51	0.59	18.68	0.094
45. BD (1) C15- C19	750. RY*(3)Ru51	0.58	8.88	0.065
45. BD (1) C15- C19	776. RY*(29)Ru51	0.57	78.05	0.189
45. BD (1) C15- C19	780. RY*(33)Ru51	0.52	324.95	0.368
45. BD (1) C15- C19	900. BD*(1) C11- C15	1.46	1.13	0.036
45. BD (1) C15- C19	902. BD*(1) C11-Ru51	3.43	0.64	0.045
45. BD (1) C15- C19	903. BD*(1) C17- C19	0.77	1.09	0.026
45. BD (1) C15- C19	905. BD*(1) C17- H34	2.35	1.02	0.044
46. BD (1) C15- H33	318. RY*(1) C11	1.71	1.69	0.048
46. BD (1) C15- H33	438. RY*(1) C19	0.90	2.03	0.038
46. BD (1) C15- H33	444. RY*(7) C19	0.54	6.71	0.054
46. BD (1) C15- H33	897. BD*(1) C 9- C11	3.79	0.94	0.053

46. BD (1) C15- H33	903. BD*(1) C17- C19	3.73	0.92	0.052
50. BD (1) C17- C19	350. RY*(3) C13	1.01	2.36	0.044
50. BD (1) C17- C19	381. RY*(4) C15	0.71	1.65	0.031
50. BD (1) C17- C19	898. BD*(1) C13- C17	0.95	1.11	0.029
50. BD (1) C17- C19	899. BD*(1) C13- H30	2.53	1.01	0.045
50. BD (1) C17- C19	907. BD*(1) C15- C19	0.81	1.10	0.027
50. BD (1) C17- C19	908. BD*(1) C15- H33	2.17	1.02	0.042
51. BD (2) C17- C19	349. RY*(2) C13	0.57	0.75	0.020
51. BD (2) C17- C19	352. RY*(5) C13	0.52	2.01	0.032
51. BD (2) C17- C19	379. RY*(2) C15	0.66	0.72	0.021
51. BD (2) C17- C19	896. BD*(2) C 9- C13	16.27	0.23	0.055
51. BD (2) C17- C19	901. BD*(2) C11- C15	12.38	0.24	0.050
52. BD (1) C17- H34	348. RY*(1) C13	0.96	2.00	0.039
52. BD (1) C17- H34	438. RY*(1) C19	0.96	2.05	0.040
52. BD (1) C17- H34	895. BD*(1) C 9- C13	4.02	0.94	0.055
52. BD (1) C17- H34	907. BD*(1) C15- C19	3.72	0.94	0.053
56. BD (1) C19- H35	378. RY*(1) C15	0.89	2.11	0.039
56. BD (1) C19- H35	408. RY*(1) C17	0.93	2.17	0.040
56. BD (1) C19- H35	898. BD*(1) C13- C17	3.66	0.95	0.053
56. BD (1) C19- H35	900. BD*(1) C11- C15	4.82	0.96	0.061
73. CR (1) C 1	186. RY*(4) C 2	0.91	11.22	0.090
73. CR (1) C 1	199. RY*(2) C 3	1.04	11.50	0.098
73. CR (1) C 1	890. BD*(1) C 2- N49	0.68	10.23	0.075
74. CR (1) C 2	168. RY*(1) C 1	0.75	11.49	0.083
74. CR (1) C 2	170. RY*(3) C 1	0.64	11.68	0.077
74. CR (1) C 2	892. BD*(1) C 7- N49	1.08	10.24	0.095
75. CR (1) C 3	170. RY*(3) C 1	1.36	11.65	0.112
75. CR (1) C 3	230. RY*(3) C 5	1.33	11.45	0.110
76. CR (1) C 4	646. RY*(4) O44	0.85	10.62	0.085
77. CR (1) C 5	199. RY*(2) C 3	1.17	11.50	0.104
77. CR (1) C 5	260. RY*(3) C 7	1.14	11.76	0.104
77. CR (1) C 5	892. BD*(1) C 7- N49	0.67	10.21	0.074
77. CR (1) C 5	894. BD*(1) C 7- C 9	0.93	10.21	0.087
79. CR (1) C 7	228. RY*(1) C 5	0.61	11.36	0.074
79. CR (1) C 7	288. RY*(1) C 9	0.54	11.27	0.070
79. CR (1) C 7	720. RY*(3) N49	0.54	11.95	0.072
79. CR (1) C 7	890. BD*(1) C 2- N49	0.94	10.27	0.088
79. CR (1) C 7	895. BD*(1) C 9- C13	0.61	10.32	0.071
79. CR (1) C 7	897. BD*(1) C 9- C11	0.61	10.33	0.072
81. CR (1) C 9	258. RY*(1) C 7	0.56	11.33	0.072
81. CR (1) C 9	320. RY*(3) C11	0.86	10.79	0.086
81. CR (1) C 9	348. RY*(1) C13	0.52	11.31	0.068
81. CR (1) C 9	350. RY*(3) C13	0.59	11.51	0.073
81. CR (1) C 9	876. BD*(1) C 5- C 7	0.80	10.24	0.081
81. CR (1) C 9	892. BD*(1) C 7- N49	0.51	10.19	0.065
81. CR (1) C 9	902. BD*(1) C11-Ru51	0.59	9.79	0.074
82. CR (1) C10	706. RY*(4) O48	0.96	10.61	0.090
83. CR (1) C11	288. RY*(1) C 9	0.53	11.22	0.069
83. CR (1) C11	290. RY*(3) C 9	0.90	11.59	0.091
83. CR (1) C11	380. RY*(3) C15	1.04	11.54	0.098
83. CR (1) C11	894. BD*(1) C 7- C 9	0.68	10.20	0.075
83. CR (1) C11	895. BD*(1) C 9- C13	0.73	10.26	0.078
83. CR (1) C11	902. BD*(1) C11-Ru51	0.51	9.80	0.068
83. CR (1) C11	907. BD*(1) C15- C19	0.59	10.26	0.070
85. CR (1) C13	290. RY*(3) C 9	0.93	11.58	0.092
85. CR (1) C13	410. RY*(3) C17	1.25	11.68	0.108
85. CR (1) C13	894. BD*(1) C 7- C 9	0.77	10.19	0.079
85. CR (1) C13	897. BD*(1) C 9- C11	0.92	10.26	0.087
87. CR (1) C15	320. RY*(3) C11	0.89	10.77	0.088
87. CR (1) C15	321. RY*(4) C11	0.57	12.02	0.074
87. CR (1) C15	440. RY*(3) C19	0.91	11.64	0.092
87. CR (1) C15	902. BD*(1) C11-Ru51	0.79	9.78	0.085
89. CR (1) C17	350. RY*(3) C13	1.29	11.50	0.109
89. CR (1) C17	440. RY*(3) C19	1.28	11.64	0.109
89. CR (1) C17	895. BD*(1) C 9- C13	0.57	10.25	0.069
91. CR (1) C19	380. RY*(3) C15	0.80	11.52	0.086
91. CR (1) C19	381. RY*(4) C15	0.61	10.79	0.073
91. CR (1) C19	410. RY*(3) C17	0.86	11.68	0.089
91. CR (1) C19	900. BD*(1) C11- C15	0.86	10.27	0.084
99. CR (1) O44	213. RY*(1) C 4	4.35	20.84	0.270
99. CR (1) O44	912. BD*(1) C 4-Ru51	0.70	18.65	0.112
103. CR (1) O48	303. RY*(1) C10	4.87	20.66	0.284
103. CR (1) O48	913. BD*(1) C10-Ru51	0.61	18.70	0.104
104. CR (1) N49	183. RY*(1) C 2	0.89	15.39	0.105
104. CR (1) N49	185. RY*(3) C 2	0.93	15.68	0.108
104. CR (1) N49	258. RY*(1) C 7	0.98	15.44	0.110
104. CR (1) N49	260. RY*(3) C 7	0.97	15.86	0.111
104. CR (1) N49	913. BD*(1) C10-Ru51	4.69	14.00	0.250
107. CR (2)Ru51	776. RY*(29)Ru51	1.12	191.09	0.413
107. CR (2)Ru51	780. RY*(33)Ru51	2.49	437.99	0.932
107. CR (2)Ru51	785. RY*(38)Ru51	3.32	709.83	1.371
107. CR (2)Ru51	788. RY*(41)Ru51	0.81	202.60	0.361
107. CR (2)Ru51	789. RY*(42)Ru51	4.14	646.43	1.460
107. CR (2)Ru51	911. BD*(3) C 4- O44	0.87	114.26	0.282
107. CR (2)Ru51	916. BD*(3) C10- O48	0.98	114.26	0.299
108. CR (3)Ru51	748. RY*(1)Ru51	1.47	40.00	0.217
108. CR (3)Ru51	750. RY*(3)Ru51	0.84	30.20	0.142
108. CR (3)Ru51	755. RY*(8)Ru51	0.61	28.09	0.117
108. CR (3)Ru51	757. RY*(10)Ru51	1.29	43.19	0.211
108. CR (3)Ru51	759. RY*(12)Ru51	0.62	36.69	0.135
108. CR (3)Ru51	762. RY*(15)Ru51	0.76	36.17	0.148
108. CR (3)Ru51	763. RY*(16)Ru51	0.54	34.75	0.122
108. CR (3)Ru51	764. RY*(17)Ru51	0.60	32.48	0.125
108. CR (3)Ru51	767. RY*(20)Ru51	1.05	39.15	0.181
108. CR (3)Ru51	770. RY*(23)Ru51	0.51	38.10	0.125
108. CR (3)Ru51	776. RY*(29)Ru51	2.83	99.38	0.473
108. CR (3)Ru51	777. RY*(30)Ru51	0.96	47.66	0.190
108. CR (3)Ru51	780. RY*(33)Ru51	4.60	346.27	1.127
108. CR (3)Ru51	785. RY*(38)Ru51	5.34	618.11	1.622
108. CR (3)Ru51	788. RY*(41)Ru51	1.97	110.88	0.417
108. CR (3)Ru51	789. RY*(42)Ru51	12.89	554.71	2.387
108. CR (3)Ru51	890. BD*(1) C 2- N49	0.81	22.38	0.121
108. CR (3)Ru51	892. BD*(1) C 7- N49	0.69	22.36	0.112
108. CR (3)Ru51	897. BD*(1) C 9- C11	0.60	22.44	0.104
108. CR (3)Ru51	900. BD*(1) C11- C15	1.48	22.45	0.164
108. CR (3)Ru51	902. BD*(1) C11-Ru51	0.77	21.97	0.125
108. CR (3)Ru51	911. BD*(3) C 4- O44	3.69	22.54	0.258
108. CR (3)Ru51	916. BD*(3) C10- O48	4.14	22.54	0.274
109. CR (4)Ru51	213. RY*(1) C 4	3.22	6.87	0.133
109. CR (4)Ru51	303. RY*(1) C10	3.96	6.69	0.145
109. CR (4)Ru51	309. RY*(7) C10	0.55	11.29	0.070
109. CR (4)Ru51	318. RY*(1) C11	0.65	5.85	0.055
109. CR (4)Ru51	748. RY*(1)Ru51	1.47	22.67	0.163
109. CR (4)Ru51	750. RY*(3)Ru51	0.99	12.87	0.101
109. CR (4)Ru51	752. RY*(5)Ru51	0.63	8.77	0.067
109. CR (4)Ru51	755. RY*(8)Ru51	0.88	10.75	0.087

109. CR (4)Ru51	757. RY*(10)Ru51	1.39	25.85	0.169
109. CR (4)Ru51	759. RY*(12)Ru51	0.89	19.35	0.118
109. CR (4)Ru51	760. RY*(13)Ru51	0.67	9.39	0.071
109. CR (4)Ru51	762. RY*(15)Ru51	1.02	18.83	0.124
109. CR (4)Ru51	763. RY*(16)Ru51	0.87	17.41	0.110
109. CR (4)Ru51	764. RY*(17)Ru51	0.81	15.14	0.099
109. CR (4)Ru51	767. RY*(20)Ru51	1.35	21.81	0.153
109. CR (4)Ru51	770. RY*(23)Ru51	0.66	20.76	0.105
109. CR (4)Ru51	772. RY*(25)Ru51	0.54	9410.66	2.023
109. CR (4)Ru51	776. RY*(29)Ru51	1.90	82.04	0.354
109. CR (4)Ru51	777. RY*(30)Ru51	1.10	30.32	0.164
109. CR (4)Ru51	780. RY*(33)Ru51	2.05	328.94	0.735
109. CR (4)Ru51	785. RY*(38)Ru51	2.08	600.77	1.002
109. CR (4)Ru51	788. RY*(41)Ru51	0.72	93.54	0.233
109. CR (4)Ru51	789. RY*(42)Ru51	2.50	537.37	1.038
109. CR (4)Ru51	890. BD*(1) C 2- N49	2.43	5.04	0.099
109. CR (4)Ru51	892. BD*(1) C 7- N49	2.10	5.03	0.092
109. CR (4)Ru51	897. BD*(1) C 9- C11	1.48	5.10	0.078
109. CR (4)Ru51	900. BD*(1) C11- C15	4.02	5.11	0.128
109. CR (4)Ru51	902. BD*(1) C11-Ru51	2.49	4.63	0.103
109. CR (4)Ru51	911. BD*(3) C 4- O44	10.38	5.20	0.207
109. CR (4)Ru51	915. BD*(2) C10- O48	0.54	4.60	0.047
109. CR (4)Ru51	916. BD*(3) C10- O48	11.48	5.20	0.218
112. CR (7)Ru51	890. BD*(1) C 2- N49	0.51	2.28	0.030
112. CR (7)Ru51	900. BD*(1) C11- C15	0.57	2.35	0.033
112. CR (7)Ru51	902. BD*(1) C11-Ru51	2.48	1.86	0.065
112. CR (7)Ru51	913. BD*(1) C10-Ru51	3.07	1.95	0.075
112. CR (7)Ru51	916. BD*(3) C10- O48	1.52	2.43	0.054
115. CR (10)Ru51	902. BD*(1) C11-Ru51	2.63	1.87	0.067
115. CR (10)Ru51	911. BD*(3) C 4- O44	0.92	2.44	0.042
115. CR (10)Ru51	912. BD*(1) C 4-Ru51	4.33	1.92	0.089
115. CR (10)Ru51	913. BD*(1) C10-Ru51	1.47	1.96	0.052
115. CR (10)Ru51	915. BD*(2) C10- O48	1.06	1.84	0.042
118. CR (13)Ru51	902. BD*(1) C11-Ru51	1.22	1.86	0.046
118. CR (13)Ru51	911. BD*(3) C 4- O44	1.61	2.43	0.056
118. CR (13)Ru51	912. BD*(1) C 4-Ru51	3.75	1.91	0.083
118. CR (13)Ru51	913. BD*(1) C10-Ru51	1.52	1.95	0.053
118. CR (13)Ru51	914. BD*(1) C10- O48	0.62	1.83	0.032
118. CR (13)Ru51	916. BD*(3) C10- O48	0.85	2.44	0.041
148. LP (1) O44	213. RY*(1) C 4	6.15	2.94	0.120
148. LP (1) O44	215. RY*(3) C 4	0.99	2.28	0.043
148. LP (1) O44	219. RY*(7) C 4	0.76	7.31	0.067
148. LP (1) O44	220. RY*(8) C 4	0.77	4.76	0.054
148. LP (1) O44	912. BD*(1) C 4-Ru51	3.29	0.76	0.049
154. LP (1) O48	303. RY*(1) C10	7.84	2.76	0.131
154. LP (1) O48	310. RY*(8) C10	1.58	4.66	0.077
154. LP (1) O48	913. BD*(1) C10-Ru51	3.10	0.79	0.048
155. LP (1) N49	183. RY*(1) C 2	2.01	1.87	0.060
155. LP (1) N49	185. RY*(3) C 2	0.90	2.16	0.043
155. LP (1) N49	258. RY*(1) C 7	1.93	1.92	0.059
155. LP (1) N49	260. RY*(3) C 7	1.21	2.34	0.052
155. LP (1) N49	305. RY*(3) C10	0.57	2.99	0.040
155. LP (1) N49	748. RY*(1)Ru51	1.31	18.43	0.152
155. LP (1) N49	750. RY*(3)Ru51	1.01	8.63	0.091
155. LP (1) N49	755. RY*(8)Ru51	1.24	6.51	0.088
155. LP (1) N49	757. RY*(10)Ru51	1.45	21.62	0.173
155. LP (1) N49	762. RY*(15)Ru51	0.77	14.59	0.104
155. LP (1) N49	764. RY*(17)Ru51	1.00	10.90	0.102
155. LP (1) N49	767. RY*(20)Ru51	1.26	17.58	0.146
155. LP (1) N49	776. RY*(29)Ru51	1.01	77.80	0.274
155. LP (1) N49	777. RY*(30)Ru51	0.90	26.08	0.150
155. LP (1) N49	780. RY*(33)Ru51	0.91	324.70	0.533
155. LP (1) N49	785. RY*(38)Ru51	0.67	596.54	0.617
155. LP (1) N49	876. BD*(1) C 5- C 7	7.26	0.83	0.076
155. LP (1) N49	887. BD*(1) C 1- C 2	6.78	0.84	0.073
155. LP (1) N49	891. BD*(1) C 2- H27	2.62	0.75	0.043
155. LP (1) N49	894. BD*(1) C 7- C 9	1.67	0.79	0.035
155. LP (1) N49	895. BD*(1) C 9- C13	0.53	0.85	0.021
155. LP (1) N49	900. BD*(1) C11- C15	1.55	0.88	0.036
155. LP (1) N49	902. BD*(1) C11-Ru51	1.70	0.39	0.023
155. LP (1) N49	910. BD*(2) C 4- O44	0.98	0.35	0.017
155. LP (1) N49	911. BD*(3) C 4- O44	1.08	0.96	0.031
155. LP (1) N49	913. BD*(1) C10-Ru51	74.90	0.48	0.170
157. LP (1)Ru51	216. RY*(4) C 4	0.93	1.99	0.041
157. LP (1)Ru51	306. RY*(4) C10	1.25	1.98	0.047
157. LP (1)Ru51	319. RY*(2) C11	0.55	0.95	0.022
157. LP (1)Ru51	320. RY*(3) C11	0.67	1.22	0.027
157. LP (1)Ru51	720. RY*(3) N49	1.80	2.32	0.061
157. LP (1)Ru51	900. BD*(1) C11- C15	0.57	0.71	0.019
157. LP (1)Ru51	901. BD*(2) C11- C15	2.40	0.23	0.021
157. LP (1)Ru51	909. BD*(1) C 4- O44	8.39	0.19	0.036
157. LP (1)Ru51	914. BD*(1) C10- O48	8.65	0.19	0.037
157. LP (1)Ru51	915. BD*(2) C10- O48	11.09	0.20	0.042
158. LP (2)Ru51	216. RY*(4) C 4	1.92	2.00	0.060
158. LP (2)Ru51	306. RY*(4) C10	0.94	1.99	0.042
158. LP (2)Ru51	319. RY*(2) C11	1.55	0.96	0.037
158. LP (2)Ru51	320. RY*(3) C11	0.53	1.22	0.024
158. LP (2)Ru51	720. RY*(3) N49	0.72	2.33	0.040
158. LP (2)Ru51	901. BD*(2) C11- C15	4.27	0.23	0.028
158. LP (2)Ru51	902. BD*(1) C11-Ru51	1.11	0.23	0.014
158. LP (2)Ru51	909. BD*(1) C 4- O44	19.98	0.20	0.056
158. LP (2)Ru51	914. BD*(1) C10- O48	2.78	0.20	0.021
158. LP (2)Ru51	915. BD*(2) C10- O48	6.54	0.20	0.033
159. LP (3)Ru51	214. RY*(2) C 4	2.13	1.70	0.059
159. LP (3)Ru51	304. RY*(2) C10	2.65	1.13	0.053
159. LP (3)Ru51	719. RY*(2) N49	2.52	1.07	0.051
159. LP (3)Ru51	893. BD*(2) C 7- N49	3.74	0.18	0.024
159. LP (3)Ru51	909. BD*(1) C 4- O44	0.70	0.21	0.011
159. LP (3)Ru51	910. BD*(2) C 4- O44	23.68	0.20	0.064
159. LP (3)Ru51	914. BD*(1) C10- O48	14.27	0.21	0.050
159. LP (3)Ru51	915. BD*(2) C10- O48	8.68	0.21	0.039

from unit 1 to unit 2

1. BD (1) C 1- C 2	570. RY*(3) H29	0.11	2.08	0.013
1. BD (1) C 1- C 2	805. RY*(10)Ru52	62.56	0.01	0.025
2. BD (2) C 1- C 2	884. BD*(2) C 6- O46	0.07	0.23	0.004
4. BD (1) C 1- H42	796. RY*(1)Ru52	0.23	0.34	0.008
4. BD (1) C 1- H42	797. RY*(2)Ru52	0.05	0.95	0.006
5. BD (1) C 2- H27	570. RY*(3) H29	0.12	1.90	0.014
5. BD (1) C 2- H27	799. RY*(4)Ru52	0.09	2.19	0.012
5. BD (1) C 2- H27	811. RY*(16)Ru52	0.07	6.49	0.020
5. BD (1) C 2- H27	820. RY*(25)Ru52	0.08	765.54	0.229
5. BD (1) C 2- H27	821. RY*(26)Ru52	0.08	12899.80	0.905
5. BD (1) C 2- H27	833. RY*(38)Ru52	0.09	3361.89	0.498
5. BD (1) C 2- H27	836. RY*(41)Ru52	0.05	777.18	0.183
5. BD (1) C 2- H27	884. BD*(2) C 6- O46	0.12	0.46	0.007

6. BD (1) C 2- N49	338. RY*(6) C12	0.11	3.55	0.018
6. BD (1) C 2- N49	569. RY*(2) H29	0.06	2.69	0.011
6. BD (1) C 2- N49	570. RY*(3) H29	0.27	2.19	0.022
6. BD (1) C 2- N49	796. RY*(1)Ru52	0.15	0.62	0.009
6. BD (1) C 2- N49	797. RY*(2)Ru52	0.07	1.23	0.008
6. BD (1) C 2- N49	799. RY*(4)Ru52	0.07	2.49	0.012
6. BD (1) C 2- N49	805. RY*(10)Ru52	14.25	0.13	0.038
6. BD (1) C 2- N49	811. RY*(16)Ru52	0.07	6.78	0.019
6. BD (1) C 2- N49	813. RY*(18)Ru52	0.14	6.23	0.026
6. BD (1) C 2- N49	833. RY*(38)Ru52	0.05	3362.19	0.373
7. BD (1) C 3- C 5	805. RY*(10)Ru52	3.00	0.01	0.006
10. BD (1) C 4- O44	796. RY*(1)Ru52	0.73	0.23	0.012
10. BD (1) C 4- O44	797. RY*(2)Ru52	0.39	0.85	0.016
10. BD (1) C 4- O44	801. RY*(6)Ru52	0.05	1.50	0.008
10. BD (1) C 4- O44	814. RY*(19)Ru52	0.06	5.57	0.017
10. BD (1) C 4- O44	820. RY*(25)Ru52	0.06	765.45	0.190
10. BD (1) C 4- O44	821. RY*(26)Ru52	0.06	12899.71	0.756
10. BD (1) C 4- O44	833. RY*(38)Ru52	0.06	3361.80	0.415
10. BD (1) C 4- O44	840. RY*(45)Ru52	0.05	51.20	0.045
12. BD (3) C 4- O44	255. RY*(13) C 6	0.05	3.76	0.012
12. BD (3) C 4- O44	285. RY*(13) C 8	0.13	3.69	0.020
12. BD (3) C 4- O44	338. RY*(6) C12	0.58	3.85	0.042
12. BD (3) C 4- O44	341. RY*(9) C12	0.09	5.85	0.021
12. BD (3) C 4- O44	344. RY*(12) C12	0.07	3.70	0.014
12. BD (3) C 4- O44	364. RY*(2) C14	0.24	1.65	0.018
12. BD (3) C 4- O44	373. RY*(11) C14	0.10	3.75	0.018
12. BD (3) C 4- O44	393. RY*(1) C16	0.06	2.12	0.010
12. BD (3) C 4- O44	396. RY*(4) C16	0.05	3.23	0.011
12. BD (3) C 4- O44	568. RY*(1) H29	0.59	2.34	0.033
12. BD (3) C 4- O44	569. RY*(2) H29	0.15	2.99	0.019
12. BD (3) C 4- O44	570. RY*(3) H29	1.89	2.49	0.061
12. BD (3) C 4- O44	734. RY*(2) N50	0.11	1.91	0.013
12. BD (3) C 4- O44	735. RY*(3) N50	0.10	3.20	0.016
12. BD (3) C 4- O44	796. RY*(1)Ru52	1.53	0.92	0.034
12. BD (3) C 4- O44	797. RY*(2)Ru52	0.20	1.54	0.016
12. BD (3) C 4- O44	799. RY*(4)Ru52	0.55	2.79	0.035
12. BD (3) C 4- O44	800. RY*(5)Ru52	0.15	4.09	0.022
12. BD (3) C 4- O44	804. RY*(9)Ru52	0.23	3.27	0.025
12. BD (3) C 4- O44	805. RY*(10)Ru52	14.90	0.43	0.071
12. BD (3) C 4- O44	809. RY*(14)Ru52	0.06	6.31	0.017
12. BD (3) C 4- O44	811. RY*(16)Ru52	0.18	7.09	0.032
12. BD (3) C 4- O44	812. RY*(17)Ru52	0.08	4.98	0.017
12. BD (3) C 4- O44	813. RY*(18)Ru52	0.33	6.53	0.041
12. BD (3) C 4- O44	816. RY*(21)Ru52	0.05	14.43	0.025
12. BD (3) C 4- O44	833. RY*(38)Ru52	0.05	3362.49	0.378
13. BD (1) C 4-Ru51	338. RY*(6) C12	0.11	3.31	0.018
13. BD (1) C 4-Ru51	364. RY*(2) C14	0.11	1.10	0.010
13. BD (1) C 4-Ru51	570. RY*(3) H29	0.17	1.95	0.017
13. BD (1) C 4-Ru51	796. RY*(1)Ru52	1.82	0.38	0.024
13. BD (1) C 4-Ru51	799. RY*(4)Ru52	0.44	2.25	0.029
13. BD (1) C 4-Ru51	800. RY*(5)Ru52	0.05	3.54	0.012
13. BD (1) C 4-Ru51	801. RY*(6)Ru52	0.08	1.65	0.010
13. BD (1) C 4-Ru51	816. RY*(21)Ru52	0.05	13.88	0.025
13. BD (1) C 4-Ru51	834. RY*(39)Ru52	0.05	18.44	0.028
13. BD (1) C 4-Ru51	881. BD*(1) C 8-Ru52	0.10	0.59	0.007
13. BD (1) C 4-Ru51	926. BD*(1) C16-Ru52	0.09	0.53	0.006
21. BD (1) C 7- N49	568. RY*(1) H29	0.07	2.02	0.010
21. BD (1) C 7- N49	570. RY*(3) H29	0.10	2.17	0.013
21. BD (1) C 7- N49	796. RY*(1)Ru52	0.77	0.61	0.019
21. BD (1) C 7- N49	797. RY*(2)Ru52	0.22	1.22	0.015
21. BD (1) C 7- N49	798. RY*(3)Ru52	0.06	1.46	0.008
21. BD (1) C 7- N49	805. RY*(10)Ru52	0.43	0.11	0.006
21. BD (1) C 7- N49	818. RY*(23)Ru52	0.07	7.30	0.020
21. BD (1) C 7- N49	820. RY*(25)Ru52	0.07	765.82	0.210
21. BD (1) C 7- N49	821. RY*(26)Ru52	0.06	12900.08	0.816
21. BD (1) C 7- N49	833. RY*(38)Ru52	0.08	3362.17	0.451
22. BD (2) C 7- N49	796. RY*(1)Ru52	0.50	0.15	0.008
22. BD (2) C 7- N49	798. RY*(3)Ru52	0.06	1.00	0.007
22. BD (2) C 7- N49	803. RY*(8)Ru52	0.06	1.38	0.009
22. BD (2) C 7- N49	818. RY*(23)Ru52	0.05	6.84	0.018
27. BD (1) C 9- C11	568. RY*(1) H29	0.06	1.87	0.010
27. BD (1) C 9- C11	570. RY*(3) H29	0.16	2.02	0.016
27. BD (1) C 9- C11	796. RY*(1)Ru52	1.00	0.45	0.019
27. BD (1) C 9- C11	797. RY*(2)Ru52	0.19	1.07	0.013
29. BD (2) C 9- C13	796. RY*(1)Ru52	0.08	0.07	0.002
31. BD (2) C10- O48	334. RY*(2) C12	0.17	1.05	0.012
31. BD (2) C10- O48	336. RY*(4) C12	0.12	1.70	0.013
31. BD (2) C10- O48	347. RY*(15) C12	0.06	26.55	0.036
31. BD (2) C10- O48	364. RY*(2) C14	0.06	0.97	0.007
31. BD (2) C10- O48	570. RY*(3) H29	0.09	1.81	0.012
31. BD (2) C10- O48	796. RY*(1)Ru52	0.40	0.24	0.009
31. BD (2) C10- O48	797. RY*(2)Ru52	0.07	0.86	0.007
31. BD (2) C10- O48	864. BD*(2) C12- C14	0.06	0.37	0.005
32. BD (3) C10- O48	253. RY*(11) C 6	0.06	2.91	0.012
32. BD (3) C10- O48	255. RY*(13) C 6	0.08	3.75	0.016
32. BD (3) C10- O48	273. RY*(1) C 8	0.07	2.42	0.012
32. BD (3) C10- O48	279. RY*(7) C 8	0.09	5.40	0.020
32. BD (3) C10- O48	285. RY*(13) C 8	0.10	3.68	0.017
32. BD (3) C10- O48	334. RY*(2) C12	0.06	1.72	0.009
32. BD (3) C10- O48	336. RY*(4) C12	0.21	2.37	0.020
32. BD (3) C10- O48	338. RY*(6) C12	0.62	3.84	0.043
32. BD (3) C10- O48	341. RY*(9) C12	0.14	5.84	0.026
32. BD (3) C10- O48	343. RY*(11) C12	0.07	5.74	0.017
32. BD (3) C10- O48	344. RY*(12) C12	0.12	3.69	0.019
32. BD (3) C10- O48	364. RY*(2) C14	0.18	1.64	0.015
32. BD (3) C10- O48	373. RY*(11) C14	0.08	3.74	0.016
32. BD (3) C10- O48	393. RY*(1) C16	0.07	2.11	0.011
32. BD (3) C10- O48	457. RY*(5) C20	0.05	2.80	0.011
32. BD (3) C10- O48	568. RY*(1) H29	0.70	2.33	0.036
32. BD (3) C10- O48	569. RY*(2) H29	0.25	2.98	0.025
32. BD (3) C10- O48	570. RY*(3) H29	2.13	2.48	0.065
32. BD (3) C10- O48	580. RY*(3) H31	0.07	2.17	0.011
32. BD (3) C10- O48	734. RY*(2) N50	0.15	1.90	0.015
32. BD (3) C10- O48	735. RY*(3) N50	0.07	3.19	0.014
32. BD (3) C10- O48	740. RY*(8) N50	0.08	15.80	0.031
32. BD (3) C10- O48	745. RY*(13) N50	0.07	6.13	0.019
32. BD (3) C10- O48	796. RY*(1)Ru52	3.61	0.92	0.051
32. BD (3) C10- O48	797. RY*(2)Ru52	0.85	1.53	0.032
32. BD (3) C10- O48	798. RY*(3)Ru52	0.08	1.77	0.011
32. BD (3) C10- O48	799. RY*(4)Ru52	0.32	2.78	0.027
32. BD (3) C10- O48	800. RY*(5)Ru52	0.22	4.08	0.027
32. BD (3) C10- O48	804. RY*(9)Ru52	0.14	3.26	0.019
32. BD (3) C10- O48	805. RY*(10)Ru52	4.29	0.42	0.038
32. BD (3) C10- O48	809. RY*(14)Ru52	0.08	6.30	0.020
32. BD (3) C10- O48	811. RY*(16)Ru52	0.05	7.08	0.017
32. BD (3) C10- O48	813. RY*(18)Ru52	0.34	6.52	0.042

32. BD (3) C10- O48	814. RY*(19)Ru52	0.24	6.25	0.035
32. BD (3) C10- O48	818. RY*(23)Ru52	0.08	7.61	0.022
32. BD (3) C10- O48	834. RY*(39)Ru52	0.07	18.98	0.032
33. BD (1) C10-Ru51	334. RY*(2) C12	0.30	1.19	0.017
33. BD (1) C10-Ru51	336. RY*(4) C12	0.11	1.84	0.013
33. BD (1) C10-Ru51	796. RY*(1)Ru52	0.72	0.38	0.015
33. BD (1) C10-Ru51	798. RY*(3)Ru52	0.08	1.23	0.009
33. BD (1) C10-Ru51	799. RY*(4)Ru52	0.20	2.25	0.019
33. BD (1) C10-Ru51	801. RY*(6)Ru52	0.23	1.65	0.018
33. BD (1) C10-Ru51	803. RY*(8)Ru52	0.21	1.61	0.017
33. BD (1) C10-Ru51	804. RY*(9)Ru52	0.24	2.73	0.023
33. BD (1) C10-Ru51	812. RY*(17)Ru52	0.10	4.44	0.019
33. BD (1) C10-Ru51	817. RY*(22)Ru52	0.09	9.71	0.026
33. BD (1) C10-Ru51	840. RY*(45)Ru52	0.06	51.35	0.049
33. BD (1) C10-Ru51	863. BD*(1) C12- C14	0.07	0.99	0.007
33. BD (1) C10-Ru51	864. BD*(2) C12- C14	0.06	0.51	0.005
33. BD (1) C10-Ru51	881. BD*(1) C 8-Ru52	0.23	0.60	0.011
33. BD (1) C10-Ru51	882. BD*(1) C 6-Ru52	0.06	0.63	0.006
33. BD (1) C10-Ru51	926. BD*(1) C16-Ru52	0.17	0.54	0.009
34. BD (1) C11- C15	253. RY*(11) C 6	0.06	2.46	0.011
34. BD (1) C11- C15	338. RY*(6) C12	0.20	3.39	0.023
34. BD (1) C11- C15	364. RY*(2) C14	0.11	1.19	0.010
34. BD (1) C11- C15	568. RY*(1) H29	0.17	1.87	0.016
34. BD (1) C11- C15	569. RY*(2) H29	0.09	2.53	0.013
34. BD (1) C11- C15	570. RY*(3) H29	0.71	2.03	0.034
34. BD (1) C11- C15	796. RY*(1)Ru52	0.80	0.46	0.017
34. BD (1) C11- C15	799. RY*(4)Ru52	0.21	2.33	0.020
34. BD (1) C11- C15	804. RY*(9)Ru52	0.06	2.81	0.011
34. BD (1) C11- C15	813. RY*(18)Ru52	0.13	6.07	0.025
35. BD (2) C11- C15	796. RY*(1)Ru52	0.79	0.06	0.007
35. BD (2) C11- C15	797. RY*(2)Ru52	0.08	0.67	0.007
36. BD (1) C11-Ru51	394. RY*(2) C16	0.05	0.97	0.007
36. BD (1) C11-Ru51	802. RY*(7)Ru52	0.07	3.42	0.015
36. BD (1) C11-Ru51	926. BD*(1) C16-Ru52	0.17	0.36	0.007
45. BD (1) C15- C19	570. RY*(3) H29	0.09	2.04	0.012
45. BD (1) C15- C19	796. RY*(1)Ru52	0.08	0.47	0.006
108. CR (3)Ru51	805. RY*(10)Ru52	0.05	21.30	0.030
108. CR (3)Ru51	882. BD*(1) C 6-Ru52	0.05	22.05	0.033
109. CR (4)Ru51	570. RY*(3) H29	0.09	6.03	0.021
109. CR (4)Ru51	805. RY*(10)Ru52	0.15	3.96	0.022
109. CR (4)Ru51	882. BD*(1) C 6-Ru52	0.12	4.71	0.023
109. CR (4)Ru51	926. BD*(1) C16-Ru52	0.10	4.61	0.021
148. LP (1) O44	805. RY*(10)Ru52	5.94	0.04	0.013
154. LP (1) O48	796. RY*(1)Ru52	0.13	0.53	0.007
154. LP (1) O48	805. RY*(10)Ru52	0.49	0.03	0.004
155. LP (1) N49	338. RY*(6) C12	0.08	3.15	0.015
155. LP (1) N49	570. RY*(3) H29	0.16	1.79	0.016
155. LP (1) N49	796. RY*(1)Ru52	2.69	0.22	0.024
155. LP (1) N49	797. RY*(2)Ru52	0.56	0.83	0.021
155. LP (1) N49	798. RY*(3)Ru52	0.07	1.07	0.008
155. LP (1) N49	803. RY*(8)Ru52	0.06	1.45	0.009
155. LP (1) N49	882. BD*(1) C 6-Ru52	0.09	0.47	0.006
157. LP (1)Ru51	273. RY*(1) C 8	0.13	1.56	0.014
157. LP (1)Ru51	428. RY*(6) C18	0.05	2.60	0.011
157. LP (1)Ru51	570. RY*(3) H29	0.08	1.62	0.011
157. LP (1)Ru51	676. RY*(4) O46	0.08	0.69	0.007
157. LP (1)Ru51	691. RY*(4) O47	0.06	0.65	0.006
157. LP (1)Ru51	733. RY*(1) N50	0.15	1.76	0.015
157. LP (1)Ru51	796. RY*(1)Ru52	25.62	0.05	0.035
157. LP (1)Ru51	797. RY*(2)Ru52	3.10	0.66	0.043
157. LP (1)Ru51	798. RY*(3)Ru52	0.29	0.90	0.015
157. LP (1)Ru51	799. RY*(4)Ru52	0.23	1.92	0.020
157. LP (1)Ru51	800. RY*(5)Ru52	0.14	3.21	0.020
157. LP (1)Ru51	801. RY*(6)Ru52	0.75	1.32	0.030
157. LP (1)Ru51	804. RY*(9)Ru52	0.21	2.40	0.021
157. LP (1)Ru51	807. RY*(12)Ru52	0.05	7.25	0.018
157. LP (1)Ru51	810. RY*(15)Ru52	0.34	6.28	0.044
157. LP (1)Ru51	811. RY*(16)Ru52	0.22	6.21	0.035
157. LP (1)Ru51	812. RY*(17)Ru52	0.15	4.10	0.023
157. LP (1)Ru51	813. RY*(18)Ru52	0.07	5.66	0.019
157. LP (1)Ru51	814. RY*(19)Ru52	0.34	5.39	0.041
157. LP (1)Ru51	817. RY*(22)Ru52	0.06	9.37	0.022
157. LP (1)Ru51	818. RY*(23)Ru52	0.28	6.74	0.041
157. LP (1)Ru51	819. RY*(24)Ru52	0.28	29463.54	2.738
157. LP (1)Ru51	820. RY*(25)Ru52	0.57	765.26	0.631
157. LP (1)Ru51	821. RY*(26)Ru52	0.53	12899.53	2.478
157. LP (1)Ru51	833. RY*(38)Ru52	0.61	3361.62	1.364
157. LP (1)Ru51	836. RY*(41)Ru52	0.36	776.90	0.499
157. LP (1)Ru51	837. RY*(42)Ru52	0.23	3154.64	0.813
157. LP (1)Ru51	840. RY*(45)Ru52	0.18	51.02	0.090
157. LP (1)Ru51	841. RY*(46)Ru52	0.12	186.33	0.143
157. LP (1)Ru51	926. BD*(1) C16-Ru52	0.28	0.21	0.007
158. LP (2)Ru51	243. RY*(1) C 6	0.06	1.69	0.009
158. LP (2)Ru51	273. RY*(1) C 8	0.11	1.56	0.013
158. LP (2)Ru51	393. RY*(1) C16	0.11	1.25	0.011
158. LP (2)Ru51	676. RY*(4) O46	0.05	0.70	0.006
158. LP (2)Ru51	733. RY*(1) N50	0.08	1.77	0.011
158. LP (2)Ru51	796. RY*(1)Ru52	16.95	0.06	0.030
158. LP (2)Ru51	797. RY*(2)Ru52	2.06	0.67	0.036
158. LP (2)Ru51	798. RY*(3)Ru52	0.26	0.91	0.015
158. LP (2)Ru51	799. RY*(4)Ru52	0.33	1.92	0.024
158. LP (2)Ru51	800. RY*(5)Ru52	0.18	3.22	0.023
158. LP (2)Ru51	801. RY*(6)Ru52	0.25	1.32	0.018
158. LP (2)Ru51	802. RY*(7)Ru52	0.13	3.26	0.020
158. LP (2)Ru51	803. RY*(8)Ru52	0.08	1.29	0.010
158. LP (2)Ru51	804. RY*(9)Ru52	0.44	2.40	0.031
158. LP (2)Ru51	806. RY*(11)Ru52	0.07	6.64	0.020
158. LP (2)Ru51	810. RY*(15)Ru52	0.13	6.28	0.028
158. LP (2)Ru51	811. RY*(16)Ru52	0.11	6.22	0.025
158. LP (2)Ru51	814. RY*(19)Ru52	0.22	5.39	0.033
158. LP (2)Ru51	816. RY*(21)Ru52	0.06	13.56	0.028
158. LP (2)Ru51	817. RY*(22)Ru52	0.27	9.38	0.049
158. LP (2)Ru51	819. RY*(24)Ru52	0.13	29463.54	1.918
158. LP (2)Ru51	820. RY*(25)Ru52	0.26	765.27	0.431
158. LP (2)Ru51	821. RY*(26)Ru52	0.26	12899.53	1.753
158. LP (2)Ru51	833. RY*(38)Ru52	0.29	3361.62	0.957
158. LP (2)Ru51	836. RY*(41)Ru52	0.17	776.90	0.348
158. LP (2)Ru51	837. RY*(42)Ru52	0.11	3154.64	0.568
158. LP (2)Ru51	840. RY*(45)Ru52	0.39	51.03	0.136
158. LP (2)Ru51	841. RY*(46)Ru52	0.26	186.34	0.211
158. LP (2)Ru51	882. BD*(1) C 6-Ru52	0.29	0.31	0.008
158. LP (2)Ru51	926. BD*(1) C16-Ru52	0.07	0.21	0.004
159. LP (3)Ru51	796. RY*(1)Ru52	1.53	0.07	0.010
159. LP (3)Ru51	802. RY*(7)Ru52	0.05	3.27	0.013
159. LP (3)Ru51	803. RY*(8)Ru52	0.06	1.30	0.008

from unit 1 to unit 3

1. BD (1) C 1- C 2	638. RY*(1) H43	0.13	2.17	0.015
1. BD (1) C 1- C 2	640. RY*(3) H43	0.12	2.75	0.016
5. BD (1) C 2- H27	638. RY*(1) H43	0.13	1.99	0.014
5. BD (1) C 2- H27	640. RY*(3) H43	0.22	2.57	0.021
5. BD (1) C 2- H27	659. RY*(2) O45	0.05	1.98	0.009
5. BD (1) C 2- H27	661. RY*(4) O45	0.08	4.36	0.017
6. BD (1) C 2- N49	638. RY*(1) H43	0.27	2.28	0.022
6. BD (1) C 2- N49	640. RY*(3) H43	0.35	2.86	0.028
6. BD (1) C 2- N49	659. RY*(2) O45	0.07	2.28	0.011
6. BD (1) C 2- N49	661. RY*(4) O45	0.21	4.65	0.028
6. BD (1) C 2- N49	662. RY*(5) O45	0.05	3.01	0.011
6. BD (1) C 2- N49	665. RY*(8) O45	0.12	2.57	0.015
12. BD (3) C 4- O44	638. RY*(1) H43	2.17	2.58	0.067
12. BD (3) C 4- O44	640. RY*(3) H43	3.19	3.16	0.090
12. BD (3) C 4- O44	641. RY*(4) H43	0.31	3.68	0.030
12. BD (3) C 4- O44	642. RY*(5) H43	0.57	3.52	0.040
12. BD (3) C 4- O44	658. RY*(1) O45	0.34	3.43	0.030
12. BD (3) C 4- O44	659. RY*(2) O45	0.14	2.58	0.017
12. BD (3) C 4- O44	660. RY*(3) O45	0.19	3.20	0.022
12. BD (3) C 4- O44	661. RY*(4) O45	0.16	4.96	0.025
12. BD (3) C 4- O44	662. RY*(5) O45	0.91	3.31	0.049
12. BD (3) C 4- O44	663. RY*(6) O45	0.11	3.71	0.018
12. BD (3) C 4- O44	665. RY*(8) O45	0.11	2.87	0.016
12. BD (3) C 4- O44	666. RY*(9) O45	0.10	3.41	0.016
12. BD (3) C 4- O44	667. RY*(10) O45	0.25	5.93	0.034
12. BD (3) C 4- O44	668. RY*(11) O45	0.49	6.19	0.049
12. BD (3) C 4- O44	669. RY*(12) O45	0.27	5.38	0.034
13. BD (1) C 4-Ru51	638. RY*(1) H43	0.12	2.04	0.014
13. BD (1) C 4-Ru51	640. RY*(3) H43	0.51	2.62	0.033
13. BD (1) C 4-Ru51	641. RY*(4) H43	0.09	3.14	0.015
13. BD (1) C 4-Ru51	642. RY*(5) H43	0.14	2.97	0.019
13. BD (1) C 4-Ru51	658. RY*(1) O45	0.65	2.89	0.040
13. BD (1) C 4-Ru51	659. RY*(2) O45	0.09	2.03	0.013
13. BD (1) C 4-Ru51	660. RY*(3) O45	1.41	2.65	0.056
13. BD (1) C 4-Ru51	661. RY*(4) O45	0.08	4.41	0.017
13. BD (1) C 4-Ru51	663. RY*(6) O45	0.16	3.16	0.020
13. BD (1) C 4-Ru51	664. RY*(7) O45	0.09	2.75	0.014
13. BD (1) C 4-Ru51	666. RY*(9) O45	0.16	2.87	0.019
13. BD (1) C 4-Ru51	667. RY*(10) O45	0.28	5.38	0.036
13. BD (1) C 4-Ru51	668. RY*(11) O45	0.10	5.65	0.022
13. BD (1) C 4-Ru51	669. RY*(12) O45	0.07	4.83	0.017
13. BD (1) C 4-Ru51	672. RY*(15) O45	0.12	76.16	0.086
21. BD (1) C 7- N49	638. RY*(1) H43	0.11	2.26	0.014
21. BD (1) C 7- N49	662. RY*(5) O45	0.07	2.99	0.013
27. BD (1) C 9- C11	638. RY*(1) H43	0.16	2.11	0.016
27. BD (1) C 9- C11	640. RY*(3) H43	0.24	2.69	0.023
27. BD (1) C 9- C11	658. RY*(1) O45	0.05	2.96	0.011
27. BD (1) C 9- C11	668. RY*(11) O45	0.11	5.72	0.022
31. BD (2) C10- O48	640. RY*(3) H43	0.14	2.48	0.017
32. BD (3) C10- O48	638. RY*(1) H43	2.44	2.57	0.071
32. BD (3) C10- O48	640. RY*(3) H43	3.12	3.16	0.089
32. BD (3) C10- O48	641. RY*(4) H43	0.40	3.68	0.034
32. BD (3) C10- O48	642. RY*(5) H43	0.56	3.51	0.040
32. BD (3) C10- O48	658. RY*(1) O45	0.28	3.43	0.028
32. BD (3) C10- O48	660. RY*(3) O45	0.45	3.19	0.034
32. BD (3) C10- O48	661. RY*(4) O45	0.16	4.95	0.025
32. BD (3) C10- O48	662. RY*(5) O45	0.92	3.30	0.049
32. BD (3) C10- O48	663. RY*(6) O45	0.09	3.70	0.017
32. BD (3) C10- O48	664. RY*(7) O45	0.06	3.29	0.012
32. BD (3) C10- O48	665. RY*(8) O45	0.13	2.86	0.017
32. BD (3) C10- O48	666. RY*(9) O45	0.11	3.40	0.017
32. BD (3) C10- O48	667. RY*(10) O45	0.18	5.92	0.029
32. BD (3) C10- O48	668. RY*(11) O45	0.50	6.19	0.050
32. BD (3) C10- O48	669. RY*(12) O45	0.17	5.37	0.027
32. BD (3) C10- O48	671. RY*(14) O45	0.05	5.71	0.016
33. BD (1) C10-Ru51	639. RY*(2) H43	0.08	2.24	0.012
33. BD (1) C10-Ru51	641. RY*(4) H43	0.10	3.14	0.016
33. BD (1) C10-Ru51	658. RY*(1) O45	0.77	2.89	0.043
33. BD (1) C10-Ru51	659. RY*(2) O45	0.26	2.04	0.021
33. BD (1) C10-Ru51	660. RY*(3) O45	2.07	2.66	0.067
33. BD (1) C10-Ru51	661. RY*(4) O45	0.26	4.42	0.031
33. BD (1) C10-Ru51	662. RY*(5) O45	0.14	2.77	0.018
33. BD (1) C10-Ru51	663. RY*(6) O45	0.06	3.16	0.012
33. BD (1) C10-Ru51	664. RY*(7) O45	0.18	2.76	0.020
33. BD (1) C10-Ru51	667. RY*(10) O45	0.15	5.39	0.026
33. BD (1) C10-Ru51	669. RY*(12) O45	0.16	4.83	0.025
33. BD (1) C10-Ru51	670. RY*(13) O45	0.06	92.64	0.067
33. BD (1) C10-Ru51	672. RY*(15) O45	0.14	76.16	0.094
34. BD (1) C11- C15	638. RY*(1) H43	0.71	2.12	0.035
34. BD (1) C11- C15	640. RY*(3) H43	0.68	2.70	0.039
34. BD (1) C11- C15	642. RY*(5) H43	0.10	3.05	0.016
34. BD (1) C11- C15	659. RY*(2) O45	0.13	2.12	0.015
34. BD (1) C11- C15	660. RY*(3) O45	0.13	2.74	0.017
34. BD (1) C11- C15	661. RY*(4) O45	0.12	4.50	0.021
34. BD (1) C11- C15	662. RY*(5) O45	0.39	2.85	0.030
34. BD (1) C11- C15	665. RY*(8) O45	0.06	2.41	0.011
34. BD (1) C11- C15	669. RY*(12) O45	0.18	4.91	0.026
36. BD (1) C11-Ru51	639. RY*(2) H43	0.06	2.06	0.010
36. BD (1) C11-Ru51	658. RY*(1) O45	0.30	2.72	0.026
36. BD (1) C11-Ru51	659. RY*(2) O45	0.07	1.87	0.011
36. BD (1) C11-Ru51	660. RY*(3) O45	0.19	2.48	0.020
36. BD (1) C11-Ru51	661. RY*(4) O45	0.63	4.24	0.048
36. BD (1) C11-Ru51	670. RY*(13) O45	0.22	92.46	0.132
36. BD (1) C11-Ru51	672. RY*(15) O45	0.29	75.99	0.137
45. BD (1) C15- C19	638. RY*(1) H43	0.06	2.13	0.010
45. BD (1) C15- C19	640. RY*(3) H43	0.12	2.71	0.016
46. BD (1) C15- H33	660. RY*(3) O45	0.05	2.57	0.010
108. CR (3)Ru51	640. RY*(3) H43	0.06	24.03	0.033
109. CR (4)Ru51	638. RY*(1) H43	0.13	6.12	0.025
109. CR (4)Ru51	640. RY*(3) H43	0.15	6.70	0.028
109. CR (4)Ru51	661. RY*(4) O45	0.05	8.49	0.019
115. CR (10)Ru51	934. BD*(1) H43- O45	0.16	2.29	0.017
148. LP (1) O44	640. RY*(3) H43	0.07	2.77	0.012
155. LP (1) N49	638. RY*(1) H43	0.14	1.88	0.016
155. LP (1) N49	640. RY*(3) H43	0.15	2.46	0.019
155. LP (1) N49	662. RY*(5) O45	0.08	2.61	0.014
157. LP (1)Ru51	638. RY*(1) H43	0.06	1.71	0.009
157. LP (1)Ru51	659. RY*(2) O45	1.28	1.71	0.044
157. LP (1)Ru51	668. RY*(11) O45	0.19	5.32	0.030
158. LP (2)Ru51	658. RY*(1) O45	0.56	2.57	0.036
158. LP (2)Ru51	659. RY*(2) O45	0.36	1.71	0.024
158. LP (2)Ru51	668. RY*(11) O45	0.08	5.33	0.020
158. LP (2)Ru51	934. BD*(1) H43- O45	0.28	0.66	0.013
159. LP (3)Ru51	934. BD*(1) H43- O45	0.05	0.67	0.006

from unit 1 to unit 4

1. BD (1) C 1- C 2	846. RY*(3)C153	0.15	6.70	0.028
1. BD (1) C 1- C 2	847. RY*(4)C153	0.27	3.06	0.026
1. BD (1) C 1- C 2	848. RY*(5)C153	0.23	7.16	0.036
1. BD (1) C 1- C 2	853. RY*(10)C153	0.06	5.22	0.016
5. BD (1) C 2- H27	845. RY*(2)C153	0.06	1.41	0.008
5. BD (1) C 2- H27	846. RY*(3)C153	0.24	6.52	0.035
5. BD (1) C 2- H27	847. RY*(4)C153	0.40	2.88	0.030
5. BD (1) C 2- H27	848. RY*(5)C153	0.38	6.98	0.046
6. BD (1) C 2- N49	845. RY*(2)C153	0.06	1.71	0.009
6. BD (1) C 2- N49	846. RY*(3)C153	0.41	6.81	0.047
6. BD (1) C 2- N49	847. RY*(4)C153	0.51	3.18	0.036
6. BD (1) C 2- N49	848. RY*(5)C153	0.77	7.27	0.067
6. BD (1) C 2- N49	851. RY*(8)C153	0.35	1.91	0.023
6. BD (1) C 2- N49	852. RY*(9)C153	0.14	2.48	0.017
6. BD (1) C 2- N49	853. RY*(10)C153	0.28	5.33	0.035
6. BD (1) C 2- N49	854. RY*(11)C153	0.07	5.90	0.018
6. BD (1) C 2- N49	856. RY*(13)C153	0.15	6.11	0.027
12. BD (3) C 4- O44	844. RY*(1)C153	0.07	1.72	0.010
12. BD (3) C 4- O44	845. RY*(2)C153	0.24	2.01	0.020
12. BD (3) C 4- O44	846. RY*(3)C153	3.05	7.12	0.132
12. BD (3) C 4- O44	847. RY*(4)C153	4.14	3.48	0.107
12. BD (3) C 4- O44	848. RY*(5)C153	4.04	7.58	0.156
12. BD (3) C 4- O44	849. RY*(6)C153	0.09	2.36	0.013
12. BD (3) C 4- O44	851. RY*(8)C153	0.27	2.21	0.022
12. BD (3) C 4- O44	853. RY*(10)C153	1.07	5.64	0.070
12. BD (3) C 4- O44	854. RY*(11)C153	0.13	6.20	0.026
12. BD (3) C 4- O44	855. RY*(12)C153	0.09	6.35	0.021
12. BD (3) C 4- O44	856. RY*(13)C153	0.36	6.42	0.043
13. BD (1) C 4-Ru51	845. RY*(2)C153	0.13	1.46	0.013
13. BD (1) C 4-Ru51	846. RY*(3)C153	0.56	6.57	0.055
13. BD (1) C 4-Ru51	847. RY*(4)C153	0.90	2.93	0.047
13. BD (1) C 4-Ru51	848. RY*(5)C153	0.77	7.03	0.067
13. BD (1) C 4-Ru51	849. RY*(6)C153	0.13	1.81	0.014
13. BD (1) C 4-Ru51	853. RY*(10)C153	0.12	5.09	0.022
13. BD (1) C 4-Ru51	856. RY*(13)C153	0.06	5.87	0.016
13. BD (1) C 4-Ru51	858. RY*(15)C153	0.05	170.72	0.084
13. BD (1) C 4-Ru51	860. RY*(17)C153	0.06	49.51	0.048
14. BD (1) C 5- C 7	847. RY*(4)C153	0.09	3.06	0.015
14. BD (1) C 5- C 7	848. RY*(5)C153	0.10	7.15	0.024
20. BD (1) C 7- C 9	845. RY*(2)C153	0.07	1.54	0.009
20. BD (1) C 7- C 9	847. RY*(4)C153	0.14	3.00	0.019
20. BD (1) C 7- C 9	848. RY*(5)C153	0.14	7.10	0.028
20. BD (1) C 7- C 9	853. RY*(10)C153	0.05	5.16	0.015
21. BD (1) C 7- N49	845. RY*(2)C153	0.08	1.69	0.010
21. BD (1) C 7- N49	846. RY*(3)C153	0.09	6.80	0.022
21. BD (1) C 7- N49	847. RY*(4)C153	0.36	3.16	0.030
21. BD (1) C 7- N49	848. RY*(5)C153	0.29	7.26	0.041
21. BD (1) C 7- N49	853. RY*(10)C153	0.24	5.32	0.032
22. BD (2) C 7- N49	846. RY*(3)C153	0.08	6.34	0.022
22. BD (2) C 7- N49	850. RY*(7)C153	0.17	3.97	0.025
22. BD (2) C 7- N49	852. RY*(9)C153	0.08	2.00	0.012
22. BD (2) C 7- N49	853. RY*(10)C153	0.18	4.86	0.029
22. BD (2) C 7- N49	858. RY*(15)C153	0.08	170.49	0.115
22. BD (2) C 7- N49	860. RY*(17)C153	0.11	49.28	0.072
22. BD (2) C 7- N49	861. RY*(18)C153	0.12	16.28	0.043
27. BD (1) C 9- C11	845. RY*(2)C153	0.08	1.54	0.010
27. BD (1) C 9- C11	846. RY*(3)C153	0.18	6.64	0.031
27. BD (1) C 9- C11	847. RY*(4)C153	0.39	3.01	0.031
27. BD (1) C 9- C11	848. RY*(5)C153	0.41	7.11	0.049
27. BD (1) C 9- C11	851. RY*(8)C153	0.11	1.74	0.013
27. BD (1) C 9- C11	852. RY*(9)C153	0.06	2.31	0.010
27. BD (1) C 9- C11	853. RY*(10)C153	0.34	5.17	0.038
27. BD (1) C 9- C11	856. RY*(13)C153	0.06	5.95	0.016
30. BD (1) C10- O48	847. RY*(4)C153	0.09	2.79	0.014
30. BD (1) C10- O48	853. RY*(10)C153	0.10	4.95	0.020
30. BD (1) C10- O48	861. RY*(18)C153	0.05	16.37	0.026
31. BD (2) C10- O48	847. RY*(4)C153	0.08	2.80	0.013
31. BD (2) C10- O48	853. RY*(10)C153	0.16	4.96	0.025
31. BD (2) C10- O48	856. RY*(13)C153	0.06	5.74	0.016
32. BD (3) C10- O48	844. RY*(1)C153	0.12	1.71	0.013
32. BD (3) C10- O48	845. RY*(2)C153	0.35	2.00	0.024
32. BD (3) C10- O48	846. RY*(3)C153	4.00	7.11	0.151
32. BD (3) C10- O48	847. RY*(4)C153	4.88	3.47	0.116
32. BD (3) C10- O48	848. RY*(5)C153	4.36	7.57	0.162
32. BD (3) C10- O48	851. RY*(8)C153	0.20	2.20	0.019
32. BD (3) C10- O48	852. RY*(9)C153	0.07	2.77	0.013
32. BD (3) C10- O48	853. RY*(10)C153	1.56	5.63	0.084
32. BD (3) C10- O48	854. RY*(11)C153	0.10	6.19	0.022
32. BD (3) C10- O48	855. RY*(12)C153	0.09	6.34	0.022
32. BD (3) C10- O48	856. RY*(13)C153	0.48	6.41	0.049
33. BD (1) C10-Ru51	845. RY*(2)C153	0.14	1.47	0.013
33. BD (1) C10-Ru51	846. RY*(3)C153	0.45	6.57	0.049
33. BD (1) C10-Ru51	847. RY*(4)C153	0.18	2.94	0.021
33. BD (1) C10-Ru51	848. RY*(5)C153	0.29	7.04	0.041
33. BD (1) C10-Ru51	849. RY*(6)C153	0.46	1.82	0.026
33. BD (1) C10-Ru51	850. RY*(7)C153	0.68	4.21	0.049
33. BD (1) C10-Ru51	853. RY*(10)C153	0.12	5.10	0.023
33. BD (1) C10-Ru51	858. RY*(15)C153	0.16	170.73	0.149
33. BD (1) C10-Ru51	860. RY*(17)C153	0.21	49.52	0.093
33. BD (1) C10-Ru51	861. RY*(18)C153	0.17	16.52	0.049
34. BD (1) C11- C15	845. RY*(2)C153	0.15	1.55	0.014
34. BD (1) C11- C15	846. RY*(3)C153	0.76	6.65	0.064
34. BD (1) C11- C15	847. RY*(4)C153	2.54	3.02	0.078
34. BD (1) C11- C15	848. RY*(5)C153	1.02	7.11	0.077
34. BD (1) C11- C15	851. RY*(8)C153	0.14	1.75	0.014
34. BD (1) C11- C15	852. RY*(9)C153	0.06	2.32	0.010
34. BD (1) C11- C15	853. RY*(10)C153	0.98	5.17	0.064
34. BD (1) C11- C15	855. RY*(12)C153	0.06	5.89	0.017
34. BD (1) C11- C15	856. RY*(13)C153	0.20	5.95	0.031
34. BD (1) C11- C15	861. RY*(18)C153	0.07	16.59	0.031
35. BD (2) C11- C15	850. RY*(7)C153	0.06	3.88	0.015
35. BD (2) C11- C15	853. RY*(10)C153	0.09	4.77	0.020
35. BD (2) C11- C15	860. RY*(17)C153	0.06	49.19	0.056
35. BD (2) C11- C15	861. RY*(18)C153	0.07	16.19	0.034
36. BD (1) C11-Ru51	845. RY*(2)C153	0.16	1.29	0.013
36. BD (1) C11-Ru51	849. RY*(6)C153	0.26	1.64	0.019
36. BD (1) C11-Ru51	850. RY*(7)C153	0.17	4.03	0.024
36. BD (1) C11-Ru51	852. RY*(9)C153	0.13	2.06	0.015
36. BD (1) C11-Ru51	853. RY*(10)C153	0.08	4.92	0.019
36. BD (1) C11-Ru51	860. RY*(17)C153	0.06	49.34	0.051
36. BD (1) C11-Ru51	861. RY*(18)C153	0.06	16.34	0.029
45. BD (1) C15- C19	846. RY*(3)C153	0.11	6.66	0.025
45. BD (1) C15- C19	847. RY*(4)C153	0.22	3.02	0.023
45. BD (1) C15- C19	848. RY*(5)C153	0.14	7.12	0.028
45. BD (1) C15- C19	853. RY*(10)C153	0.08	5.18	0.018

46. BD (1) C15- H33	846. RY*(3)C153	0.09	6.49	0.022
46. BD (1) C15- H33	847. RY*(4)C153	0.20	2.85	0.022
46. BD (1) C15- H33	848. RY*(5)C153	0.13	6.95	0.027
108. CR (3)Ru51	846. RY*(3)C153	0.14	27.99	0.056
108. CR (3)Ru51	847. RY*(4)C153	0.15	24.35	0.055
108. CR (3)Ru51	848. RY*(5)C153	0.21	28.45	0.068
108. CR (3)Ru51	853. RY*(10)C153	0.06	26.51	0.037
109. CR (4)Ru51	846. RY*(3)C153	0.26	10.65	0.047
109. CR (4)Ru51	847. RY*(4)C153	0.18	7.01	0.032
109. CR (4)Ru51	848. RY*(5)C153	0.35	11.11	0.056
109. CR (4)Ru51	853. RY*(10)C153	0.14	9.17	0.032
148. LP (1) O44	846. RY*(3)C153	0.06	6.72	0.018
148. LP (1) O44	847. RY*(4)C153	0.12	3.09	0.017
148. LP (1) O44	848. RY*(5)C153	0.08	7.19	0.022
154. LP (1) O48	846. RY*(3)C153	0.07	6.72	0.020
154. LP (1) O48	847. RY*(4)C153	0.05	3.08	0.011
154. LP (1) O48	848. RY*(5)C153	0.13	7.18	0.027
155. LP (1) N49	845. RY*(2)C153	0.06	1.31	0.009
155. LP (1) N49	846. RY*(3)C153	0.20	6.41	0.035
155. LP (1) N49	847. RY*(4)C153	0.28	2.78	0.027
155. LP (1) N49	848. RY*(5)C153	0.38	6.87	0.050
155. LP (1) N49	851. RY*(8)C153	0.09	1.51	0.011
155. LP (1) N49	853. RY*(10)C153	0.13	4.93	0.025
157. LP (1)Ru51	845. RY*(2)C153	0.13	1.14	0.012
157. LP (1)Ru51	847. RY*(4)C153	0.26	2.61	0.025
157. LP (1)Ru51	852. RY*(9)C153	0.05	1.91	0.009
158. LP (2)Ru51	845. RY*(2)C153	0.55	1.14	0.024
158. LP (2)Ru51	846. RY*(3)C153	0.18	6.25	0.032
158. LP (2)Ru51	848. RY*(5)C153	0.22	6.71	0.037
158. LP (2)Ru51	850. RY*(7)C153	0.07	3.88	0.016
158. LP (2)Ru51	852. RY*(9)C153	0.15	1.91	0.016
158. LP (2)Ru51	858. RY*(15)C153	0.09	170.40	0.119
158. LP (2)Ru51	860. RY*(17)C153	0.12	49.19	0.073
158. LP (2)Ru51	861. RY*(18)C153	0.09	16.19	0.036
159. LP (3)Ru51	844. RY*(1)C153	0.39	0.86	0.018

from unit 2 to unit 1

17. BD (2) C 6- O46	184. RY*(2) C 2	0.14	1.03	0.011
17. BD (2) C 6- O46	186. RY*(4) C 2	0.06	1.82	0.009
17. BD (2) C 6- O46	720. RY*(3) N49	0.05	2.51	0.010
18. BD (3) C 6- O46	169. RY*(2) C 1	0.06	1.63	0.009
18. BD (3) C 6- O46	184. RY*(2) C 2	0.14	1.73	0.014
18. BD (3) C 6- O46	185. RY*(3) C 2	0.05	2.88	0.011
18. BD (3) C 6- O46	188. RY*(6) C 2	0.25	4.74	0.031
18. BD (3) C 6- O46	190. RY*(8) C 2	0.06	9.86	0.022
18. BD (3) C 6- O46	560. RY*(3) H27	0.16	2.05	0.016
18. BD (3) C 6- O46	748. RY*(1)Ru51	0.14	19.15	0.046
18. BD (3) C 6- O46	750. RY*(3)Ru51	0.05	9.35	0.020
18. BD (3) C 6- O46	754. RY*(7)Ru51	0.07	5.29	0.017
18. BD (3) C 6- O46	761. RY*(14)Ru51	0.06	8.62	0.020
18. BD (3) C 6- O46	766. RY*(19)Ru51	0.15	7.93	0.031
18. BD (3) C 6- O46	776. RY*(29)Ru51	0.06	78.52	0.059
19. BD (1) C 6-Ru52	184. RY*(2) C 2	0.29	1.18	0.017
19. BD (1) C 6-Ru52	186. RY*(4) C 2	0.05	1.97	0.009
19. BD (1) C 6-Ru52	188. RY*(6) C 2	0.12	4.19	0.020
19. BD (1) C 6-Ru52	190. RY*(8) C 2	0.05	9.31	0.020
19. BD (1) C 6-Ru52	318. RY*(1) C11	0.10	1.77	0.012
19. BD (1) C 6-Ru52	558. RY*(1) H27	0.31	1.90	0.022
19. BD (1) C 6-Ru52	559. RY*(2) H27	0.07	2.52	0.012
19. BD (1) C 6-Ru52	560. RY*(3) H27	0.33	1.49	0.020
19. BD (1) C 6-Ru52	751. RY*(4)Ru51	0.20	1.79	0.017
19. BD (1) C 6-Ru52	755. RY*(8)Ru51	0.10	6.67	0.023
19. BD (1) C 6-Ru52	756. RY*(9)Ru51	0.23	3.14	0.024
19. BD (1) C 6-Ru52	757. RY*(10)Ru51	0.10	21.78	0.042
19. BD (1) C 6-Ru52	758. RY*(11)Ru51	0.07	7.37	0.021
19. BD (1) C 6-Ru52	792. RY*(45)Ru51	0.07	51.49	0.054
19. BD (1) C 6-Ru52	902. BD*(1) C11-Ru51	0.14	0.56	0.008
19. BD (1) C 6-Ru52	912. BD*(1) C 4-Ru51	0.16	0.61	0.010
23. BD (1) C 8- O47	748. RY*(1)Ru51	0.08	18.45	0.033
23. BD (1) C 8- O47	755. RY*(8)Ru51	0.15	6.53	0.028
23. BD (1) C 8- O47	756. RY*(9)Ru51	0.12	3.00	0.017
23. BD (1) C 8- O47	757. RY*(10)Ru51	0.12	21.63	0.046
23. BD (1) C 8- O47	759. RY*(12)Ru51	0.06	15.13	0.026
23. BD (1) C 8- O47	764. RY*(17)Ru51	0.08	10.92	0.026
23. BD (1) C 8- O47	767. RY*(20)Ru51	0.07	17.59	0.031
23. BD (1) C 8- O47	769. RY*(22)Ru51	0.05	9.30	0.019
23. BD (1) C 8- O47	770. RY*(23)Ru51	0.07	16.54	0.031
23. BD (1) C 8- O47	776. RY*(29)Ru51	0.11	77.82	0.081
23. BD (1) C 8- O47	777. RY*(30)Ru51	0.07	26.10	0.039
23. BD (1) C 8- O47	780. RY*(33)Ru51	0.09	324.72	0.149
23. BD (1) C 8- O47	785. RY*(38)Ru51	0.07	596.55	0.181
23. BD (1) C 8- O47	792. RY*(45)Ru51	0.06	51.34	0.049
25. BD (3) C 8- O47	169. RY*(2) C 1	0.05	1.64	0.008
25. BD (3) C 8- O47	188. RY*(6) C 2	0.06	4.75	0.015
25. BD (3) C 8- O47	560. RY*(3) H27	0.41	2.06	0.026
25. BD (3) C 8- O47	750. RY*(3)Ru51	0.06	9.36	0.021
25. BD (3) C 8- O47	752. RY*(5)Ru51	0.08	5.26	0.018
25. BD (3) C 8- O47	753. RY*(6)Ru51	0.10	4.21	0.018
25. BD (3) C 8- O47	755. RY*(8)Ru51	0.20	7.24	0.034
25. BD (3) C 8- O47	757. RY*(10)Ru51	0.25	22.34	0.067
25. BD (3) C 8- O47	760. RY*(13)Ru51	0.10	5.88	0.021
25. BD (3) C 8- O47	763. RY*(16)Ru51	0.09	13.90	0.032
25. BD (3) C 8- O47	764. RY*(17)Ru51	0.09	11.63	0.029
25. BD (3) C 8- O47	765. RY*(18)Ru51	0.10	7.80	0.025
25. BD (3) C 8- O47	766. RY*(19)Ru51	0.10	7.94	0.025
25. BD (3) C 8- O47	767. RY*(20)Ru51	0.15	18.30	0.047
25. BD (3) C 8- O47	776. RY*(29)Ru51	0.06	78.53	0.061
25. BD (3) C 8- O47	777. RY*(30)Ru51	0.08	26.81	0.041
25. BD (3) C 8- O47	780. RY*(33)Ru51	0.08	325.43	0.145
25. BD (3) C 8- O47	785. RY*(38)Ru51	0.06	597.26	0.171
26. BD (1) C 8-Ru52	184. RY*(2) C 2	0.07	1.18	0.008
26. BD (1) C 8-Ru52	188. RY*(6) C 2	0.06	4.19	0.015
26. BD (1) C 8-Ru52	558. RY*(1) H27	0.32	1.91	0.022
26. BD (1) C 8-Ru52	560. RY*(3) H27	0.63	1.50	0.028
26. BD (1) C 8-Ru52	720. RY*(3) N49	0.05	2.65	0.011
26. BD (1) C 8-Ru52	751. RY*(4)Ru51	0.08	1.79	0.011
26. BD (1) C 8-Ru52	755. RY*(8)Ru51	0.17	6.68	0.031
26. BD (1) C 8-Ru52	757. RY*(10)Ru51	0.12	21.78	0.046
26. BD (1) C 8-Ru52	758. RY*(11)Ru51	0.08	7.37	0.022
26. BD (1) C 8-Ru52	760. RY*(13)Ru51	0.09	5.32	0.020
26. BD (1) C 8-Ru52	764. RY*(17)Ru51	0.06	11.07	0.022
26. BD (1) C 8-Ru52	765. RY*(18)Ru51	0.16	7.24	0.031
26. BD (1) C 8-Ru52	766. RY*(19)Ru51	0.11	7.38	0.026
26. BD (1) C 8-Ru52	767. RY*(20)Ru51	0.08	17.74	0.034
26. BD (1) C 8-Ru52	774. RY*(27)Ru51	0.05	49.75	0.046
38. BD (2) C12- C14	915. BD*(2) C10- O48	0.10	0.25	0.005

39. BD (1) C12- H29	213. RY*(1) C 4	0.06	2.76	0.012
39. BD (1) C12- H29	219. RY*(7) C 4	0.08	7.12	0.022
39. BD (1) C12- H29	303. RY*(1) C10	0.09	2.58	0.014
39. BD (1) C12- H29	748. RY*(1)Ru51	0.20	18.56	0.054
39. BD (1) C12- H29	750. RY*(3)Ru51	0.20	8.76	0.037
39. BD (1) C12- H29	752. RY*(5)Ru51	0.11	4.66	0.020
39. BD (1) C12- H29	753. RY*(6)Ru51	0.06	3.61	0.013
39. BD (1) C12- H29	755. RY*(8)Ru51	0.20	6.64	0.033
39. BD (1) C12- H29	757. RY*(10)Ru51	0.23	21.74	0.063
39. BD (1) C12- H29	759. RY*(12)Ru51	0.11	15.24	0.037
39. BD (1) C12- H29	760. RY*(13)Ru51	0.13	5.28	0.023
39. BD (1) C12- H29	762. RY*(15)Ru51	0.12	14.72	0.038
39. BD (1) C12- H29	763. RY*(16)Ru51	0.10	13.30	0.032
39. BD (1) C12- H29	764. RY*(17)Ru51	0.17	11.03	0.039
39. BD (1) C12- H29	767. RY*(20)Ru51	0.23	17.70	0.057
39. BD (1) C12- H29	768. RY*(21)Ru51	0.06	17.35	0.028
39. BD (1) C12- H29	770. RY*(23)Ru51	0.09	16.65	0.035
39. BD (1) C12- H29	772. RY*(25)Ru51	0.11	9406.55	0.916
39. BD (1) C12- H29	773. RY*(26)Ru51	0.06	37514.10	1.399
39. BD (1) C12- H29	776. RY*(29)Ru51	0.20	77.93	0.111
39. BD (1) C12- H29	777. RY*(30)Ru51	0.18	26.21	0.061
39. BD (1) C12- H29	780. RY*(33)Ru51	0.19	324.83	0.226
39. BD (1) C12- H29	785. RY*(38)Ru51	0.15	596.66	0.272
39. BD (1) C12- H29	789. RY*(42)Ru51	0.11	533.26	0.215
39. BD (1) C12- H29	915. BD*(2) C10- O48	0.15	0.49	0.008
40. BD (1) C12- N50	560. RY*(3) H27	0.05	1.74	0.009
40. BD (1) C12- N50	748. RY*(1)Ru51	0.05	18.84	0.028
40. BD (1) C12- N50	750. RY*(3)Ru51	0.06	9.04	0.021
40. BD (1) C12- N50	753. RY*(6)Ru51	0.06	3.89	0.014
40. BD (1) C12- N50	755. RY*(8)Ru51	0.07	6.92	0.019
40. BD (1) C12- N50	757. RY*(10)Ru51	0.09	22.03	0.040
40. BD (1) C12- N50	762. RY*(15)Ru51	0.05	15.00	0.025
40. BD (1) C12- N50	767. RY*(20)Ru51	0.08	17.99	0.035
40. BD (1) C12- N50	776. RY*(29)Ru51	0.06	78.21	0.062
40. BD (1) C12- N50	777. RY*(30)Ru51	0.05	26.50	0.033
40. BD (1) C12- N50	780. RY*(33)Ru51	0.06	325.11	0.127
40. BD (1) C12- N50	785. RY*(38)Ru51	0.05	596.95	0.155
47. BD (1) C16- C18	560. RY*(3) H27	0.12	1.58	0.012
48. BD (1) C16- C22	188. RY*(6) C 2	0.06	4.26	0.014
49. BD (1) C16-Ru52	184. RY*(2) C 2	0.06	1.01	0.007
49. BD (1) C16-Ru52	188. RY*(6) C 2	0.09	4.02	0.017
49. BD (1) C16-Ru52	558. RY*(1) H27	0.23	1.74	0.018
49. BD (1) C16-Ru52	560. RY*(3) H27	0.72	1.33	0.029
49. BD (1) C16-Ru52	720. RY*(3) N49	0.07	2.48	0.012
49. BD (1) C16-Ru52	753. RY*(6)Ru51	0.15	3.48	0.021
49. BD (1) C16-Ru52	757. RY*(10)Ru51	0.05	21.61	0.031
49. BD (1) C16-Ru52	902. BD*(1) C11-Ru51	0.08	0.39	0.005
59. BD (1) C20- N50	188. RY*(6) C 2	0.09	4.42	0.017
59. BD (1) C20- N50	748. RY*(1)Ru51	0.14	18.82	0.046
59. BD (1) C20- N50	750. RY*(3)Ru51	0.08	9.02	0.023
59. BD (1) C20- N50	755. RY*(8)Ru51	0.11	6.90	0.025
59. BD (1) C20- N50	757. RY*(10)Ru51	0.08	22.01	0.037
59. BD (1) C20- N50	759. RY*(12)Ru51	0.07	15.50	0.030
59. BD (1) C20- N50	763. RY*(16)Ru51	0.06	13.56	0.025
59. BD (1) C20- N50	764. RY*(17)Ru51	0.07	11.29	0.025
59. BD (1) C20- N50	767. RY*(20)Ru51	0.08	17.96	0.034
59. BD (1) C20- N50	772. RY*(25)Ru51	0.06	9406.81	0.660
59. BD (1) C20- N50	776. RY*(29)Ru51	0.11	78.19	0.084
59. BD (1) C20- N50	777. RY*(30)Ru51	0.08	26.47	0.041
59. BD (1) C20- N50	780. RY*(33)Ru51	0.10	325.09	0.163
59. BD (1) C20- N50	785. RY*(38)Ru51	0.08	596.93	0.196
59. BD (1) C20- N50	789. RY*(42)Ru51	0.06	533.53	0.155
60. BD (2) C20- N50	748. RY*(1)Ru51	0.10	18.36	0.041
60. BD (2) C20- N50	750. RY*(3)Ru51	0.10	8.56	0.028
60. BD (2) C20- N50	759. RY*(12)Ru51	0.06	15.04	0.028
60. BD (2) C20- N50	762. RY*(15)Ru51	0.07	14.52	0.030
60. BD (2) C20- N50	766. RY*(19)Ru51	0.07	7.15	0.022
60. BD (2) C20- N50	767. RY*(20)Ru51	0.10	17.50	0.040
60. BD (2) C20- N50	776. RY*(29)Ru51	0.09	77.73	0.079
60. BD (2) C20- N50	777. RY*(30)Ru51	0.08	26.01	0.043
60. BD (2) C20- N50	780. RY*(33)Ru51	0.07	324.63	0.148
60. BD (2) C20- N50	785. RY*(38)Ru51	0.06	596.47	0.176
126. CR (3)Ru52	913. BD*(1) C10-Ru51	0.05	22.01	0.033
127. CR (4)Ru52	902. BD*(1) C11-Ru51	0.10	4.63	0.020
127. CR (4)Ru52	913. BD*(1) C10-Ru51	0.13	4.72	0.024
156. LP (1) N50	188. RY*(6) C 2	0.11	4.03	0.021
156. LP (1) N50	558. RY*(1) H27	0.06	1.75	0.010
156. LP (1) N50	560. RY*(3) H27	0.11	1.34	0.012
156. LP (1) N50	748. RY*(1)Ru51	0.11	18.44	0.044
156. LP (1) N50	750. RY*(3)Ru51	0.06	8.64	0.023
156. LP (1) N50	766. RY*(19)Ru51	0.07	7.22	0.022
156. LP (1) N50	776. RY*(29)Ru51	0.07	77.81	0.074
156. LP (1) N50	780. RY*(33)Ru51	0.06	324.71	0.134
156. LP (1) N50	913. BD*(1) C10-Ru51	0.08	0.49	0.006
160. LP (1)Ru52	188. RY*(6) C 2	0.16	3.86	0.023
160. LP (1)Ru52	213. RY*(1) C 4	0.09	2.46	0.014
160. LP (1)Ru52	219. RY*(7) C 4	0.11	6.83	0.026
160. LP (1)Ru52	293. RY*(6) C 9	0.06	4.09	0.015
160. LP (1)Ru52	303. RY*(1) C10	0.06	2.28	0.011
160. LP (1)Ru52	329. RY*(12) C11	0.05	3.35	0.013
160. LP (1)Ru52	383. RY*(6) C15	0.11	3.67	0.019
160. LP (1)Ru52	561. RY*(4) H27	0.15	2.00	0.016
160. LP (1)Ru52	646. RY*(4) O44	0.11	0.92	0.009
160. LP (1)Ru52	706. RY*(4) O48	0.08	0.92	0.008
160. LP (1)Ru52	748. RY*(1)Ru51	0.36	18.26	0.076
160. LP (1)Ru52	750. RY*(3)Ru51	0.24	8.46	0.043
160. LP (1)Ru52	752. RY*(5)Ru51	0.06	4.37	0.015
160. LP (1)Ru52	755. RY*(8)Ru51	0.67	6.34	0.062
160. LP (1)Ru52	756. RY*(9)Ru51	0.34	2.81	0.029
160. LP (1)Ru52	757. RY*(10)Ru51	0.54	21.45	0.102
160. LP (1)Ru52	759. RY*(12)Ru51	0.24	14.94	0.057
160. LP (1)Ru52	760. RY*(13)Ru51	0.22	4.98	0.031
160. LP (1)Ru52	761. RY*(14)Ru51	0.12	7.74	0.029
160. LP (1)Ru52	762. RY*(15)Ru51	0.13	14.42	0.040
160. LP (1)Ru52	763. RY*(16)Ru51	0.18	13.00	0.045
160. LP (1)Ru52	764. RY*(17)Ru51	0.32	10.74	0.056
160. LP (1)Ru52	765. RY*(18)Ru51	0.13	6.90	0.028
160. LP (1)Ru52	767. RY*(20)Ru51	0.37	17.41	0.076
160. LP (1)Ru52	768. RY*(21)Ru51	0.16	17.06	0.049
160. LP (1)Ru52	769. RY*(22)Ru51	0.06	9.12	0.023
160. LP (1)Ru52	770. RY*(23)Ru51	0.21	16.36	0.056
160. LP (1)Ru52	772. RY*(25)Ru51	0.23	9406.25	1.399
160. LP (1)Ru52	773. RY*(26)Ru51	0.13	37513.81	2.128
160. LP (1)Ru52	776. RY*(29)Ru51	0.45	77.63	0.176
160. LP (1)Ru52	777. RY*(30)Ru51	0.34	25.92	0.089
160. LP (1)Ru52	780. RY*(33)Ru51	0.40	324.53	0.341

160. LP (1)Ru52	785. RY*(38)Ru51	0.32	596.37	0.414
160. LP (1)Ru52	788. RY*(41)Ru51	0.09	89.14	0.083
160. LP (1)Ru52	789. RY*(42)Ru51	0.23	532.97	0.330
160. LP (1)Ru52	792. RY*(45)Ru51	0.11	51.16	0.072
160. LP (1)Ru52	793. RY*(46)Ru51	0.07	186.24	0.104
161. LP (2)Ru52	188. RY*(6) C 2	0.22	3.86	0.028
161. LP (2)Ru52	213. RY*(1) C 4	0.16	2.47	0.019
161. LP (2)Ru52	219. RY*(7) C 4	0.28	6.83	0.042
161. LP (2)Ru52	224. RY*(12) C 4	0.06	3.57	0.014
161. LP (2)Ru52	225. RY*(13) C 4	0.09	2.76	0.015
161. LP (2)Ru52	264. RY*(7) C 7	0.12	4.24	0.021
161. LP (2)Ru52	293. RY*(6) C 9	0.13	4.10	0.022
161. LP (2)Ru52	303. RY*(1) C10	0.17	2.28	0.019
161. LP (2)Ru52	305. RY*(3) C10	0.13	2.82	0.019
161. LP (2)Ru52	309. RY*(7) C10	0.16	6.89	0.032
161. LP (2)Ru52	310. RY*(8) C10	0.06	4.19	0.016
161. LP (2)Ru52	313. RY*(11) C10	0.10	1.99	0.014
161. LP (2)Ru52	318. RY*(1) C11	0.06	1.45	0.009
161. LP (2)Ru52	329. RY*(12) C11	0.10	3.35	0.018
161. LP (2)Ru52	383. RY*(6) C15	0.20	3.68	0.026
161. LP (2)Ru52	630. RY*(3) H41	0.06	1.44	0.009
161. LP (2)Ru52	646. RY*(4) O44	0.22	0.93	0.014
161. LP (2)Ru52	647. RY*(5) O44	0.10	2.61	0.016
161. LP (2)Ru52	706. RY*(4) O48	0.10	0.93	0.009
161. LP (2)Ru52	708. RY*(6) O48	0.07	2.10	0.012
161. LP (2)Ru52	721. RY*(4) N49	0.08	4.76	0.019
161. LP (2)Ru52	748. RY*(1)Ru51	0.66	18.26	0.106
161. LP (2)Ru52	750. RY*(3)Ru51	0.48	8.46	0.061
161. LP (2)Ru52	752. RY*(5)Ru51	0.07	4.37	0.016
161. LP (2)Ru52	753. RY*(6)Ru51	0.11	3.32	0.019
161. LP (2)Ru52	755. RY*(8)Ru51	1.30	6.35	0.088
161. LP (2)Ru52	756. RY*(9)Ru51	1.05	2.82	0.052
161. LP (2)Ru52	757. RY*(10)Ru51	1.03	21.45	0.144
161. LP (2)Ru52	758. RY*(11)Ru51	0.06	7.04	0.020
161. LP (2)Ru52	759. RY*(12)Ru51	0.55	14.95	0.087
161. LP (2)Ru52	760. RY*(13)Ru51	0.36	4.99	0.041
161. LP (2)Ru52	761. RY*(14)Ru51	0.45	7.74	0.057
161. LP (2)Ru52	762. RY*(15)Ru51	0.23	14.43	0.055
161. LP (2)Ru52	763. RY*(16)Ru51	0.34	13.01	0.064
161. LP (2)Ru52	764. RY*(17)Ru51	0.71	10.74	0.084
161. LP (2)Ru52	765. RY*(18)Ru51	0.16	6.91	0.032
161. LP (2)Ru52	767. RY*(20)Ru51	0.70	17.41	0.106
161. LP (2)Ru52	768. RY*(21)Ru51	0.32	17.06	0.071
161. LP (2)Ru52	769. RY*(22)Ru51	0.47	9.12	0.063
161. LP (2)Ru52	770. RY*(23)Ru51	0.69	16.36	0.102
161. LP (2)Ru52	772. RY*(25)Ru51	0.50	9406.26	2.086
161. LP (2)Ru52	773. RY*(26)Ru51	0.30	37513.81	3.211
161. LP (2)Ru52	776. RY*(29)Ru51	1.08	77.64	0.280
161. LP (2)Ru52	777. RY*(30)Ru51	0.81	25.92	0.139
161. LP (2)Ru52	780. RY*(33)Ru51	0.86	324.53	0.509
161. LP (2)Ru52	781. RY*(34)Ru51	0.05	50.39	0.049
161. LP (2)Ru52	785. RY*(38)Ru51	0.69	596.37	0.620
161. LP (2)Ru52	788. RY*(41)Ru51	0.19	89.14	0.126
161. LP (2)Ru52	789. RY*(42)Ru51	0.49	532.97	0.491
161. LP (2)Ru52	792. RY*(45)Ru51	0.54	51.16	0.161
161. LP (2)Ru52	793. RY*(46)Ru51	0.32	186.24	0.236
161. LP (2)Ru52	913. BD*(1) C10-Ru51	0.15	0.32	0.006
161. LP (2)Ru52	916. BD*(3) C10- O48	0.06	0.80	0.006
162. LP (3)Ru52	749. RY*(2)Ru51	0.07	1.11	0.009
162. LP (3)Ru52	756. RY*(9)Ru51	0.08	2.83	0.015

within unit 2

16. BD (1) C 6- O46	798. RY*(3)Ru52	0.64	1.10	0.024
17. BD (2) C 6- O46	796. RY*(1)Ru52	1.55	0.24	0.017
18. BD (3) C 6- O46	243. RY*(1) C 6	2.55	2.58	0.073
18. BD (3) C 6- O46	245. RY*(3) C 6	1.22	3.69	0.060
18. BD (3) C 6- O46	249. RY*(7) C 6	1.03	7.35	0.078
18. BD (3) C 6- O46	251. RY*(9) C 6	0.77	4.13	0.050
18. BD (3) C 6- O46	256. RY*(14) C 6	0.84	46.48	0.176
18. BD (3) C 6- O46	257. RY*(15) C 6	1.41	26.56	0.173
18. BD (3) C 6- O46	279. RY*(7) C 8	0.58	5.43	0.050
18. BD (3) C 6- O46	733. RY*(1) N50	0.69	2.65	0.038
18. BD (3) C 6- O46	796. RY*(1)Ru52	3.22	0.94	0.049
18. BD (3) C 6- O46	797. RY*(2)Ru52	0.95	1.55	0.034
18. BD (3) C 6- O46	799. RY*(4)Ru52	1.05	2.81	0.048
18. BD (3) C 6- O46	800. RY*(5)Ru52	1.52	4.10	0.071
18. BD (3) C 6- O46	802. RY*(7)Ru52	1.37	4.15	0.067
18. BD (3) C 6- O46	803. RY*(8)Ru52	6.46	2.17	0.106
18. BD (3) C 6- O46	804. RY*(9)Ru52	0.89	3.28	0.048
18. BD (3) C 6- O46	805. RY*(10)Ru52	40.23	0.44	0.119
18. BD (3) C 6- O46	807. RY*(12)Ru52	3.42	8.14	0.149
18. BD (3) C 6- O46	809. RY*(14)Ru52	0.76	6.33	0.062
18. BD (3) C 6- O46	810. RY*(15)Ru52	0.87	7.17	0.071
18. BD (3) C 6- O46	811. RY*(16)Ru52	1.07	7.10	0.078
18. BD (3) C 6- O46	817. RY*(22)Ru52	1.73	10.26	0.119
18. BD (3) C 6- O46	818. RY*(23)Ru52	2.15	7.63	0.114
18. BD (3) C 6- O46	819. RY*(24)Ru52	4.46	29464.43	10.247
18. BD (3) C 6- O46	820. RY*(25)Ru52	9.13	766.15	2.365
18. BD (3) C 6- O46	821. RY*(26)Ru52	8.98	12900.41	9.623
18. BD (3) C 6- O46	828. RY*(33)Ru52	1.11	156.43	0.372
18. BD (3) C 6- O46	829. RY*(34)Ru52	0.82	50.75	0.182
18. BD (3) C 6- O46	832. RY*(37)Ru52	0.52	187.32	0.279
18. BD (3) C 6- O46	833. RY*(38)Ru52	10.34	3362.50	5.269
18. BD (3) C 6- O46	836. RY*(41)Ru52	6.08	777.79	1.943
18. BD (3) C 6- O46	837. RY*(42)Ru52	3.46	3155.52	2.952
18. BD (3) C 6- O46	840. RY*(45)Ru52	0.65	51.91	0.164
19. BD (1) C 6-Ru52	257. RY*(15) C 6	0.63	26.01	0.116
19. BD (1) C 6-Ru52	273. RY*(1) C 8	0.59	1.89	0.030
19. BD (1) C 6-Ru52	274. RY*(2) C 8	1.78	2.49	0.060
19. BD (1) C 6-Ru52	279. RY*(7) C 8	1.52	4.87	0.078
19. BD (1) C 6-Ru52	393. RY*(1) C16	1.46	1.57	0.043
19. BD (1) C 6-Ru52	428. RY*(6) C18	0.77	2.93	0.043
19. BD (1) C 6-Ru52	675. RY*(3) O46	1.65	2.39	0.057
19. BD (1) C 6-Ru52	676. RY*(4) O46	1.23	1.02	0.032
19. BD (1) C 6-Ru52	733. RY*(1) N50	1.00	2.09	0.042
19. BD (1) C 6-Ru52	796. RY*(1)Ru52	48.31	0.38	0.123
19. BD (1) C 6-Ru52	797. RY*(2)Ru52	17.36	0.99	0.119
19. BD (1) C 6-Ru52	798. RY*(3)Ru52	3.85	1.23	0.063
19. BD (1) C 6-Ru52	801. RY*(6)Ru52	3.41	1.65	0.068
19. BD (1) C 6-Ru52	803. RY*(8)Ru52	3.35	1.61	0.067
19. BD (1) C 6-Ru52	810. RY*(15)Ru52	2.30	6.61	0.112
19. BD (1) C 6-Ru52	811. RY*(16)Ru52	0.89	6.54	0.070
19. BD (1) C 6-Ru52	812. RY*(17)Ru52	3.97	4.44	0.121
19. BD (1) C 6-Ru52	814. RY*(19)Ru52	1.56	5.72	0.086
19. BD (1) C 6-Ru52	818. RY*(23)Ru52	1.33	7.07	0.088
19. BD (1) C 6-Ru52	828. RY*(33)Ru52	1.74	155.87	0.474

19. BD (1) C 6-Ru52	879. BD*(2) C 8- O47	1.98	0.51	0.029
19. BD (1) C 6-Ru52	880. BD*(3) C 8- O47	1.75	1.11	0.040
19. BD (1) C 6-Ru52	881. BD*(1) C 8-Ru52	11.60	0.60	0.080
19. BD (1) C 6-Ru52	882. BD*(1) C 6-Ru52	0.86	0.63	0.022
19. BD (1) C 6-Ru52	885. BD*(3) C 6- O46	0.56	1.12	0.023
19. BD (1) C 6-Ru52	926. BD*(1) C16-Ru52	12.22	0.54	0.076
19. BD (1) C 6-Ru52	927. BD*(1) C16- C22	2.05	1.03	0.041
23. BD (1) C 8- O47	796. RY*(1)Ru52	1.30	0.24	0.016
24. BD (2) C 8- O47	796. RY*(1)Ru52	1.10	0.23	0.014
24. BD (2) C 8- O47	798. RY*(3)Ru52	1.42	1.09	0.035
25. BD (3) C 8- O47	273. RY*(1) C 8	1.74	2.45	0.058
25. BD (3) C 8- O47	280. RY*(8) C 8	1.12	5.10	0.067
25. BD (3) C 8- O47	281. RY*(9) C 8	0.50	3.88	0.040
25. BD (3) C 8- O47	286. RY*(14) C 8	0.55	46.70	0.143
25. BD (3) C 8- O47	287. RY*(15) C 8	0.82	27.71	0.135
25. BD (3) C 8- O47	796. RY*(1)Ru52	2.60	0.95	0.044
25. BD (3) C 8- O47	797. RY*(2)Ru52	0.71	1.56	0.030
25. BD (3) C 8- O47	798. RY*(3)Ru52	0.71	1.80	0.032
25. BD (3) C 8- O47	800. RY*(5)Ru52	2.40	4.11	0.089
25. BD (3) C 8- O47	803. RY*(8)Ru52	1.43	2.18	0.050
25. BD (3) C 8- O47	805. RY*(10)Ru52	168.84	0.45	0.246
25. BD (3) C 8- O47	807. RY*(12)Ru52	1.35	8.15	0.094
25. BD (3) C 8- O47	808. RY*(13)Ru52	0.53	3.50	0.039
25. BD (3) C 8- O47	812. RY*(17)Ru52	1.51	5.00	0.078
25. BD (3) C 8- O47	816. RY*(21)Ru52	0.90	14.45	0.102
25. BD (3) C 8- O47	817. RY*(22)Ru52	2.26	10.27	0.136
25. BD (3) C 8- O47	818. RY*(23)Ru52	6.66	7.64	0.202
25. BD (3) C 8- O47	819. RY*(24)Ru52	4.27	29464.43	10.024
25. BD (3) C 8- O47	820. RY*(25)Ru52	8.87	766.16	2.330
25. BD (3) C 8- O47	821. RY*(26)Ru52	8.43	12900.42	9.321
25. BD (3) C 8- O47	828. RY*(33)Ru52	0.73	156.44	0.302
25. BD (3) C 8- O47	833. RY*(38)Ru52	9.75	3362.51	5.117
25. BD (3) C 8- O47	836. RY*(41)Ru52	5.78	777.80	1.894
25. BD (3) C 8- O47	837. RY*(42)Ru52	3.35	3155.53	2.906
25. BD (3) C 8- O47	840. RY*(45)Ru52	1.01	51.92	0.204
25. BD (3) C 8- O47	841. RY*(46)Ru52	0.55	187.23	0.287
26. BD (1) C 8-Ru52	167. LP*(1) C16	0.53	0.45	0.018
26. BD (1) C 8-Ru52	243. RY*(1) C 6	1.34	2.02	0.047
26. BD (1) C 8-Ru52	244. RY*(2) C 6	0.90	1.41	0.032
26. BD (1) C 8-Ru52	245. RY*(3) C 6	3.22	3.14	0.091
26. BD (1) C 8-Ru52	247. RY*(5) C 6	0.57	2.36	0.034
26. BD (1) C 8-Ru52	249. RY*(7) C 6	1.43	6.80	0.090
26. BD (1) C 8-Ru52	250. RY*(8) C 6	0.83	4.41	0.055
26. BD (1) C 8-Ru52	286. RY*(14) C 8	0.51	46.13	0.140
26. BD (1) C 8-Ru52	287. RY*(15) C 8	0.55	27.14	0.111
26. BD (1) C 8-Ru52	338. RY*(6) C12	0.86	3.31	0.048
26. BD (1) C 8-Ru52	394. RY*(2) C16	0.78	1.15	0.027
26. BD (1) C 8-Ru52	404. RY*(12) C16	0.66	3.43	0.044
26. BD (1) C 8-Ru52	428. RY*(6) C18	1.21	2.94	0.054
26. BD (1) C 8-Ru52	690. RY*(3) O47	0.71	2.23	0.036
26. BD (1) C 8-Ru52	691. RY*(4) O47	1.69	0.98	0.037
26. BD (1) C 8-Ru52	733. RY*(1) N50	1.71	2.10	0.054
26. BD (1) C 8-Ru52	796. RY*(1)Ru52	98.73	0.38	0.177
26. BD (1) C 8-Ru52	797. RY*(2)Ru52	35.11	1.00	0.170
26. BD (1) C 8-Ru52	798. RY*(3)Ru52	9.36	1.24	0.098
26. BD (1) C 8-Ru52	799. RY*(4)Ru52	3.44	2.25	0.080
26. BD (1) C 8-Ru52	801. RY*(6)Ru52	3.69	1.65	0.071
26. BD (1) C 8-Ru52	803. RY*(8)Ru52	9.45	1.62	0.113
26. BD (1) C 8-Ru52	804. RY*(9)Ru52	1.33	2.73	0.055
26. BD (1) C 8-Ru52	807. RY*(12)Ru52	0.61	7.59	0.062
26. BD (1) C 8-Ru52	809. RY*(14)Ru52	0.58	5.77	0.053
26. BD (1) C 8-Ru52	810. RY*(15)Ru52	4.37	6.61	0.155
26. BD (1) C 8-Ru52	811. RY*(16)Ru52	5.38	6.55	0.171
26. BD (1) C 8-Ru52	812. RY*(17)Ru52	5.55	4.44	0.143
26. BD (1) C 8-Ru52	814. RY*(19)Ru52	2.41	5.72	0.107
26. BD (1) C 8-Ru52	818. RY*(23)Ru52	4.18	7.08	0.157
26. BD (1) C 8-Ru52	820. RY*(25)Ru52	0.60	765.60	0.616
26. BD (1) C 8-Ru52	828. RY*(33)Ru52	2.12	155.87	0.524
26. BD (1) C 8-Ru52	865. BD*(1) C12- N50	0.60	0.97	0.022
26. BD (1) C 8-Ru52	881. BD*(1) C 8-Ru52	1.12	0.60	0.025
26. BD (1) C 8-Ru52	882. BD*(1) C 6-Ru52	13.52	0.63	0.088
26. BD (1) C 8-Ru52	883. BD*(1) C 6- O46	1.87	0.53	0.029
26. BD (1) C 8-Ru52	884. BD*(2) C 6- O46	1.36	0.52	0.025
26. BD (1) C 8-Ru52	885. BD*(3) C 6- O46	2.30	1.12	0.046
26. BD (1) C 8-Ru52	921. BD*(1) C20- N50	0.80	0.94	0.025
26. BD (1) C 8-Ru52	926. BD*(1) C16-Ru52	13.24	0.54	0.079
26. BD (1) C 8-Ru52	927. BD*(1) C16- C22	0.60	1.03	0.022
26. BD (1) C 8-Ru52	928. BD*(1) C16- C18	0.78	1.04	0.026
37. BD (1) C12- C14	469. RY*(2) C21	0.93	2.39	0.042
37. BD (1) C12- C14	733. RY*(1) N50	1.05	2.23	0.043
37. BD (1) C12- C14	796. RY*(1)Ru52	1.01	0.52	0.020
37. BD (1) C12- C14	797. RY*(2)Ru52	0.60	1.13	0.023
37. BD (1) C12- C14	805. RY*(10)Ru52	165.50	0.02	0.055
37. BD (1) C12- C14	818. RY*(23)Ru52	0.54	7.21	0.056
37. BD (1) C12- C14	865. BD*(1) C12- N50	0.62	1.10	0.023
37. BD (1) C12- C14	867. BD*(1) C14- C21	0.71	1.11	0.025
37. BD (1) C12- C14	882. BD*(1) C 6-Ru52	0.58	0.77	0.020
37. BD (1) C12- C14	919. BD*(1) C21- H37	2.47	1.04	0.045
38. BD (2) C12- C14	470. RY*(3) C21	1.04	0.79	0.028
38. BD (2) C12- C14	734. RY*(2) N50	0.94	1.09	0.031
38. BD (2) C12- C14	864. BD*(2) C12- C14	0.67	0.23	0.011
38. BD (2) C12- C14	918. BD*(2) C21- C23	15.95	0.23	0.055
38. BD (2) C12- C14	922. BD*(2) C20- N50	10.45	0.21	0.044
39. BD (1) C12- H29	363. RY*(1) C14	0.95	2.18	0.041
39. BD (1) C12- H29	733. RY*(1) N50	1.16	2.06	0.044
39. BD (1) C12- H29	796. RY*(1)Ru52	1.07	0.35	0.017
39. BD (1) C12- H29	797. RY*(2)Ru52	0.89	0.96	0.026
39. BD (1) C12- H29	798. RY*(3)Ru52	0.59	1.20	0.024
39. BD (1) C12- H29	799. RY*(4)Ru52	0.55	2.21	0.031
39. BD (1) C12- H29	818. RY*(23)Ru52	0.84	7.04	0.069
39. BD (1) C12- H29	867. BD*(1) C14- C21	3.27	0.94	0.050
39. BD (1) C12- H29	921. BD*(1) C20- N50	6.56	0.91	0.069
40. BD (1) C12- N50	346. RY*(14) C12	0.67	40.85	0.148
40. BD (1) C12- N50	347. RY*(15) C12	0.97	26.94	0.145
40. BD (1) C12- N50	365. RY*(3) C14	0.88	2.64	0.043
40. BD (1) C12- N50	369. RY*(7) C14	0.71	4.52	0.051
40. BD (1) C12- N50	453. RY*(1) C20	0.55	2.31	0.032
40. BD (1) C12- N50	455. RY*(3) C20	1.24	2.71	0.052
40. BD (1) C12- N50	736. RY*(4) N50	0.92	5.27	0.062
40. BD (1) C12- N50	797. RY*(2)Ru52	2.71	1.24	0.052
40. BD (1) C12- N50	798. RY*(3)Ru52	1.72	1.48	0.045
40. BD (1) C12- N50	799. RY*(4)Ru52	0.60	2.50	0.035
40. BD (1) C12- N50	801. RY*(6)Ru52	2.06	1.90	0.056
40. BD (1) C12- N50	803. RY*(8)Ru52	0.62	1.86	0.030
40. BD (1) C12- N50	805. RY*(10)Ru52	18.30	0.14	0.045
40. BD (1) C12- N50	811. RY*(16)Ru52	0.51	6.79	0.053

40. BD (1) C12- N50	818. RY*(23)Ru52	2.23	7.32	0.115
40. BD (1) C12- N50	819. RY*(24)Ru52	0.57	29464.12	3.667
40. BD (1) C12- N50	820. RY*(25)Ru52	1.16	765.84	0.846
40. BD (1) C12- N50	821. RY*(26)Ru52	1.14	12900.11	3.433
40. BD (1) C12- N50	833. RY*(38)Ru52	1.30	3362.20	1.876
40. BD (1) C12- N50	836. RY*(41)Ru52	0.78	777.48	0.697
40. BD (1) C12- N50	863. BD*(1) C12- C14	1.01	1.24	0.032
40. BD (1) C12- N50	868. BD*(1) C14- H31	1.52	1.15	0.037
40. BD (1) C12- N50	882. BD*(1) C 6-Ru52	4.03	0.88	0.058
40. BD (1) C12- N50	921. BD*(1) C20- N50	0.59	1.19	0.024
40. BD (1) C12- N50	924. BD*(1) C20- C22	2.70	1.20	0.051
43. BD (1) C14- C21	500. RY*(3) C23	0.96	2.31	0.042
43. BD (1) C14- C21	805. RY*(10)Ru52	2.16	0.01	0.005
43. BD (1) C14- C21	863. BD*(1) C12- C14	0.81	1.12	0.027
43. BD (1) C14- C21	866. BD*(1) C12- H29	2.51	1.01	0.045
43. BD (1) C14- C21	917. BD*(1) C21- C23	0.81	1.12	0.027
43. BD (1) C14- C21	920. BD*(1) C23- H38	2.49	1.03	0.045
44. BD (1) C14- H31	333. RY*(1) C12	0.68	2.00	0.033
44. BD (1) C14- H31	468. RY*(1) C21	0.86	2.24	0.039
44. BD (1) C14- H31	865. BD*(1) C12- N50	5.42	0.92	0.063
44. BD (1) C14- H31	917. BD*(1) C21- C23	3.29	0.95	0.050
47. BD (1) C16- C18	396. RY*(4) C16	0.89	2.78	0.045
47. BD (1) C16- C18	435. RY*(13) C18	0.61	41.18	0.143
47. BD (1) C16- C18	437. RY*(15) C18	0.78	27.40	0.131
47. BD (1) C16- C18	483. RY*(1) C22	0.68	1.95	0.033
47. BD (1) C16- C18	487. RY*(5) C22	0.68	4.23	0.048
47. BD (1) C16- C18	515. RY*(3) C24	1.25	2.50	0.050
47. BD (1) C16- C18	733. RY*(1) N50	0.78	2.18	0.037
47. BD (1) C16- C18	796. RY*(1)Ru52	2.98	0.47	0.033
47. BD (1) C16- C18	797. RY*(2)Ru52	2.45	1.08	0.046
47. BD (1) C16- C18	802. RY*(7)Ru52	0.59	3.68	0.042
47. BD (1) C16- C18	803. RY*(8)Ru52	4.24	1.70	0.076
47. BD (1) C16- C18	806. RY*(11)Ru52	1.23	7.05	0.083
47. BD (1) C16- C18	812. RY*(17)Ru52	1.14	4.52	0.064
47. BD (1) C16- C18	817. RY*(22)Ru52	1.11	9.79	0.094
47. BD (1) C16- C18	818. RY*(23)Ru52	0.68	7.16	0.062
47. BD (1) C16- C18	819. RY*(24)Ru52	1.20	29463.96	5.328
47. BD (1) C16- C18	820. RY*(25)Ru52	2.45	765.68	1.229
47. BD (1) C16- C18	821. RY*(26)Ru52	2.29	12899.95	4.877
47. BD (1) C16- C18	822. RY*(27)Ru52	0.62	49.85	0.158
47. BD (1) C16- C18	833. RY*(38)Ru52	2.64	3362.03	2.673
47. BD (1) C16- C18	836. RY*(41)Ru52	1.56	777.32	0.988
47. BD (1) C16- C18	837. RY*(42)Ru52	0.96	3155.05	1.564
47. BD (1) C16- C18	840. RY*(45)Ru52	0.60	51.44	0.157
47. BD (1) C16- C18	924. BD*(1) C20- C22	3.69	1.04	0.055
47. BD (1) C16- C18	927. BD*(1) C16- C22	0.65	1.11	0.024
47. BD (1) C16- C18	930. BD*(1) C24- H36	2.18	1.02	0.042
47. BD (1) C16- C18	931. BD*(1) C18- C24	1.36	1.10	0.034
47. BD (1) C16- C18	933. BD*(1) C18- H32	0.66	1.02	0.023
48. BD (1) C16- C22	395. RY*(3) C16	0.70	1.58	0.030
48. BD (1) C16- C22	425. RY*(3) C18	1.02	2.26	0.043
48. BD (1) C16- C22	429. RY*(7) C18	0.59	8.48	0.063
48. BD (1) C16- C22	453. RY*(1) C20	0.66	2.13	0.034
48. BD (1) C16- C22	491. RY*(9) C22	0.73	14.20	0.092
48. BD (1) C16- C22	496. RY*(14) C22	1.00	26.17	0.145
48. BD (1) C16- C22	497. RY*(15) C22	0.83	42.36	0.169
48. BD (1) C16- C22	530. RY*(3) C25	0.74	2.34	0.037
48. BD (1) C16- C22	531. RY*(4) C25	0.89	2.15	0.039
48. BD (1) C16- C22	533. RY*(6) C25	0.63	6.21	0.056
48. BD (1) C16- C22	796. RY*(1)Ru52	10.88	0.46	0.063
48. BD (1) C16- C22	798. RY*(3)Ru52	0.76	1.31	0.028
48. BD (1) C16- C22	801. RY*(6)Ru52	0.51	1.73	0.027
48. BD (1) C16- C22	802. RY*(7)Ru52	0.57	3.67	0.041
48. BD (1) C16- C22	818. RY*(23)Ru52	1.63	7.15	0.097
48. BD (1) C16- C22	820. RY*(25)Ru52	0.71	765.67	0.662
48. BD (1) C16- C22	821. RY*(26)Ru52	0.63	12899.93	2.556
48. BD (1) C16- C22	833. RY*(38)Ru52	0.72	3362.02	1.403
48. BD (1) C16- C22	865. BD*(1) C12- N50	0.50	1.04	0.020
48. BD (1) C16- C22	871. BD*(1) C25- H39	2.27	1.00	0.043
48. BD (1) C16- C22	923. BD*(1) C20- C23	3.63	1.07	0.056
48. BD (1) C16- C22	924. BD*(1) C20- C22	1.06	1.02	0.029
48. BD (1) C16- C22	925. BD*(1) C22- C25	2.24	1.09	0.044
48. BD (1) C16- C22	928. BD*(1) C16- C18	0.51	1.11	0.021
48. BD (1) C16- C22	933. BD*(1) C18- H32	2.85	1.01	0.048
49. BD (1) C16-Ru52	243. RY*(1) C 6	1.45	1.85	0.048
49. BD (1) C16-Ru52	245. RY*(3) C 6	2.91	2.97	0.086
49. BD (1) C16-Ru52	249. RY*(7) C 6	1.00	6.63	0.076
49. BD (1) C16-Ru52	250. RY*(8) C 6	0.75	4.24	0.052
49. BD (1) C16-Ru52	273. RY*(1) C 8	0.82	1.72	0.035
49. BD (1) C16-Ru52	274. RY*(2) C 8	0.86	2.33	0.041
49. BD (1) C16-Ru52	279. RY*(7) C 8	0.84	4.70	0.058
49. BD (1) C16-Ru52	338. RY*(6) C12	0.83	3.14	0.047
49. BD (1) C16-Ru52	404. RY*(12) C16	0.69	3.26	0.044
49. BD (1) C16-Ru52	423. RY*(1) C18	0.51	1.99	0.030
49. BD (1) C16-Ru52	425. RY*(3) C18	1.28	2.02	0.047
49. BD (1) C16-Ru52	428. RY*(6) C18	0.59	2.77	0.038
49. BD (1) C16-Ru52	691. RY*(4) O47	0.79	0.81	0.023
49. BD (1) C16-Ru52	733. RY*(1) N50	1.62	1.93	0.052
49. BD (1) C16-Ru52	796. RY*(1)Ru52	147.77	0.21	0.165
49. BD (1) C16-Ru52	797. RY*(2)Ru52	50.57	0.83	0.189
49. BD (1) C16-Ru52	798. RY*(3)Ru52	11.35	1.07	0.102
49. BD (1) C16-Ru52	799. RY*(4)Ru52	5.16	2.08	0.096
49. BD (1) C16-Ru52	801. RY*(6)Ru52	2.61	1.48	0.058
49. BD (1) C16-Ru52	803. RY*(8)Ru52	7.20	1.45	0.094
49. BD (1) C16-Ru52	804. RY*(9)Ru52	0.60	2.56	0.036
49. BD (1) C16-Ru52	807. RY*(12)Ru52	0.80	7.42	0.071
49. BD (1) C16-Ru52	808. RY*(13)Ru52	0.53	2.77	0.035
49. BD (1) C16-Ru52	809. RY*(14)Ru52	0.76	5.60	0.060
49. BD (1) C16-Ru52	810. RY*(15)Ru52	2.83	6.44	0.125
49. BD (1) C16-Ru52	811. RY*(16)Ru52	4.29	6.38	0.153
49. BD (1) C16-Ru52	812. RY*(17)Ru52	4.10	4.27	0.122
49. BD (1) C16-Ru52	814. RY*(19)Ru52	2.21	5.55	0.103
49. BD (1) C16-Ru52	818. RY*(23)Ru52	3.39	6.91	0.142
49. BD (1) C16-Ru52	828. RY*(33)Ru52	2.53	155.70	0.581
49. BD (1) C16-Ru52	865. BD*(1) C12- N50	1.67	0.80	0.034
49. BD (1) C16-Ru52	878. BD*(1) C 8- O47	1.60	0.35	0.022
49. BD (1) C16-Ru52	880. BD*(3) C 8- O47	0.90	0.94	0.027
49. BD (1) C16-Ru52	881. BD*(1) C 8-Ru52	13.33	0.43	0.071
49. BD (1) C16-Ru52	882. BD*(1) C 6-Ru52	14.62	0.46	0.077
49. BD (1) C16-Ru52	884. BD*(2) C 6- O46	1.12	0.35	0.018
49. BD (1) C16-Ru52	885. BD*(3) C 6- O46	2.28	0.95	0.043
49. BD (1) C16-Ru52	923. BD*(1) C20- C23	0.61	0.82	0.021
49. BD (1) C16-Ru52	924. BD*(1) C20- C22	0.61	0.78	0.020
49. BD (1) C16-Ru52	925. BD*(1) C22- C25	6.32	0.84	0.067
49. BD (1) C16-Ru52	926. BD*(1) C16-Ru52	1.35	0.37	0.021
49. BD (1) C16-Ru52	931. BD*(1) C18- C24	5.25	0.84	0.061

49. BD (1) C16-Ru52	933. BD*(1) C18- H32	0.85	0.77	0.023
53. BD (1) C18- C24	393. RY*(1) C16	0.66	1.66	0.030
53. BD (1) C18- C24	545. RY*(3) C26	0.99	2.53	0.045
53. BD (1) C18- C24	872. BD*(1) C26- H40	2.39	1.02	0.044
53. BD (1) C18- C24	926. BD*(1) C16-Ru52	4.19	0.63	0.049
53. BD (1) C18- C24	928. BD*(1) C16- C18	1.43	1.13	0.036
53. BD (1) C18- C24	929. BD*(1) C24- C26	0.76	1.09	0.026
54. BD (2) C18- C24	167. LP*(1) C16	40.16	0.13	0.075
54. BD (2) C18- C24	394. RY*(2) C16	0.74	0.83	0.024
54. BD (2) C18- C24	424. RY*(2) C18	0.60	0.69	0.020
54. BD (2) C18- C24	544. RY*(2) C26	0.92	0.71	0.025
54. BD (2) C18- C24	870. BD*(2) C25- C26	14.36	0.22	0.051
55. BD (1) C18- H32	393. RY*(1) C16	1.50	1.49	0.042
55. BD (1) C18- H32	513. RY*(1) C24	1.02	2.02	0.041
55. BD (1) C18- H32	927. BD*(1) C16- C22	3.76	0.94	0.053
55. BD (1) C18- H32	929. BD*(1) C24- C26	3.74	0.92	0.052
57. BD (1) C20- C22	393. RY*(1) C16	0.78	1.64	0.032
57. BD (1) C20- C22	498. RY*(1) C23	0.83	2.13	0.038
57. BD (1) C20- C22	528. RY*(1) C25	0.91	2.14	0.040
57. BD (1) C20- C22	733. RY*(1) N50	0.62	2.16	0.033
57. BD (1) C20- C22	796. RY*(1)Ru52	1.39	0.45	0.023
57. BD (1) C20- C22	802. RY*(7)Ru52	0.51	3.66	0.039
57. BD (1) C20- C22	865. BD*(1) C12- N50	4.66	1.03	0.062
57. BD (1) C20- C22	869. BD*(1) C25- C26	2.09	1.09	0.043
57. BD (1) C20- C22	917. BD*(1) C21- C23	2.03	1.06	0.042
57. BD (1) C20- C22	923. BD*(1) C20- C23	1.00	1.06	0.029
57. BD (1) C20- C22	925. BD*(1) C22- C25	0.89	1.08	0.028
57. BD (1) C20- C22	927. BD*(1) C16- C22	1.08	1.10	0.031
57. BD (1) C20- C22	928. BD*(1) C16- C18	2.56	1.11	0.048
58. BD (1) C20- C23	469. RY*(2) C21	1.56	2.38	0.055
58. BD (1) C20- C23	485. RY*(3) C22	1.05	2.38	0.045
58. BD (1) C20- C23	796. RY*(1)Ru52	0.91	0.50	0.019
58. BD (1) C20- C23	882. BD*(1) C 6-Ru52	0.51	0.75	0.019
58. BD (1) C20- C23	917. BD*(1) C21- C23	0.92	1.11	0.029
58. BD (1) C20- C23	919. BD*(1) C21- H37	2.36	1.02	0.044
58. BD (1) C20- C23	924. BD*(1) C20- C22	1.09	1.07	0.031
58. BD (1) C20- C23	927. BD*(1) C16- C22	2.20	1.15	0.045
59. BD (1) C20- N50	335. RY*(3) C12	1.88	2.46	0.061
59. BD (1) C20- N50	461. RY*(9) C20	0.57	9.67	0.067
59. BD (1) C20- N50	466. RY*(14) C20	0.76	42.68	0.161
59. BD (1) C20- N50	467. RY*(15) C20	1.03	24.71	0.143
59. BD (1) C20- N50	503. RY*(6) C23	0.52	6.81	0.053
59. BD (1) C20- N50	505. RY*(8) C23	0.63	3.96	0.045
59. BD (1) C20- N50	735. RY*(3) N50	1.14	2.88	0.051
59. BD (1) C20- N50	796. RY*(1)Ru52	7.38	0.61	0.060
59. BD (1) C20- N50	805. RY*(10)Ru52	20.32	0.11	0.043
59. BD (1) C20- N50	818. RY*(23)Ru52	0.91	7.30	0.073
59. BD (1) C20- N50	866. BD*(1) C12- H29	2.08	1.11	0.043
59. BD (1) C20- N50	882. BD*(1) C 6-Ru52	4.94	0.86	0.063
59. BD (1) C20- N50	920. BD*(1) C23- H38	1.59	1.13	0.038
59. BD (1) C20- N50	923. BD*(1) C20- C23	1.01	1.22	0.031
59. BD (1) C20- N50	924. BD*(1) C20- C22	0.63	1.18	0.024
59. BD (1) C20- N50	925. BD*(1) C22- C25	2.38	1.24	0.049
60. BD (2) C20- N50	147. LP (1) C22	12.86	0.20	0.057
60. BD (2) C20- N50	334. RY*(2) C12	2.85	0.95	0.050
60. BD (2) C20- N50	484. RY*(2) C22	0.74	0.83	0.024
60. BD (2) C20- N50	499. RY*(2) C23	0.97	0.76	0.026
60. BD (2) C20- N50	734. RY*(2) N50	0.53	1.13	0.024
60. BD (2) C20- N50	797. RY*(2)Ru52	0.94	0.76	0.026
60. BD (2) C20- N50	864. BD*(2) C12- C14	20.56	0.27	0.067
60. BD (2) C20- N50	918. BD*(2) C21- C23	7.52	0.27	0.041
61. BD (1) C21- C23	365. RY*(3) C14	0.84	2.53	0.041
61. BD (1) C21- C23	453. RY*(1) C20	0.73	2.19	0.036
61. BD (1) C21- C23	805. RY*(10)Ru52	7.70	0.02	0.011
61. BD (1) C21- C23	867. BD*(1) C14- C21	0.77	1.11	0.026
61. BD (1) C21- C23	868. BD*(1) C14- H31	2.48	1.04	0.045
61. BD (1) C21- C23	923. BD*(1) C20- C23	1.07	1.12	0.031
61. BD (1) C21- C23	924. BD*(1) C20- C22	3.50	1.08	0.055
62. BD (2) C21- C23	364. RY*(2) C14	1.02	0.83	0.029
62. BD (2) C21- C23	458. RY*(6) C20	0.54	2.23	0.034
62. BD (2) C21- C23	864. BD*(2) C12- C14	12.80	0.23	0.049
62. BD (2) C21- C23	922. BD*(2) C20- N50	22.34	0.21	0.064
63. BD (1) C21- H37	363. RY*(1) C14	0.89	2.18	0.040
63. BD (1) C21- H37	498. RY*(1) C23	0.92	2.02	0.039
63. BD (1) C21- H37	863. BD*(1) C12- C14	3.38	0.95	0.051
63. BD (1) C21- H37	923. BD*(1) C20- C23	3.90	0.95	0.055
64. BD (1) C22- C25	395. RY*(3) C16	0.68	1.60	0.030
64. BD (1) C22- C25	455. RY*(3) C20	1.32	2.55	0.052
64. BD (1) C22- C25	545. RY*(3) C26	1.72	2.53	0.059
64. BD (1) C22- C25	869. BD*(1) C25- C26	1.00	1.11	0.030
64. BD (1) C22- C25	872. BD*(1) C26- H40	2.34	1.02	0.044
64. BD (1) C22- C25	921. BD*(1) C20- N50	2.87	1.03	0.049
64. BD (1) C22- C25	924. BD*(1) C20- C22	0.98	1.04	0.029
64. BD (1) C22- C25	926. BD*(1) C16-Ru52	3.51	0.63	0.045
64. BD (1) C22- C25	927. BD*(1) C16- C22	2.18	1.11	0.044
65. BD (1) C23- H38	453. RY*(1) C20	1.07	2.02	0.042
65. BD (1) C23- H38	468. RY*(1) C21	0.90	2.24	0.040
65. BD (1) C23- H38	867. BD*(1) C14- C21	3.52	0.93	0.051
65. BD (1) C23- H38	921. BD*(1) C20- N50	5.73	0.90	0.064
66. BD (1) C24- C26	426. RY*(4) C18	0.65	1.60	0.029
66. BD (1) C24- C26	530. RY*(3) C25	1.02	2.35	0.044
66. BD (1) C24- C26	869. BD*(1) C25- C26	0.95	1.11	0.029
66. BD (1) C24- C26	871. BD*(1) C25- H39	2.54	1.01	0.045
66. BD (1) C24- C26	931. BD*(1) C18- C24	0.82	1.10	0.027
66. BD (1) C24- C26	933. BD*(1) C18- H32	2.18	1.02	0.042
67. BD (1) C24- H36	423. RY*(1) C18	0.97	2.08	0.040
67. BD (1) C24- H36	543. RY*(1) C26	0.91	2.17	0.040
67. BD (1) C24- H36	869. BD*(1) C25- C26	3.66	0.95	0.053
67. BD (1) C24- H36	928. BD*(1) C16- C18	4.84	0.96	0.061
68. BD (1) C25- C26	483. RY*(1) C22	0.77	1.96	0.035
68. BD (1) C25- C26	515. RY*(3) C24	1.03	2.51	0.045
68. BD (1) C25- C26	924. BD*(1) C20- C22	3.43	1.05	0.054
68. BD (1) C25- C26	925. BD*(1) C22- C25	1.27	1.11	0.034
68. BD (1) C25- C26	929. BD*(1) C24- C26	0.87	1.10	0.028
68. BD (1) C25- C26	930. BD*(1) C24- H36	2.32	1.03	0.044
69. BD (2) C25- C26	147. LP (1) C22	34.38	0.12	0.073
69. BD (2) C25- C26	484. RY*(2) C22	0.60	0.75	0.021
69. BD (2) C25- C26	514. RY*(2) C24	0.77	0.76	0.023
69. BD (2) C25- C26	932. BD*(2) C18- C24	15.22	0.23	0.053
70. BD (1) C25- H39	483. RY*(1) C22	1.26	1.80	0.043
70. BD (1) C25- H39	543. RY*(1) C26	0.96	2.18	0.041
70. BD (1) C25- H39	927. BD*(1) C16- C22	4.99	0.96	0.062
70. BD (1) C25- H39	929. BD*(1) C24- C26	3.57	0.94	0.052
71. BD (1) C26- H40	513. RY*(1) C24	0.95	2.03	0.039
71. BD (1) C26- H40	528. RY*(1) C25	0.95	2.00	0.039
71. BD (1) C26- H40	925. BD*(1) C22- C25	4.05	0.94	0.055

71. BD (1) C26- H40	931. BD*(1) C18- C24	3.74	0.94	0.053
78. CR (1) C 6	676. RY*(4) O46	0.90	10.38	0.086
80. CR (1) C 8	691. RY*(4) O47	0.80	10.34	0.081
84. CR (1) C12	363. RY*(1) C14	0.71	11.52	0.081
84. CR (1) C12	365. RY*(3) C14	0.71	11.70	0.081
84. CR (1) C12	921. BD*(1) C20- N50	1.02	10.25	0.092
86. CR (1) C14	335. RY*(3) C12	0.62	11.50	0.075
86. CR (1) C14	336. RY*(4) C12	0.80	11.11	0.084
86. CR (1) C14	469. RY*(2) C21	1.00	11.52	0.096
86. CR (1) C14	865. BD*(1) C12- N50	0.74	10.23	0.078
88. CR (1) C16	425. RY*(3) C18	1.01	11.43	0.096
88. CR (1) C16	483. RY*(1) C22	0.54	11.11	0.069
88. CR (1) C16	485. RY*(3) C22	0.91	11.51	0.091
88. CR (1) C16	924. BD*(1) C20- C22	0.67	10.20	0.074
88. CR (1) C16	925. BD*(1) C22- C25	0.74	10.26	0.078
88. CR (1) C16	931. BD*(1) C18- C24	0.59	10.26	0.070
90. CR (1) C18	395. RY*(3) C16	1.17	10.73	0.100
90. CR (1) C18	515. RY*(3) C24	0.93	11.64	0.093
90. CR (1) C18	926. BD*(1) C16-Ru52	0.80	9.76	0.085
92. CR (1) C20	483. RY*(1) C22	0.54	11.17	0.070
92. CR (1) C20	498. RY*(1) C23	0.61	11.36	0.074
92. CR (1) C20	735. RY*(3) N50	0.53	11.96	0.071
92. CR (1) C20	865. BD*(1) C12- N50	0.92	10.27	0.087
92. CR (1) C20	925. BD*(1) C22- C25	0.61	10.32	0.071
92. CR (1) C20	927. BD*(1) C16- C22	0.61	10.33	0.072
93. CR (1) C21	365. RY*(3) C14	1.29	11.66	0.110
93. CR (1) C21	500. RY*(3) C23	1.35	11.45	0.111
93. CR (1) C21	923. BD*(1) C20- C23	0.51	10.26	0.065
94. CR (1) C22	393. RY*(1) C16	0.53	10.82	0.068
94. CR (1) C22	395. RY*(3) C16	0.74	10.75	0.079
94. CR (1) C22	453. RY*(1) C20	0.58	11.30	0.072
94. CR (1) C22	528. RY*(1) C25	0.51	11.31	0.068
94. CR (1) C22	530. RY*(3) C25	0.58	11.50	0.073
94. CR (1) C22	921. BD*(1) C20- N50	0.52	10.18	0.066
94. CR (1) C22	923. BD*(1) C20- C23	0.78	10.23	0.080
94. CR (1) C22	926. BD*(1) C16-Ru52	0.60	9.78	0.074
95. CR (1) C23	455. RY*(3) C20	1.18	11.72	0.105
95. CR (1) C23	469. RY*(2) C21	1.19	11.52	0.105
95. CR (1) C23	921. BD*(1) C20- N50	0.68	10.21	0.075
95. CR (1) C23	924. BD*(1) C20- C22	0.89	10.21	0.086
96. CR (1) C24	425. RY*(3) C18	0.82	11.42	0.086
96. CR (1) C24	426. RY*(4) C18	0.65	10.75	0.075
96. CR (1) C24	545. RY*(3) C26	0.84	11.68	0.089
96. CR (1) C24	928. BD*(1) C16- C18	0.86	10.27	0.084
97. CR (1) C25	485. RY*(3) C22	0.95	11.50	0.093
97. CR (1) C25	545. RY*(3) C26	1.27	11.68	0.109
97. CR (1) C25	924. BD*(1) C20- C22	0.77	10.19	0.080
97. CR (1) C25	927. BD*(1) C16- C22	0.91	10.27	0.087
98. CR (1) C26	515. RY*(3) C24	1.27	11.64	0.108
98. CR (1) C26	530. RY*(3) C25	1.29	11.49	0.109
98. CR (1) C26	925. BD*(1) C22- C25	0.57	10.25	0.069
101. CR (1) O46	243. RY*(1) C 6	5.01	20.07	0.284
101. CR (1) O46	882. BD*(1) C 6-Ru52	0.61	18.68	0.104
102. CR (1) O47	273. RY*(1) C 8	4.53	19.94	0.269
102. CR (1) O47	881. BD*(1) C 8-Ru52	0.69	18.65	0.111
105. CR (1) N50	333. RY*(1) C12	0.90	15.39	0.105
105. CR (1) N50	335. RY*(3) C12	1.01	15.59	0.112
105. CR (1) N50	453. RY*(1) C20	0.97	15.42	0.109
105. CR (1) N50	455. RY*(3) C20	0.94	15.81	0.109
105. CR (1) N50	882. BD*(1) C 6-Ru52	4.45	13.99	0.243
125. CR (2)Ru52	820. RY*(25)Ru52	1.46	879.79	1.012
125. CR (2)Ru52	824. RY*(29)Ru52	1.78	94.31	0.366
125. CR (2)Ru52	828. RY*(33)Ru52	3.39	270.06	0.855
125. CR (2)Ru52	836. RY*(41)Ru52	1.68	891.42	1.092
125. CR (2)Ru52	880. BD*(3) C 8- O47	0.93	115.30	0.294
125. CR (2)Ru52	885. BD*(3) C 6- O46	1.05	115.31	0.312
126. CR (3)Ru52	796. RY*(1)Ru52	1.52	21.74	0.163
126. CR (3)Ru52	797. RY*(2)Ru52	1.73	22.36	0.176
126. CR (3)Ru52	803. RY*(8)Ru52	0.63	22.97	0.108
126. CR (3)Ru52	805. RY*(10)Ru52	3.24	21.25	0.234
126. CR (3)Ru52	807. RY*(12)Ru52	0.54	28.94	0.111
126. CR (3)Ru52	810. RY*(15)Ru52	1.10	27.97	0.157
126. CR (3)Ru52	811. RY*(16)Ru52	0.63	27.90	0.118
126. CR (3)Ru52	812. RY*(17)Ru52	0.91	25.80	0.137
126. CR (3)Ru52	815. RY*(20)Ru52	1.69	17.73	0.154
126. CR (3)Ru52	818. RY*(23)Ru52	0.72	28.43	0.128
126. CR (3)Ru52	820. RY*(25)Ru52	2.41	786.95	1.230
126. CR (3)Ru52	824. RY*(29)Ru52	159.98	1.48	0.435
126. CR (3)Ru52	825. RY*(30)Ru52	0.57	20.36	0.096
126. CR (3)Ru52	828. RY*(33)Ru52	7.89	177.23	1.055
126. CR (3)Ru52	833. RY*(38)Ru52	1.55	3383.31	2.042
126. CR (3)Ru52	836. RY*(41)Ru52	3.50	798.59	1.492
126. CR (3)Ru52	865. BD*(1) C12- N50	0.83	22.32	0.122
126. CR (3)Ru52	880. BD*(3) C 8- O47	3.66	22.47	0.257
126. CR (3)Ru52	885. BD*(3) C 6- O46	4.11	22.48	0.273
126. CR (3)Ru52	921. BD*(1) C20- N50	0.62	22.30	0.106
126. CR (3)Ru52	926. BD*(1) C16-Ru52	0.80	21.90	0.127
126. CR (3)Ru52	927. BD*(1) C16- C22	0.64	22.39	0.108
126. CR (3)Ru52	928. BD*(1) C16- C18	1.47	22.40	0.163
127. CR (4)Ru52	243. RY*(1) C 6	3.14	6.10	0.123
127. CR (4)Ru52	273. RY*(1) C 8	2.35	5.96	0.106
127. CR (4)Ru52	805. RY*(10)Ru52	0.69	3.96	0.047
127. CR (4)Ru52	821. RY*(26)Ru52	0.54	12903.94	2.367
127. CR (4)Ru52	828. RY*(33)Ru52	1.13	159.95	0.381
127. CR (4)Ru52	833. RY*(38)Ru52	1.00	3366.02	1.644
127. CR (4)Ru52	865. BD*(1) C12- N50	2.48	5.04	0.100
127. CR (4)Ru52	880. BD*(3) C 8- O47	10.66	5.19	0.210
127. CR (4)Ru52	885. BD*(3) C 6- O46	11.71	5.20	0.220
127. CR (4)Ru52	921. BD*(1) C20- N50	1.92	5.02	0.088
127. CR (4)Ru52	926. BD*(1) C16-Ru52	2.47	4.61	0.102
127. CR (4)Ru52	927. BD*(1) C16- C22	1.59	5.10	0.081
127. CR (4)Ru52	928. BD*(1) C16- C18	4.05	5.11	0.129
130. CR (7)Ru52	880. BD*(3) C 8- O47	1.02	2.42	0.044
130. CR (7)Ru52	881. BD*(1) C 8-Ru52	2.35	1.91	0.065
130. CR (7)Ru52	882. BD*(1) C 6-Ru52	3.68	1.94	0.082
130. CR (7)Ru52	885. BD*(3) C 6- O46	1.98	2.43	0.062
133. CR (10)Ru52	805. RY*(10)Ru52	1.92	1.20	0.043
133. CR (10)Ru52	825. RY*(30)Ru52	7.72	0.31	0.044
133. CR (10)Ru52	878. BD*(1) C 8- O47	0.58	1.83	0.031
133. CR (10)Ru52	880. BD*(3) C 8- O47	1.00	2.42	0.044
133. CR (10)Ru52	881. BD*(1) C 8-Ru52	4.08	1.91	0.086
133. CR (10)Ru52	882. BD*(1) C 6-Ru52	1.61	1.94	0.054
133. CR (10)Ru52	884. BD*(2) C 6- O46	0.98	1.83	0.040
133. CR (10)Ru52	926. BD*(1) C16-Ru52	2.38	1.85	0.064
136. CR (13)Ru52	880. BD*(3) C 8- O47	0.68	2.42	0.036
136. CR (13)Ru52	881. BD*(1) C 8-Ru52	1.60	1.90	0.054

136. CR (13)Ru52	882. BD*(1) C 6-Ru52	0.89	1.94	0.040
136. CR (13)Ru52	883. BD*(1) C 6- O46	0.84	1.84	0.037
136. CR (13)Ru52	926. BD*(1) C16-Ru52	3.94	1.84	0.082
147. LP (1) C22	167. LP*(1) C16	1155.20	0.01	0.114
147. LP (1) C22	394. RY*(2) C16	0.99	0.71	0.033
147. LP (1) C22	457. RY*(5) C20	0.86	1.84	0.049
147. LP (1) C22	484. RY*(2) C22	2.61	0.63	0.050
147. LP (1) C22	529. RY*(2) C25	2.92	0.61	0.052
147. LP (1) C22	870. BD*(2) C25- C26	57.78	0.11	0.085
147. LP (1) C22	922. BD*(2) C20- N50	133.83	0.06	0.088
147. LP (1) C22	932. BD*(2) C18- C24	0.73	0.11	0.010
152. LP (1) O46	243. RY*(1) C 6	11.86	2.17	0.143
152. LP (1) O46	250. RY*(8) C 6	0.87	4.55	0.057
152. LP (1) O46	251. RY*(9) C 6	0.92	3.72	0.052
152. LP (1) O46	796. RY*(1)Ru52	0.94	0.53	0.020
152. LP (1) O46	805. RY*(10)Ru52	20.03	0.03	0.023
152. LP (1) O46	882. BD*(1) C 6-Ru52	3.29	0.78	0.049
153. LP (1) O47	273. RY*(1) C 8	11.34	2.04	0.136
153. LP (1) O47	274. RY*(2) C 8	0.99	2.65	0.046
153. LP (1) O47	280. RY*(8) C 8	0.90	4.69	0.058
153. LP (1) O47	796. RY*(1)Ru52	0.78	0.53	0.018
153. LP (1) O47	805. RY*(10)Ru52	5.52	0.04	0.013
153. LP (1) O47	881. BD*(1) C 8-Ru52	3.50	0.75	0.050
156. LP (1) N50	273. RY*(1) C 8	0.85	1.73	0.037
156. LP (1) N50	333. RY*(1) C12	2.30	1.88	0.064
156. LP (1) N50	338. RY*(6) C12	0.79	3.16	0.049
156. LP (1) N50	453. RY*(1) C20	2.41	1.90	0.066
156. LP (1) N50	455. RY*(3) C20	0.73	2.30	0.040
156. LP (1) N50	459. RY*(7) C20	0.82	3.73	0.054
156. LP (1) N50	796. RY*(1)Ru52	12.96	0.23	0.053
156. LP (1) N50	797. RY*(2)Ru52	3.92	0.84	0.056
156. LP (1) N50	798. RY*(3)Ru52	1.38	1.08	0.038
156. LP (1) N50	801. RY*(6)Ru52	1.17	1.50	0.041
156. LP (1) N50	807. RY*(12)Ru52	0.57	7.43	0.063
156. LP (1) N50	811. RY*(16)Ru52	0.93	6.39	0.075
156. LP (1) N50	818. RY*(23)Ru52	1.17	6.92	0.088
156. LP (1) N50	820. RY*(25)Ru52	0.69	765.44	0.710
156. LP (1) N50	821. RY*(26)Ru52	0.53	12899.70	2.547
156. LP (1) N50	833. RY*(38)Ru52	0.63	3361.79	1.419
156. LP (1) N50	863. BD*(1) C12- C14	7.44	0.83	0.076
156. LP (1) N50	866. BD*(1) C12- H29	2.79	0.73	0.044
156. LP (1) N50	879. BD*(2) C 8- O47	1.13	0.36	0.019
156. LP (1) N50	880. BD*(3) C 8- O47	0.71	0.96	0.025
156. LP (1) N50	882. BD*(1) C 6-Ru52	70.67	0.48	0.164
156. LP (1) N50	923. BD*(1) C20- C23	7.55	0.83	0.077
156. LP (1) N50	924. BD*(1) C20- C22	1.61	0.79	0.035
156. LP (1) N50	925. BD*(1) C22- C25	0.57	0.86	0.021
156. LP (1) N50	926. BD*(1) C16-Ru52	2.46	0.38	0.028
156. LP (1) N50	928. BD*(1) C16- C18	1.46	0.88	0.035
160. LP (1)Ru52	167. LP*(1) C16	4.28	0.11	0.024
160. LP (1)Ru52	246. RY*(4) C 6	1.67	1.81	0.052
160. LP (1)Ru52	394. RY*(2) C16	0.66	0.81	0.022
160. LP (1)Ru52	395. RY*(3) C16	0.75	1.18	0.028
160. LP (1)Ru52	467. RY*(15) C20	0.56	24.15	0.111
160. LP (1)Ru52	735. RY*(3) N50	2.29	2.33	0.069
160. LP (1)Ru52	796. RY*(1)Ru52	14.64	0.05	0.026
160. LP (1)Ru52	865. BD*(1) C12- N50	0.56	0.63	0.018
160. LP (1)Ru52	878. BD*(1) C 8- O47	5.66	0.19	0.029
160. LP (1)Ru52	883. BD*(1) C 6- O46	11.35	0.20	0.043
160. LP (1)Ru52	884. BD*(2) C 6- O46	10.97	0.19	0.041
160. LP (1)Ru52	921. BD*(1) C20- N50	0.51	0.61	0.017
160. LP (1)Ru52	928. BD*(1) C16- C18	0.69	0.71	0.021
161. LP (2)Ru52	167. LP*(1) C16	13.29	0.12	0.042
161. LP (2)Ru52	246. RY*(4) C 6	0.81	1.81	0.037
161. LP (2)Ru52	276. RY*(4) C 8	2.23	2.06	0.065
161. LP (2)Ru52	394. RY*(2) C16	1.75	0.82	0.036
161. LP (2)Ru52	796. RY*(1)Ru52	3.63	0.06	0.014
161. LP (2)Ru52	797. RY*(2)Ru52	1.87	0.67	0.034
161. LP (2)Ru52	878. BD*(1) C 8- O47	23.24	0.19	0.060
161. LP (2)Ru52	879. BD*(2) C 8- O47	1.39	0.19	0.015
161. LP (2)Ru52	883. BD*(1) C 6- O46	2.30	0.20	0.020
161. LP (2)Ru52	884. BD*(2) C 6- O46	3.49	0.19	0.023
161. LP (2)Ru52	926. BD*(1) C16-Ru52	0.87	0.21	0.012
162. LP (3)Ru52	244. RY*(2) C 6	3.13	1.09	0.057
162. LP (3)Ru52	275. RY*(3) C 8	3.02	1.20	0.059
162. LP (3)Ru52	734. RY*(2) N50	2.29	1.05	0.048
162. LP (3)Ru52	797. RY*(2)Ru52	0.53	0.68	0.019
162. LP (3)Ru52	818. RY*(23)Ru52	0.69	6.76	0.067
162. LP (3)Ru52	878. BD*(1) C 8- O47	1.15	0.21	0.014
162. LP (3)Ru52	879. BD*(2) C 8- O47	23.12	0.20	0.063
162. LP (3)Ru52	883. BD*(1) C 6- O46	10.62	0.21	0.044
162. LP (3)Ru52	884. BD*(2) C 6- O46	12.25	0.20	0.046
162. LP (3)Ru52	922. BD*(2) C20- N50	3.59	0.17	0.023

from unit 2 to unit 3

18. BD (3) C 6- O46	638. RY*(1) H43	0.11	2.60	0.015
18. BD (3) C 6- O46	640. RY*(3) H43	0.40	3.18	0.032
18. BD (3) C 6- O46	642. RY*(5) H43	0.05	3.53	0.012
18. BD (3) C 6- O46	661. RY*(4) O45	0.09	4.97	0.019
18. BD (3) C 6- O46	668. RY*(11) O45	0.08	6.21	0.020
19. BD (1) C 6-Ru52	638. RY*(1) H43	0.13	2.04	0.015
19. BD (1) C 6-Ru52	658. RY*(1) O45	0.26	2.89	0.025
19. BD (1) C 6-Ru52	659. RY*(2) O45	0.32	2.04	0.023
19. BD (1) C 6-Ru52	660. RY*(3) O45	1.99	2.66	0.066
19. BD (1) C 6-Ru52	661. RY*(4) O45	0.35	4.42	0.036
19. BD (1) C 6-Ru52	662. RY*(5) O45	0.28	2.77	0.025
19. BD (1) C 6-Ru52	664. RY*(7) O45	0.09	2.76	0.014
19. BD (1) C 6-Ru52	667. RY*(10) O45	0.09	5.39	0.020
19. BD (1) C 6-Ru52	669. RY*(12) O45	0.26	4.83	0.032
19. BD (1) C 6-Ru52	670. RY*(13) O45	0.05	92.63	0.062
19. BD (1) C 6-Ru52	671. RY*(14) O45	0.05	5.17	0.015
19. BD (1) C 6-Ru52	672. RY*(15) O45	0.12	76.16	0.085
19. BD (1) C 6-Ru52	934. BD*(1) H43- O45	0.12	0.98	0.010
25. BD (3) C 8- O47	640. RY*(3) H43	0.46	3.19	0.034
25. BD (3) C 8- O47	659. RY*(2) O45	0.17	2.60	0.019
25. BD (3) C 8- O47	660. RY*(3) O45	0.06	3.22	0.012
26. BD (1) C 8-Ru52	638. RY*(1) H43	0.17	2.04	0.017
26. BD (1) C 8-Ru52	640. RY*(3) H43	0.35	2.62	0.028
26. BD (1) C 8-Ru52	658. RY*(1) O45	0.08	2.89	0.014
26. BD (1) C 8-Ru52	659. RY*(2) O45	0.05	2.04	0.009
26. BD (1) C 8-Ru52	660. RY*(3) O45	0.79	2.66	0.042
26. BD (1) C 8-Ru52	661. RY*(4) O45	0.46	4.42	0.041
26. BD (1) C 8-Ru52	662. RY*(5) O45	0.09	2.77	0.015
26. BD (1) C 8-Ru52	667. RY*(10) O45	0.18	5.39	0.028
26. BD (1) C 8-Ru52	668. RY*(11) O45	0.10	5.65	0.022
26. BD (1) C 8-Ru52	669. RY*(12) O45	0.37	4.84	0.039

26. BD (1) C 8-Ru52	671. RY*(14) O45	0.08	5.18	0.019
26. BD (1) C 8-Ru52	672. RY*(15) O45	0.12	76.16	0.086
39. BD (1) C12- H29	638. RY*(1) H43	0.06	2.00	0.010
39. BD (1) C12- H29	640. RY*(3) H43	0.13	2.59	0.016
39. BD (1) C12- H29	660. RY*(3) O45	0.05	2.62	0.010
39. BD (1) C12- H29	661. RY*(4) O45	0.06	4.38	0.015
40. BD (1) C12- N50	659. RY*(2) O45	0.10	2.29	0.014
40. BD (1) C12- N50	934. BD*(1) H43- O45	0.10	1.23	0.010
47. BD (1) C16- C18	640. RY*(3) H43	0.31	2.71	0.026
47. BD (1) C16- C18	642. RY*(5) H43	0.05	3.06	0.011
47. BD (1) C16- C18	658. RY*(1) O45	0.07	2.98	0.013
47. BD (1) C16- C18	659. RY*(2) O45	0.20	2.13	0.019
49. BD (1) C16-Ru52	639. RY*(2) H43	0.12	2.07	0.015
49. BD (1) C16-Ru52	640. RY*(3) H43	0.77	2.45	0.040
49. BD (1) C16-Ru52	641. RY*(4) H43	0.08	2.97	0.015
49. BD (1) C16-Ru52	642. RY*(5) H43	0.11	2.81	0.016
49. BD (1) C16-Ru52	658. RY*(1) O45	0.64	2.72	0.039
49. BD (1) C16-Ru52	659. RY*(2) O45	0.46	1.87	0.027
49. BD (1) C16-Ru52	660. RY*(3) O45	0.30	2.49	0.025
49. BD (1) C16-Ru52	661. RY*(4) O45	0.27	4.25	0.032
49. BD (1) C16-Ru52	662. RY*(5) O45	0.06	2.60	0.011
49. BD (1) C16-Ru52	663. RY*(6) O45	0.13	3.00	0.019
49. BD (1) C16-Ru52	664. RY*(7) O45	0.12	2.59	0.016
49. BD (1) C16-Ru52	665. RY*(8) O45	0.08	2.16	0.012
49. BD (1) C16-Ru52	666. RY*(9) O45	0.12	2.70	0.017
49. BD (1) C16-Ru52	668. RY*(11) O45	0.17	5.48	0.028
49. BD (1) C16-Ru52	670. RY*(13) O45	0.21	92.47	0.129
49. BD (1) C16-Ru52	672. RY*(15) O45	0.28	75.99	0.134
59. BD (1) C20- N50	638. RY*(1) H43	0.09	2.27	0.013
130. CR (7)Ru52	934. BD*(1) H43- O45	0.05	2.29	0.010
133. CR (10)Ru52	934. BD*(1) H43- O45	0.08	2.29	0.012
156. LP (1) N50	638. RY*(1) H43	0.07	1.89	0.011
156. LP (1) N50	658. RY*(1) O45	0.05	2.74	0.012
156. LP (1) N50	659. RY*(2) O45	0.07	1.88	0.011
160. LP (1)Ru52	638. RY*(1) H43	0.05	1.71	0.009
160. LP (1)Ru52	640. RY*(3) H43	0.06	2.29	0.011
160. LP (1)Ru52	658. RY*(1) O45	0.22	2.56	0.023
160. LP (1)Ru52	659. RY*(2) O45	0.71	1.71	0.033
160. LP (1)Ru52	660. RY*(3) O45	0.19	2.33	0.020
160. LP (1)Ru52	661. RY*(4) O45	0.34	4.09	0.035
160. LP (1)Ru52	663. RY*(6) O45	0.05	2.83	0.012
160. LP (1)Ru52	664. RY*(7) O45	0.06	2.43	0.011
160. LP (1)Ru52	668. RY*(11) O45	0.27	5.32	0.036
160. LP (1)Ru52	934. BD*(1) H43- O45	0.20	0.65	0.011
161. LP (2)Ru52	638. RY*(1) H43	0.18	1.71	0.017
161. LP (2)Ru52	639. RY*(2) H43	0.07	1.91	0.011
161. LP (2)Ru52	640. RY*(3) H43	0.40	2.29	0.029
161. LP (2)Ru52	641. RY*(4) H43	0.10	2.81	0.016
161. LP (2)Ru52	658. RY*(1) O45	0.56	2.56	0.037
161. LP (2)Ru52	659. RY*(2) O45	0.31	1.71	0.022
161. LP (2)Ru52	660. RY*(3) O45	0.35	2.33	0.028
161. LP (2)Ru52	664. RY*(7) O45	0.06	2.43	0.011
161. LP (2)Ru52	667. RY*(10) O45	0.10	5.06	0.022

from unit 2 to unit 4

16. BD (1) C 6- O46	848. RY*(5)C153	0.06	6.90	0.019
17. BD (2) C 6- O46	853. RY*(10)C153	0.06	4.95	0.016
18. BD (3) C 6- O46	846. RY*(3)C153	0.20	7.13	0.034
18. BD (3) C 6- O46	847. RY*(4)C153	0.13	3.49	0.019
18. BD (3) C 6- O46	848. RY*(5)C153	0.47	7.59	0.053
18. BD (3) C 6- O46	850. RY*(7)C153	0.06	4.76	0.015
18. BD (3) C 6- O46	852. RY*(9)C153	0.09	2.79	0.014
18. BD (3) C 6- O46	853. RY*(10)C153	0.23	5.65	0.032
18. BD (3) C 6- O46	861. RY*(18)C153	0.06	17.07	0.028
19. BD (1) C 6-Ru52	845. RY*(2)C153	0.28	1.47	0.019
19. BD (1) C 6-Ru52	846. RY*(3)C153	1.42	6.57	0.088
19. BD (1) C 6-Ru52	847. RY*(4)C153	0.66	2.94	0.040
19. BD (1) C 6-Ru52	848. RY*(5)C153	1.04	7.04	0.078
19. BD (1) C 6-Ru52	849. RY*(6)C153	0.54	1.81	0.029
19. BD (1) C 6-Ru52	850. RY*(7)C153	0.54	4.21	0.043
19. BD (1) C 6-Ru52	858. RY*(15)C153	0.15	170.73	0.147
19. BD (1) C 6-Ru52	860. RY*(17)C153	0.19	49.51	0.089
19. BD (1) C 6-Ru52	861. RY*(18)C153	0.12	16.52	0.040
23. BD (1) C 8- O47	847. RY*(4)C153	0.06	2.79	0.011
25. BD (3) C 8- O47	846. RY*(3)C153	0.21	7.14	0.034
25. BD (3) C 8- O47	847. RY*(4)C153	0.87	3.50	0.049
25. BD (3) C 8- O47	848. RY*(5)C153	0.21	7.60	0.036
25. BD (3) C 8- O47	850. RY*(7)C153	0.08	4.77	0.017
25. BD (3) C 8- O47	852. RY*(9)C153	0.10	2.80	0.015
25. BD (3) C 8- O47	853. RY*(10)C153	0.24	5.66	0.033
25. BD (3) C 8- O47	856. RY*(13)C153	0.20	6.44	0.032
25. BD (3) C 8- O47	861. RY*(18)C153	0.07	17.08	0.031
26. BD (1) C 8-Ru52	846. RY*(3)C153	0.27	6.58	0.038
26. BD (1) C 8-Ru52	847. RY*(4)C153	0.50	2.94	0.035
26. BD (1) C 8-Ru52	848. RY*(5)C153	0.25	7.04	0.038
26. BD (1) C 8-Ru52	850. RY*(7)C153	0.06	4.21	0.015
26. BD (1) C 8-Ru52	852. RY*(9)C153	0.07	2.24	0.012
26. BD (1) C 8-Ru52	853. RY*(10)C153	0.25	5.10	0.032
26. BD (1) C 8-Ru52	856. RY*(13)C153	0.11	5.88	0.023
26. BD (1) C 8-Ru52	860. RY*(17)C153	0.07	49.52	0.055
26. BD (1) C 8-Ru52	861. RY*(18)C153	0.13	16.52	0.043
37. BD (1) C12- C14	847. RY*(4)C153	0.06	3.07	0.012
39. BD (1) C12- H29	847. RY*(4)C153	0.17	2.90	0.020
39. BD (1) C12- H29	848. RY*(5)C153	0.08	7.00	0.022
40. BD (1) C12- N50	847. RY*(4)C153	0.24	3.19	0.025
40. BD (1) C12- N50	852. RY*(9)C153	0.08	2.49	0.012
47. BD (1) C16- C18	846. RY*(3)C153	0.17	6.66	0.030
47. BD (1) C16- C18	848. RY*(5)C153	0.21	7.12	0.034
48. BD (1) C16- C22	846. RY*(3)C153	0.13	6.65	0.027
48. BD (1) C16- C22	848. RY*(5)C153	0.06	7.11	0.018
49. BD (1) C16-Ru52	845. RY*(2)C153	0.54	1.30	0.025
49. BD (1) C16-Ru52	846. RY*(3)C153	1.24	6.41	0.083
49. BD (1) C16-Ru52	847. RY*(4)C153	1.02	2.77	0.049
49. BD (1) C16-Ru52	848. RY*(5)C153	1.10	6.87	0.081
49. BD (1) C16-Ru52	849. RY*(6)C153	0.24	1.65	0.019
49. BD (1) C16-Ru52	850. RY*(7)C153	0.10	4.04	0.018
49. BD (1) C16-Ru52	853. RY*(10)C153	0.06	4.93	0.016
49. BD (1) C16-Ru52	858. RY*(15)C153	0.06	170.56	0.091
49. BD (1) C16-Ru52	860. RY*(17)C153	0.06	49.35	0.052
59. BD (1) C20- N50	846. RY*(3)C153	0.20	6.80	0.033
59. BD (1) C20- N50	848. RY*(5)C153	0.10	7.26	0.024
60. BD (2) C20- N50	850. RY*(7)C153	0.18	3.97	0.026
60. BD (2) C20- N50	852. RY*(9)C153	0.09	2.00	0.013
60. BD (2) C20- N50	853. RY*(10)C153	0.23	4.86	0.032
60. BD (2) C20- N50	858. RY*(15)C153	0.07	170.50	0.108
60. BD (2) C20- N50	860. RY*(17)C153	0.10	49.28	0.069

60. BD (2) C20- N50	861. RY*(18)Cl53	0.12	16.28	0.042
126. CR (3)Ru52	846. RY*(3)Cl53	0.18	27.93	0.063
126. CR (3)Ru52	847. RY*(4)Cl53	0.12	24.30	0.048
126. CR (3)Ru52	848. RY*(5)Cl53	0.21	28.40	0.068
126. CR (3)Ru52	853. RY*(10)Cl53	0.06	26.46	0.037
156. LP (1) N50	846. RY*(3)Cl53	0.31	6.42	0.044
156. LP (1) N50	848. RY*(5)Cl53	0.25	6.88	0.040
156. LP (1) N50	853. RY*(10)Cl53	0.12	4.94	0.023
160. LP (1)Ru52	846. RY*(3)Cl53	0.23	6.24	0.036
160. LP (1)Ru52	847. RY*(4)Cl53	0.08	2.61	0.014
160. LP (1)Ru52	848. RY*(5)Cl53	0.25	6.71	0.039
160. LP (1)Ru52	856. RY*(13)Cl53	0.09	5.55	0.021
161. LP (2)Ru52	845. RY*(2)Cl53	0.30	1.14	0.018
161. LP (2)Ru52	846. RY*(3)Cl53	0.08	6.25	0.022
161. LP (2)Ru52	847. RY*(4)Cl53	0.25	2.61	0.025
161. LP (2)Ru52	848. RY*(5)Cl53	0.08	6.71	0.023
161. LP (2)Ru52	850. RY*(7)Cl53	0.10	3.88	0.019
161. LP (2)Ru52	851. RY*(8)Cl53	0.21	1.34	0.016
161. LP (2)Ru52	852. RY*(9)Cl53	0.32	1.91	0.024
161. LP (2)Ru52	853. RY*(10)Cl53	0.52	4.77	0.048
161. LP (2)Ru52	855. RY*(12)Cl53	0.06	5.48	0.018
161. LP (2)Ru52	856. RY*(13)Cl53	0.12	5.55	0.025
161. LP (2)Ru52	858. RY*(15)Cl53	0.09	170.40	0.120
161. LP (2)Ru52	860. RY*(17)Cl53	0.14	49.19	0.079
161. LP (2)Ru52	861. RY*(18)Cl53	0.15	16.19	0.047
162. LP (3)Ru52	844. RY*(1)Cl53	0.45	0.86	0.019
162. LP (3)Ru52	852. RY*(9)Cl53	0.05	1.92	0.010
from unit 3 to unit 1				
72. BD (1) H43- O45	176. RY*(9) C 1	0.09	3.83	0.016
72. BD (1) H43- O45	185. RY*(3) C 2	0.14	2.42	0.016
72. BD (1) H43- O45	187. RY*(5) C 2	0.07	2.56	0.012
72. BD (1) H43- O45	188. RY*(6) C 2	0.56	4.29	0.044
72. BD (1) H43- O45	189. RY*(7) C 2	0.17	5.49	0.027
72. BD (1) H43- O45	190. RY*(8) C 2	0.10	9.41	0.027
72. BD (1) H43- O45	207. RY*(10) C 3	0.06	9.25	0.020
72. BD (1) H43- O45	213. RY*(1) C 4	0.93	2.89	0.046
72. BD (1) H43- O45	214. RY*(2) C 4	0.12	2.11	0.014
72. BD (1) H43- O45	215. RY*(3) C 4	0.08	2.23	0.012
72. BD (1) H43- O45	216. RY*(4) C 4	0.16	2.42	0.018
72. BD (1) H43- O45	219. RY*(7) C 4	0.91	7.26	0.073
72. BD (1) H43- O45	223. RY*(11) C 4	0.06	3.72	0.013
72. BD (1) H43- O45	224. RY*(12) C 4	0.13	4.00	0.020
72. BD (1) H43- O45	225. RY*(13) C 4	0.07	3.19	0.013
72. BD (1) H43- O45	258. RY*(1) C 7	0.06	2.19	0.010
72. BD (1) H43- O45	260. RY*(3) C 7	0.07	2.61	0.012
72. BD (1) H43- O45	264. RY*(7) C 7	0.18	4.67	0.026
72. BD (1) H43- O45	290. RY*(3) C 9	0.13	2.44	0.016
72. BD (1) H43- O45	291. RY*(4) C 9	0.06	1.80	0.009
72. BD (1) H43- O45	292. RY*(5) C 9	0.06	2.59	0.011
72. BD (1) H43- O45	293. RY*(6) C 9	0.34	4.52	0.035
72. BD (1) H43- O45	296. RY*(9) C 9	0.06	14.37	0.027
72. BD (1) H43- O45	297. RY*(10) C 9	0.06	4.67	0.015
72. BD (1) H43- O45	303. RY*(1) C10	0.48	2.71	0.032
72. BD (1) H43- O45	306. RY*(4) C10	0.11	2.42	0.015
72. BD (1) H43- O45	309. RY*(7) C10	0.16	7.31	0.031
72. BD (1) H43- O45	310. RY*(8) C10	0.16	4.62	0.024
72. BD (1) H43- O45	314. RY*(12) C10	0.05	3.38	0.012
72. BD (1) H43- O45	315. RY*(13) C10	0.07	3.43	0.014
72. BD (1) H43- O45	318. RY*(1) C11	0.10	1.87	0.012
72. BD (1) H43- O45	319. RY*(2) C11	0.08	1.38	0.009
72. BD (1) H43- O45	321. RY*(4) C11	0.35	2.90	0.029
72. BD (1) H43- O45	323. RY*(6) C11	0.06	3.05	0.012
72. BD (1) H43- O45	325. RY*(8) C11	0.11	5.27	0.022
72. BD (1) H43- O45	326. RY*(9) C11	0.20	14.62	0.048
72. BD (1) H43- O45	329. RY*(12) C11	0.13	3.78	0.020
72. BD (1) H43- O45	330. RY*(13) C11	0.17	4.12	0.024
72. BD (1) H43- O45	332. RY*(15) C11	0.08	27.17	0.041
72. BD (1) H43- O45	379. RY*(2) C15	0.07	1.14	0.008
72. BD (1) H43- O45	380. RY*(3) C15	0.11	2.39	0.015
72. BD (1) H43- O45	383. RY*(6) C15	0.58	4.10	0.044
72. BD (1) H43- O45	384. RY*(7) C15	0.12	8.82	0.029
72. BD (1) H43- O45	558. RY*(1) H27	0.14	2.00	0.015
72. BD (1) H43- O45	559. RY*(2) H27	0.08	2.62	0.013
72. BD (1) H43- O45	560. RY*(3) H27	0.17	1.60	0.015
72. BD (1) H43- O45	561. RY*(4) H27	0.26	2.43	0.023
72. BD (1) H43- O45	565. RY*(3) H28	0.07	2.30	0.012
72. BD (1) H43- O45	592. RY*(5) H33	0.06	4.76	0.015
72. BD (1) H43- O45	595. RY*(3) H34	0.13	2.07	0.015
72. BD (1) H43- O45	630. RY*(3) H41	0.13	1.86	0.014
72. BD (1) H43- O45	645. RY*(3) O44	0.10	2.40	0.014
72. BD (1) H43- O45	646. RY*(4) O44	0.47	1.36	0.022
72. BD (1) H43- O45	647. RY*(5) O44	0.25	3.04	0.024
72. BD (1) H43- O45	648. RY*(6) O44	0.10	3.50	0.017
72. BD (1) H43- O45	705. RY*(3) O48	0.12	2.63	0.016
72. BD (1) H43- O45	706. RY*(4) O48	0.36	1.35	0.020
72. BD (1) H43- O45	707. RY*(5) O48	0.13	2.73	0.017
72. BD (1) H43- O45	708. RY*(6) O48	0.12	2.53	0.015
72. BD (1) H43- O45	718. RY*(1) N49	0.22	2.55	0.021
72. BD (1) H43- O45	720. RY*(3) N49	0.08	2.75	0.013
72. BD (1) H43- O45	726. RY*(9) N49	0.08	5.14	0.018
72. BD (1) H43- O45	748. RY*(1)Ru51	2.78	18.69	0.204
72. BD (1) H43- O45	749. RY*(2)Ru51	0.92	1.53	0.033
72. BD (1) H43- O45	750. RY*(3)Ru51	1.66	8.89	0.109
72. BD (1) H43- O45	751. RY*(4)Ru51	0.26	1.89	0.020
72. BD (1) H43- O45	752. RY*(5)Ru51	1.25	4.80	0.069
72. BD (1) H43- O45	755. RY*(8)Ru51	2.24	6.77	0.110
72. BD (1) H43- O45	756. RY*(9)Ru51	0.36	3.24	0.030
72. BD (1) H43- O45	757. RY*(10)Ru51	2.77	21.88	0.220
72. BD (1) H43- O45	759. RY*(12)Ru51	1.45	15.37	0.134
72. BD (1) H43- O45	760. RY*(13)Ru51	1.31	5.41	0.075
72. BD (1) H43- O45	761. RY*(14)Ru51	0.52	8.17	0.058
72. BD (1) H43- O45	762. RY*(15)Ru51	1.09	14.86	0.114
72. BD (1) H43- O45	763. RY*(16)Ru51	1.23	13.43	0.115
72. BD (1) H43- O45	764. RY*(17)Ru51	1.95	11.17	0.132
72. BD (1) H43- O45	765. RY*(18)Ru51	0.54	7.34	0.056
72. BD (1) H43- O45	766. RY*(19)Ru51	0.31	7.48	0.043
72. BD (1) H43- O45	767. RY*(20)Ru51	2.62	17.84	0.194
72. BD (1) H43- O45	768. RY*(21)Ru51	0.37	17.49	0.072
72. BD (1) H43- O45	770. RY*(23)Ru51	1.37	16.79	0.136
72. BD (1) H43- O45	772. RY*(25)Ru51	1.38	9406.68	3.220
72. BD (1) H43- O45	773. RY*(26)Ru51	0.8037	514.24	4.887
72. BD (1) H43- O45	774. RY*(27)Ru51	0.07	49.85	0.052
72. BD (1) H43- O45	776. RY*(29)Ru51	2.60	78.06	0.403
72. BD (1) H43- O45	777. RY*(30)Ru51	2.13	26.35	0.212
72. BD (1) H43- O45	780. RY*(33)Ru51	2.42	324.96	0.793

72. BD (1) H43- O45	781. RY*(34)Ru51	0.07	50.82	0.052
72. BD (1) H43- O45	785. RY*(38)Ru51	1.89	596.80	0.950
72. BD (1) H43- O45	788. RY*(41)Ru51	0.48	89.57	0.186
72. BD (1) H43- O45	789. RY*(42)Ru51	1.31	533.40	0.748
72. BD (1) H43- O45	902. BD*(1) C11-Ru51	5.96	0.66	0.060
72. BD (1) H43- O45	911. BD*(3) C 4- O44	0.07	1.23	0.009
72. BD (1) H43- O45	916. BD*(3) C10- O48	0.07	1.23	0.008
100. CR (1) O45	750. RY*(3)Ru51	0.05	26.86	0.034
100. CR (1) O45	751. RY*(4)Ru51	0.06	19.85	0.030
100. CR (1) O45	902. BD*(1) C11-Ru51	3.16	18.62	0.234
149. LP (1) O45	185. RY*(3) C 2	0.10	2.20	0.014
149. LP (1) O45	188. RY*(6) C 2	0.06	4.07	0.014
149. LP (1) O45	213. RY*(1) C 4	0.13	2.67	0.016
149. LP (1) O45	219. RY*(7) C 4	0.19	7.04	0.033
149. LP (1) O45	303. RY*(1) C10	0.16	2.49	0.018
149. LP (1) O45	309. RY*(7) C10	0.06	7.09	0.019
149. LP (1) O45	311. RY*(9) C10	0.06	4.32	0.015
149. LP (1) O45	318. RY*(1) C11	0.11	1.65	0.012
149. LP (1) O45	319. RY*(2) C11	0.07	1.16	0.008
149. LP (1) O45	383. RY*(6) C15	0.15	3.88	0.022
149. LP (1) O45	558. RY*(1) H27	0.12	1.78	0.013
149. LP (1) O45	559. RY*(2) H27	0.06	2.39	0.010
149. LP (1) O45	560. RY*(3) H27	0.06	1.37	0.008
149. LP (1) O45	646. RY*(4) O44	0.12	1.13	0.010
149. LP (1) O45	647. RY*(5) O44	0.06	2.82	0.012
149. LP (1) O45	706. RY*(4) O48	0.12	1.13	0.011
149. LP (1) O45	721. RY*(4) N49	0.06	4.96	0.015
149. LP (1) O45	726. RY*(9) N49	0.06	4.92	0.015
149. LP (1) O45	748. RY*(1)Ru51	0.46	18.47	0.082
149. LP (1) O45	750. RY*(3)Ru51	0.51	8.67	0.060
149. LP (1) O45	751. RY*(4)Ru51	0.07	1.67	0.009
149. LP (1) O45	752. RY*(5)Ru51	0.11	4.57	0.020
149. LP (1) O45	755. RY*(8)Ru51	0.63	6.55	0.058
149. LP (1) O45	757. RY*(10)Ru51	0.88	21.66	0.124
149. LP (1) O45	759. RY*(12)Ru51	0.43	15.15	0.073
149. LP (1) O45	760. RY*(13)Ru51	0.60	5.19	0.050
149. LP (1) O45	761. RY*(14)Ru51	0.76	7.94	0.070
149. LP (1) O45	762. RY*(15)Ru51	0.05	14.63	0.025
149. LP (1) O45	763. RY*(16)Ru51	0.22	13.21	0.049
149. LP (1) O45	764. RY*(17)Ru51	0.24	10.95	0.046
149. LP (1) O45	765. RY*(18)Ru51	0.17	7.11	0.031
149. LP (1) O45	766. RY*(19)Ru51	0.07	7.26	0.020
149. LP (1) O45	767. RY*(20)Ru51	0.61	17.62	0.093
149. LP (1) O45	768. RY*(21)Ru51	0.14	17.27	0.045
149. LP (1) O45	770. RY*(23)Ru51	0.17	16.57	0.048
149. LP (1) O45	772. RY*(25)Ru51	0.26	9406.46	1.399
149. LP (1) O45	773. RY*(26)Ru51	0.15	37514.02	2.152
149. LP (1) O45	776. RY*(29)Ru51	0.56	77.84	0.188
149. LP (1) O45	777. RY*(30)Ru51	0.45	26.13	0.098
149. LP (1) O45	780. RY*(33)Ru51	0.48	324.74	0.356
149. LP (1) O45	785. RY*(38)Ru51	0.36	596.58	0.417
149. LP (1) O45	786. RY*(39)Ru51	0.19	18.29	0.053
149. LP (1) O45	787. RY*(40)Ru51	0.10	54.30	0.065
149. LP (1) O45	788. RY*(41)Ru51	0.09	89.35	0.082
149. LP (1) O45	789. RY*(42)Ru51	0.24	533.18	0.320
149. LP (1) O45	790. RY*(43)Ru51	0.08	18.64	0.035
149. LP (1) O45	792. RY*(45)Ru51	0.05	51.37	0.046
149. LP (1) O45	887. BD*(1) C 1- C 2	0.37	0.88	0.016
149. LP (1) O45	891. BD*(1) C 2- H27	1.60	0.79	0.032
149. LP (1) O45	892. BD*(1) C 7- N49	0.36	0.83	0.015
149. LP (1) O45	902. BD*(1) C11-Ru51	8.09	0.43	0.057
149. LP (1) O45	911. BD*(3) C 4- O44	0.05	1.00	0.006
149. LP (1) O45	912. BD*(1) C 4-Ru51	0.09	0.48	0.006
149. LP (1) O45	913. BD*(1) C10-Ru51	0.90	0.52	0.021
150. LP (2) O45	219. RY*(7) C 4	0.08	7.16	0.023
150. LP (2) O45	321. RY*(4) C11	0.08	2.80	0.014
150. LP (2) O45	326. RY*(9) C11	0.09	14.52	0.033
150. LP (2) O45	332. RY*(15) C11	0.06	27.07	0.038
150. LP (2) O45	383. RY*(6) C15	0.08	4.00	0.017
150. LP (2) O45	560. RY*(3) H27	0.11	1.50	0.012
150. LP (2) O45	646. RY*(4) O44	0.06	1.26	0.008
150. LP (2) O45	706. RY*(4) O48	0.05	1.25	0.008
150. LP (2) O45	748. RY*(1)Ru51	0.24	18.59	0.062
150. LP (2) O45	749. RY*(2)Ru51	0.07	1.43	0.009
150. LP (2) O45	750. RY*(3)Ru51	0.61	8.79	0.068
150. LP (2) O45	752. RY*(5)Ru51	0.11	4.70	0.022
150. LP (2) O45	753. RY*(6)Ru51	0.10	3.64	0.017
150. LP (2) O45	755. RY*(8)Ru51	0.22	6.67	0.036
150. LP (2) O45	756. RY*(9)Ru51	0.18	3.14	0.023
150. LP (2) O45	757. RY*(10)Ru51	0.36	21.78	0.083
150. LP (2) O45	758. RY*(11)Ru51	0.07	7.37	0.021
150. LP (2) O45	759. RY*(12)Ru51	0.22	15.27	0.055
150. LP (2) O45	760. RY*(13)Ru51	0.08	5.31	0.019
150. LP (2) O45	761. RY*(14)Ru51	0.25	8.07	0.042
150. LP (2) O45	763. RY*(16)Ru51	0.38	13.33	0.067
150. LP (2) O45	764. RY*(17)Ru51	0.34	11.07	0.058
150. LP (2) O45	766. RY*(19)Ru51	0.05	7.38	0.019
150. LP (2) O45	767. RY*(20)Ru51	0.35	17.74	0.074
150. LP (2) O45	768. RY*(21)Ru51	0.24	17.39	0.060
150. LP (2) O45	770. RY*(23)Ru51	0.10	16.69	0.038
150. LP (2) O45	772. RY*(25)Ru51	0.12	9406.58	0.997
150. LP (2) O45	773. RY*(26)Ru51	0.08	37514.14	1.612
150. LP (2) O45	776. RY*(29)Ru51	0.30	77.96	0.144
150. LP (2) O45	777. RY*(30)Ru51	0.30	26.25	0.083
150. LP (2) O45	778. RY*(31)Ru51	0.11	19.17	0.043
150. LP (2) O45	780. RY*(33)Ru51	0.26	324.86	0.275
150. LP (2) O45	785. RY*(38)Ru51	0.18	596.70	0.308
150. LP (2) O45	788. RY*(41)Ru51	0.05	89.47	0.063
150. LP (2) O45	789. RY*(42)Ru51	0.11	533.30	0.226
150. LP (2) O45	794. RY*(47)Ru51	0.08	19.96	0.037
150. LP (2) O45	891. BD*(1) C 2- H27	0.10	0.91	0.009
150. LP (2) O45	892. BD*(1) C 7- N49	0.21	0.95	0.013
150. LP (2) O45	900. BD*(1) C11- C15	0.05	1.04	0.007
150. LP (2) O45	901. BD*(2) C11- C15	0.09	0.56	0.006
150. LP (2) O45	902. BD*(1) C11-Ru51	26.63	0.56	0.111
150. LP (2) O45	909. BD*(1) C 4- O44	0.22	0.52	0.010
150. LP (2) O45	911. BD*(3) C 4- O44	0.15	1.13	0.012
150. LP (2) O45	912. BD*(1) C 4-Ru51	1.24	0.61	0.025
150. LP (2) O45	913. BD*(1) C10-Ru51	0.21	0.65	0.011
150. LP (2) O45	915. BD*(2) C10- O48	0.18	0.53	0.009
150. LP (2) O45	916. BD*(3) C10- O48	0.30	1.13	0.017
151. LP (3) O45	185. RY*(3) C 2	0.11	2.05	0.014
151. LP (3) O45	187. RY*(5) C 2	0.05	2.19	0.010
151. LP (3) O45	188. RY*(6) C 2	0.50	3.92	0.042
151. LP (3) O45	189. RY*(7) C 2	0.05	5.11	0.016
151. LP (3) O45	190. RY*(8) C 2	0.06	9.04	0.023

151. LP (3) O45	192. RY*(10) C 2	0.06	3.54	0.014
151. LP (3) O45	213. RY*(1) C 4	0.21	2.52	0.022
151. LP (3) O45	214. RY*(2) C 4	0.07	1.74	0.010
151. LP (3) O45	219. RY*(7) C 4	0.34	6.89	0.046
151. LP (3) O45	222. RY*(10) C 4	0.08	1.94	0.012
151. LP (3) O45	264. RY*(7) C 7	0.10	4.30	0.020
151. LP (3) O45	290. RY*(3) C 9	0.07	2.07	0.011
151. LP (3) O45	293. RY*(6) C 9	0.10	4.15	0.020
151. LP (3) O45	303. RY*(1) C10	0.07	2.34	0.012
151. LP (3) O45	309. RY*(7) C10	0.07	6.94	0.020
151. LP (3) O45	310. RY*(8) C10	0.05	4.25	0.014
151. LP (3) O45	311. RY*(9) C10	0.05	4.17	0.014
151. LP (3) O45	313. RY*(11) C10	0.08	2.05	0.012
151. LP (3) O45	318. RY*(1) C11	0.05	1.50	0.009
151. LP (3) O45	321. RY*(4) C11	0.13	2.53	0.017
151. LP (3) O45	326. RY*(9) C11	0.19	14.25	0.049
151. LP (3) O45	332. RY*(15) C11	0.10	26.80	0.050
151. LP (3) O45	381. RY*(4) C15	0.05	1.29	0.008
151. LP (3) O45	383. RY*(6) C15	0.37	3.73	0.036
151. LP (3) O45	384. RY*(7) C15	0.07	8.45	0.022
151. LP (3) O45	558. RY*(1) H27	0.06	1.63	0.010
151. LP (3) O45	561. RY*(4) H27	0.11	2.06	0.014
151. LP (3) O45	595. RY*(3) H34	0.07	1.69	0.010
151. LP (3) O45	630. RY*(3) H41	0.07	1.49	0.010
151. LP (3) O45	635. RY*(3) H42	0.05	1.34	0.008
151. LP (3) O45	646. RY*(4) O44	0.30	0.98	0.016
151. LP (3) O45	647. RY*(5) O44	0.13	2.67	0.018
151. LP (3) O45	706. RY*(4) O48	0.19	0.98	0.013
151. LP (3) O45	707. RY*(5) O48	0.05	2.36	0.011
151. LP (3) O45	708. RY*(6) O48	0.05	2.16	0.010
151. LP (3) O45	718. RY*(1) N49	0.06	2.18	0.011
151. LP (3) O45	726. RY*(9) N49	0.07	4.77	0.017
151. LP (3) O45	748. RY*(1)Ru51	1.46	18.32	0.155
151. LP (3) O45	750. RY*(3)Ru51	0.82	8.52	0.080
151. LP (3) O45	752. RY*(5)Ru51	0.28	4.42	0.033
151. LP (3) O45	755. RY*(8)Ru51	1.34	6.40	0.088
151. LP (3) O45	756. RY*(9)Ru51	0.50	2.87	0.036
151. LP (3) O45	757. RY*(10)Ru51	1.08	21.51	0.145
151. LP (3) O45	758. RY*(11)Ru51	0.06	7.10	0.020
151. LP (3) O45	759. RY*(12)Ru51	0.82	15.00	0.106
151. LP (3) O45	760. RY*(13)Ru51	0.66	5.04	0.055
151. LP (3) O45	761. RY*(14)Ru51	0.66	7.80	0.068
151. LP (3) O45	762. RY*(15)Ru51	0.45	14.48	0.077
151. LP (3) O45	763. RY*(16)Ru51	0.55	13.06	0.081
151. LP (3) O45	764. RY*(17)Ru51	0.65	10.80	0.080
151. LP (3) O45	765. RY*(18)Ru51	0.11	6.96	0.027
151. LP (3) O45	766. RY*(19)Ru51	0.28	7.11	0.043
151. LP (3) O45	767. RY*(20)Ru51	1.11	17.47	0.132
151. LP (3) O45	768. RY*(21)Ru51	0.20	17.12	0.055
151. LP (3) O45	770. RY*(23)Ru51	0.55	16.42	0.091
151. LP (3) O45	772. RY*(25)Ru51	0.55	9406.31	2.175
151. LP (3) O45	773. RY*(26)Ru51	0.34	37513.87	3.412
151. LP (3) O45	776. RY*(29)Ru51	1.31	77.69	0.303
151. LP (3) O45	777. RY*(30)Ru51	1.16	25.98	0.165
151. LP (3) O45	780. RY*(33)Ru51	1.08	324.59	0.563
151. LP (3) O45	785. RY*(38)Ru51	0.81	596.43	0.661
151. LP (3) O45	788. RY*(41)Ru51	0.22	89.20	0.135
151. LP (3) O45	789. RY*(42)Ru51	0.54	533.03	0.510
151. LP (3) O45	892. BD*(1) C 7- N49	0.26	0.68	0.012
151. LP (3) O45	900. BD*(1) C11- C15	0.11	0.77	0.009
151. LP (3) O45	902. BD*(1) C11-Ru51	25.53	0.28	0.077
151. LP (3) O45	909. BD*(1) C 4- O44	0.48	0.25	0.010
151. LP (3) O45	911. BD*(3) C 4- O44	0.53	0.86	0.020
151. LP (3) O45	913. BD*(1) C10-Ru51	0.41	0.38	0.011
151. LP (3) O45	914. BD*(1) C10- O48	0.36	0.25	0.009
151. LP (3) O45	915. BD*(2) C10- O48	0.07	0.26	0.004
151. LP (3) O45	916. BD*(3) C10- O48	0.45	0.86	0.019
from unit 3 to unit 2				
72. BD (1) H43- O45	243. RY*(1) C 6	0.15	2.12	0.016
72. BD (1) H43- O45	277. RY*(5) C 8	0.06	2.52	0.011
72. BD (1) H43- O45	338. RY*(6) C12	0.05	3.41	0.012
72. BD (1) H43- O45	364. RY*(2) C14	0.06	1.21	0.008
72. BD (1) H43- O45	393. RY*(1) C16	0.07	1.67	0.010
72. BD (1) H43- O45	404. RY*(12) C16	0.05	3.53	0.012
72. BD (1) H43- O45	459. RY*(7) C20	0.07	3.99	0.015
72. BD (1) H43- O45	483. RY*(1) C22	0.06	1.96	0.010
72. BD (1) H43- O45	487. RY*(5) C22	0.06	4.24	0.014
72. BD (1) H43- O45	568. RY*(1) H29	0.06	1.90	0.010
72. BD (1) H43- O45	570. RY*(3) H29	0.46	2.05	0.028
72. BD (1) H43- O45	675. RY*(3) O46	0.05	2.49	0.010
72. BD (1) H43- O45	676. RY*(4) O46	0.09	1.12	0.009
72. BD (1) H43- O45	699. RY*(12) O47	0.05	1.93	0.009
72. BD (1) H43- O45	733. RY*(1) N50	0.15	2.19	0.016
72. BD (1) H43- O45	735. RY*(3) N50	0.15	2.76	0.018
72. BD (1) H43- O45	796. RY*(1)Ru52	0.14	0.48	0.007
72. BD (1) H43- O45	797. RY*(2)Ru52	3.43	1.10	0.055
72. BD (1) H43- O45	798. RY*(3)Ru52	0.95	1.33	0.032
72. BD (1) H43- O45	799. RY*(4)Ru52	1.22	2.35	0.048
72. BD (1) H43- O45	800. RY*(5)Ru52	0.29	3.65	0.029
72. BD (1) H43- O45	801. RY*(6)Ru52	1.05	1.75	0.038
72. BD (1) H43- O45	802. RY*(7)Ru52	0.10	3.69	0.017
72. BD (1) H43- O45	803. RY*(8)Ru52	0.41	1.71	0.024
72. BD (1) H43- O45	808. RY*(13)Ru52	0.09	3.04	0.014
72. BD (1) H43- O45	810. RY*(15)Ru52	0.21	6.71	0.033
72. BD (1) H43- O45	811. RY*(16)Ru52	0.52	6.64	0.052
72. BD (1) H43- O45	812. RY*(17)Ru52	0.30	4.54	0.033
72. BD (1) H43- O45	813. RY*(18)Ru52	0.42	6.09	0.045
72. BD (1) H43- O45	814. RY*(19)Ru52	0.28	5.82	0.036
72. BD (1) H43- O45	816. RY*(21)Ru52	0.24	13.99	0.052
72. BD (1) H43- O45	818. RY*(23)Ru52	1.50	7.17	0.093
72. BD (1) H43- O45	819. RY*(24)Ru52	0.61	29463.97	3.797
72. BD (1) H43- O45	820. RY*(25)Ru52	1.28	765.69	0.886
72. BD (1) H43- O45	821. RY*(26)Ru52	1.17	12899.96	3.480
72. BD (1) H43- O45	828. RY*(33)Ru52	0.06	155.97	0.087
72. BD (1) H43- O45	829. RY*(34)Ru52	0.10	50.30	0.063
72. BD (1) H43- O45	832. RY*(37)Ru52	0.07	186.86	0.099
72. BD (1) H43- O45	833. RY*(38)Ru52	1.36	3362.05	1.911
72. BD (1) H43- O45	836. RY*(41)Ru52	0.81	777.33	0.711
72. BD (1) H43- O45	837. RY*(42)Ru52	0.49	3155.07	1.112
72. BD (1) H43- O45	863. BD*(1) C12- C14	0.08	1.09	0.008
72. BD (1) H43- O45	866. BD*(1) C12- H29	0.07	0.99	0.007
72. BD (1) H43- O45	882. BD*(1) C 6-Ru52	0.06	0.73	0.007
72. BD (1) H43- O45	926. BD*(1) C16-Ru52	3.69	0.64	0.046
100. CR (1) O45	801. RY*(6)Ru52	0.07	19.72	0.034
100. CR (1) O45	926. BD*(1) C16-Ru52	3.17	18.60	0.234

149. LP (1) O45	273. RY*(1) C 8	0.06	1.77	0.009
149. LP (1) O45	428. RY*(6) C18	0.07	2.81	0.013
149. LP (1) O45	568. RY*(1) H29	0.06	1.67	0.009
149. LP (1) O45	570. RY*(3) H29	0.10	1.83	0.012
149. LP (1) O45	676. RY*(4) O46	0.05	0.90	0.006
149. LP (1) O45	796. RY*(1)Ru52	2.76	0.26	0.024
149. LP (1) O45	797. RY*(2)Ru52	0.67	0.87	0.022
149. LP (1) O45	798. RY*(3)Ru52	0.08	1.11	0.008
149. LP (1) O45	799. RY*(4)Ru52	0.11	2.13	0.014
149. LP (1) O45	801. RY*(6)Ru52	0.42	1.53	0.023
149. LP (1) O45	802. RY*(7)Ru52	0.22	3.47	0.025
149. LP (1) O45	803. RY*(8)Ru52	0.65	1.49	0.028
149. LP (1) O45	808. RY*(13)Ru52	0.44	2.82	0.032
149. LP (1) O45	809. RY*(14)Ru52	0.09	5.65	0.020
149. LP (1) O45	810. RY*(15)Ru52	0.75	6.49	0.063
149. LP (1) O45	811. RY*(16)Ru52	0.28	6.42	0.038
149. LP (1) O45	812. RY*(17)Ru52	0.25	4.31	0.030
149. LP (1) O45	813. RY*(18)Ru52	0.05	5.87	0.015
149. LP (1) O45	816. RY*(21)Ru52	0.09	13.77	0.031
149. LP (1) O45	818. RY*(23)Ru52	0.35	6.95	0.045
149. LP (1) O45	819. RY*(24)Ru52	0.1929463.75		2.127
149. LP (1) O45	820. RY*(25)Ru52	0.43	765.47	0.514
149. LP (1) O45	821. RY*(26)Ru52	0.3612899.74		1.946
149. LP (1) O45	833. RY*(38)Ru52	0.42	3361.83	1.070
149. LP (1) O45	834. RY*(39)Ru52	0.11	18.32	0.041
149. LP (1) O45	835. RY*(40)Ru52	0.08	54.34	0.057
149. LP (1) O45	836. RY*(41)Ru52	0.27	777.11	0.411
149. LP (1) O45	837. RY*(42)Ru52	0.15	3154.85	0.616
149. LP (1) O45	842. RY*(47)Ru52	0.06	19.91	0.030
149. LP (1) O45	866. BD*(1) C12- H29	0.54	0.76	0.018
149. LP (1) O45	883. BD*(1) C 6- O46	0.07	0.41	0.005
149. LP (1) O45	884. BD*(2) C 6- O46	0.06	0.40	0.005
149. LP (1) O45	926. BD*(1) C16-Ru52	8.04	0.42	0.055
150. LP (2) O45	167. LP*(1) C16	0.10	0.44	0.007
150. LP (2) O45	243. RY*(1) C 6	0.24	2.02	0.020
150. LP (2) O45	273. RY*(1) C 8	0.33	1.89	0.023
150. LP (2) O45	279. RY*(7) C 8	0.12	4.87	0.022
150. LP (2) O45	394. RY*(2) C16	0.07	1.14	0.008
150. LP (2) O45	395. RY*(3) C16	0.06	1.51	0.009
150. LP (2) O45	404. RY*(12) C16	0.16	3.43	0.022
150. LP (2) O45	405. RY*(13) C16	0.09	3.80	0.018
150. LP (2) O45	406. RY*(14) C16	0.08	27.07	0.045
150. LP (2) O45	407. RY*(15) C16	0.08	40.32	0.054
150. LP (2) O45	428. RY*(6) C18	0.07	2.93	0.014
150. LP (2) O45	570. RY*(3) H29	0.11	1.95	0.014
150. LP (2) O45	676. RY*(4) O46	0.10	1.02	0.009
150. LP (2) O45	691. RY*(4) O47	0.08	0.98	0.008
150. LP (2) O45	733. RY*(1) N50	0.17	2.09	0.018
150. LP (2) O45	796. RY*(1)Ru52	6.66	0.38	0.047
150. LP (2) O45	797. RY*(2)Ru52	1.79	1.00	0.040
150. LP (2) O45	798. RY*(3)Ru52	0.44	1.23	0.022
150. LP (2) O45	799. RY*(4)Ru52	0.13	2.25	0.016
150. LP (2) O45	801. RY*(6)Ru52	1.51	1.65	0.047
150. LP (2) O45	802. RY*(7)Ru52	0.11	3.59	0.018
150. LP (2) O45	803. RY*(8)Ru52	0.71	1.61	0.032
150. LP (2) O45	804. RY*(9)Ru52	0.22	2.73	0.023
150. LP (2) O45	809. RY*(14)Ru52	0.05	5.77	0.016
150. LP (2) O45	810. RY*(15)Ru52	0.84	6.61	0.070
150. LP (2) O45	811. RY*(16)Ru52	0.13	6.54	0.027
150. LP (2) O45	812. RY*(17)Ru52	0.29	4.44	0.033
150. LP (2) O45	813. RY*(18)Ru52	0.38	5.99	0.045
150. LP (2) O45	814. RY*(19)Ru52	0.19	5.72	0.031
150. LP (2) O45	818. RY*(23)Ru52	0.41	7.07	0.050
150. LP (2) O45	819. RY*(24)Ru52	0.1229463.87		1.779
150. LP (2) O45	820. RY*(25)Ru52	0.30	765.59	0.454
150. LP (2) O45	821. RY*(26)Ru52	0.2012899.86		1.499
150. LP (2) O45	833. RY*(38)Ru52	0.24	3361.95	0.840
150. LP (2) O45	834. RY*(39)Ru52	0.10	18.44	0.041
150. LP (2) O45	835. RY*(40)Ru52	0.06	54.46	0.055
150. LP (2) O45	836. RY*(41)Ru52	0.16	777.23	0.334
150. LP (2) O45	837. RY*(42)Ru52	0.10	3154.97	0.540
150. LP (2) O45	838. RY*(43)Ru52	0.07	19.16	0.034
150. LP (2) O45	863. BD*(1) C12- C14	0.06	0.99	0.007
150. LP (2) O45	878. BD*(1) C 8- O47	0.25	0.52	0.010
150. LP (2) O45	880. BD*(3) C 8- O47	0.14	1.11	0.012
150. LP (2) O45	881. BD*(1) C 8-Ru52	0.77	0.60	0.020
150. LP (2) O45	882. BD*(1) C 6-Ru52	0.16	0.63	0.009
150. LP (2) O45	883. BD*(1) C 6- O46	0.14	0.53	0.008
150. LP (2) O45	884. BD*(2) C 6- O46	0.27	0.52	0.011
150. LP (2) O45	885. BD*(3) C 6- O46	0.23	1.12	0.015
150. LP (2) O45	921. BD*(1) C20- N50	0.24	0.94	0.014
150. LP (2) O45	926. BD*(1) C16-Ru52	30.84	0.54	0.117
150. LP (2) O45	928. BD*(1) C16- C18	0.07	1.04	0.008
151. LP (3) O45	243. RY*(1) C 6	0.22	1.75	0.019
151. LP (3) O45	249. RY*(7) C 6	0.13	6.52	0.027
151. LP (3) O45	273. RY*(1) C 8	0.44	1.62	0.025
151. LP (3) O45	279. RY*(7) C 8	0.26	4.60	0.033
151. LP (3) O45	338. RY*(6) C12	0.31	3.04	0.029
151. LP (3) O45	393. RY*(1) C16	0.33	1.30	0.020
151. LP (3) O45	394. RY*(2) C16	0.08	0.87	0.008
151. LP (3) O45	395. RY*(3) C16	0.14	1.24	0.013
151. LP (3) O45	404. RY*(12) C16	0.09	3.16	0.016
151. LP (3) O45	406. RY*(14) C16	0.07	26.80	0.040
151. LP (3) O45	407. RY*(15) C16	0.07	40.04	0.049
151. LP (3) O45	428. RY*(6) C18	0.13	2.66	0.018
151. LP (3) O45	459. RY*(7) C20	0.05	3.62	0.013
151. LP (3) O45	483. RY*(1) C22	0.05	1.59	0.009
151. LP (3) O45	568. RY*(1) H29	0.06	1.52	0.009
151. LP (3) O45	570. RY*(3) H29	0.21	1.68	0.018
151. LP (3) O45	676. RY*(4) O46	0.11	0.75	0.009
151. LP (3) O45	691. RY*(4) O47	0.18	0.71	0.011
151. LP (3) O45	733. RY*(1) N50	0.14	1.82	0.015
151. LP (3) O45	796. RY*(1)Ru52	37.56	0.11	0.062
151. LP (3) O45	797. RY*(2)Ru52	4.45	0.72	0.054
151. LP (3) O45	798. RY*(3)Ru52	0.51	0.96	0.021
151. LP (3) O45	799. RY*(4)Ru52	0.36	1.98	0.025
151. LP (3) O45	800. RY*(5)Ru52	0.09	3.27	0.016
151. LP (3) O45	801. RY*(6)Ru52	0.39	1.38	0.022
151. LP (3) O45	802. RY*(7)Ru52	0.81	3.32	0.049
151. LP (3) O45	803. RY*(8)Ru52	0.69	1.34	0.029
151. LP (3) O45	804. RY*(9)Ru52	0.05	2.46	0.011
151. LP (3) O45	807. RY*(12)Ru52	0.11	7.31	0.028
151. LP (3) O45	808. RY*(13)Ru52	0.11	2.67	0.016
151. LP (3) O45	809. RY*(14)Ru52	0.06	5.50	0.017
151. LP (3) O45	810. RY*(15)Ru52	0.52	6.34	0.055
151. LP (3) O45	811. RY*(16)Ru52	0.20	6.27	0.034

151. LP (3) O45	812. RY*(17)Ru52	0.44	4.17	0.041
151. LP (3) O45	814. RY*(19)Ru52	0.32	5.45	0.040
151. LP (3) O45	816. RY*(21)Ru52	0.11	13.62	0.037
151. LP (3) O45	817. RY*(22)Ru52	0.08	9.44	0.026
151. LP (3) O45	818. RY*(23)Ru52	0.76	6.80	0.068
151. LP (3) O45	819. RY*(24)Ru52	0.29	29463.60	2.804
151. LP (3) O45	820. RY*(25)Ru52	0.64	765.32	0.669
151. LP (3) O45	821. RY*(26)Ru52	0.53	12899.59	2.496
151. LP (3) O45	822. RY*(27)Ru52	0.06	49.49	0.052
151. LP (3) O45	833. RY*(38)Ru52	0.63	3361.68	1.384
151. LP (3) O45	836. RY*(41)Ru52	0.38	776.96	0.519
151. LP (3) O45	837. RY*(42)Ru52	0.24	3154.70	0.836
151. LP (3) O45	878. BD*(1) C 8- O47	0.33	0.25	0.008
151. LP (3) O45	880. BD*(3) C 8- O47	0.17	0.84	0.011
151. LP (3) O45	881. BD*(1) C 8-Ru52	0.09	0.33	0.005
151. LP (3) O45	883. BD*(1) C 6- O46	0.33	0.26	0.008
151. LP (3) O45	884. BD*(2) C 6- O46	0.09	0.25	0.004
151. LP (3) O45	885. BD*(3) C 6- O46	0.16	0.85	0.011
151. LP (3) O45	921. BD*(1) C20- N50	0.12	0.67	0.008
151. LP (3) O45	926. BD*(1) C16-Ru52	12.37	0.27	0.052
within unit 3				
72. BD (1) H43- O45	638. RY*(1) H43	0.61	2.14	0.032
72. BD (1) H43- O45	640. RY*(3) H43	0.83	2.72	0.042
149. LP (1) O45	639. RY*(2) H43	0.53	2.11	0.030
150. LP (2) O45	641. RY*(4) H43	0.65	3.14	0.043
151. LP (3) O45	638. RY*(1) H43	0.51	1.77	0.029
151. LP (3) O45	640. RY*(3) H43	1.04	2.35	0.047
from unit 3 to unit 4				
72. BD (1) H43- O45	845. RY*(2)C153	0.09	1.57	0.010
72. BD (1) H43- O45	846. RY*(3)C153	0.33	6.67	0.042
72. BD (1) H43- O45	847. RY*(4)C153	1.43	3.04	0.059
72. BD (1) H43- O45	848. RY*(5)C153	0.45	7.14	0.051
72. BD (1) H43- O45	856. RY*(13)C153	0.20	5.98	0.031
149. LP (1) O45	845. RY*(2)C153	0.07	1.35	0.009
149. LP (1) O45	846. RY*(3)C153	0.10	6.45	0.023
149. LP (1) O45	847. RY*(4)C153	0.46	2.82	0.032
149. LP (1) O45	848. RY*(5)C153	0.14	6.91	0.028
149. LP (1) O45	851. RY*(8)C153	0.07	1.55	0.009
150. LP (2) O45	847. RY*(4)C153	0.41	2.94	0.033
150. LP (2) O45	851. RY*(8)C153	0.06	1.67	0.009
151. LP (3) O45	845. RY*(2)C153	0.08	1.20	0.009
151. LP (3) O45	846. RY*(3)C153	0.66	6.30	0.061
151. LP (3) O45	847. RY*(4)C153	0.06	2.67	0.012
151. LP (3) O45	848. RY*(5)C153	0.87	6.76	0.073
151. LP (3) O45	853. RY*(10)C153	0.30	4.83	0.036
151. LP (3) O45	856. RY*(13)C153	0.06	5.61	0.018
from unit 4 to unit 1				
142. CR (1)C153	912. BD*(1) C 4-Ru51	0.82	100.57	0.282
143. CR (2)C153	901. BD*(2) C11- C15	0.11	9.83	0.032
143. CR (2)C153	902. BD*(1) C11-Ru51	0.14	9.83	0.036
143. CR (2)C153	912. BD*(1) C 4-Ru51	6.09	9.88	0.240
145. CR (4)C153	912. BD*(1) C 4-Ru51	0.31	7.02	0.046
146. CR (5)C153	912. BD*(1) C 4-Ru51	0.26	7.01	0.042
163. LP (1)C153	213. RY*(1) C 4	0.22	2.98	0.023
163. LP (1)C153	219. RY*(7) C 4	0.19	7.35	0.033
163. LP (1)C153	314. RY*(12) C10	0.05	3.47	0.012
163. LP (1)C153	383. RY*(6) C15	0.08	4.20	0.017
163. LP (1)C153	646. RY*(4) O44	0.06	1.45	0.009
163. LP (1)C153	706. RY*(4) O48	0.08	1.44	0.010
163. LP (1)C153	718. RY*(1) N49	0.07	2.64	0.012
163. LP (1)C153	748. RY*(1)Ru51	0.43	18.78	0.081
163. LP (1)C153	750. RY*(3)Ru51	0.24	8.98	0.042
163. LP (1)C153	751. RY*(4)Ru51	0.13	1.98	0.014
163. LP (1)C153	752. RY*(5)Ru51	0.24	4.89	0.030
163. LP (1)C153	753. RY*(6)Ru51	0.10	3.84	0.018
163. LP (1)C153	755. RY*(8)Ru51	0.51	6.87	0.053
163. LP (1)C153	757. RY*(10)Ru51	0.48	21.97	0.091
163. LP (1)C153	758. RY*(11)Ru51	0.05	7.56	0.017
163. LP (1)C153	759. RY*(12)Ru51	0.08	15.46	0.032
163. LP (1)C153	760. RY*(13)Ru51	0.54	5.51	0.049
163. LP (1)C153	762. RY*(15)Ru51	0.45	14.95	0.073
163. LP (1)C153	763. RY*(16)Ru51	0.48	13.53	0.072
163. LP (1)C153	764. RY*(17)Ru51	0.07	11.26	0.025
163. LP (1)C153	765. RY*(18)Ru51	0.14	7.43	0.029
163. LP (1)C153	767. RY*(20)Ru51	0.43	17.93	0.078
163. LP (1)C153	768. RY*(21)Ru51	0.23	17.58	0.057
163. LP (1)C153	770. RY*(23)Ru51	0.16	16.88	0.046
163. LP (1)C153	772. RY*(25)Ru51	0.20	9406.78	1.213
163. LP (1)C153	773. RY*(26)Ru51	0.11	37514.33	1.843
163. LP (1)C153	776. RY*(29)Ru51	0.35	78.15	0.149
163. LP (1)C153	777. RY*(30)Ru51	0.26	26.44	0.074
163. LP (1)C153	780. RY*(33)Ru51	0.35	325.05	0.301
163. LP (1)C153	785. RY*(38)Ru51	0.26	596.89	0.355
163. LP (1)C153	786. RY*(39)Ru51	0.10	18.61	0.039
163. LP (1)C153	787. RY*(40)Ru51	0.05	54.62	0.049
163. LP (1)C153	788. RY*(41)Ru51	0.06	89.66	0.068
163. LP (1)C153	789. RY*(42)Ru51	0.17	533.49	0.273
163. LP (1)C153	900. BD*(1) C11- C15	0.13	1.23	0.011
163. LP (1)C153	901. BD*(2) C11- C15	0.45	0.75	0.018
163. LP (1)C153	902. BD*(1) C11-Ru51	0.09	0.75	0.008
163. LP (1)C153	912. BD*(1) C 4-Ru51	12.73	0.80	0.099
163. LP (1)C153	914. BD*(1) C10- O48	0.12	0.71	0.009
163. LP (1)C153	916. BD*(3) C10- O48	0.11	1.32	0.011
164. LP (2)C153	751. RY*(4)Ru51	0.10	1.49	0.011
164. LP (2)C153	761. RY*(14)Ru51	0.12	7.77	0.028
164. LP (2)C153	778. RY*(31)Ru51	0.08	18.88	0.034
164. LP (2)C153	782. RY*(35)Ru51	0.06	18.69	0.030
164. LP (2)C153	794. RY*(47)Ru51	0.07	19.67	0.034
164. LP (2)C153	890. BD*(1) C 2- N49	0.06	0.68	0.006
164. LP (2)C153	897. BD*(1) C 9- C11	0.10	0.73	0.008
164. LP (2)C153	900. BD*(1) C11- C15	0.07	0.75	0.006
164. LP (2)C153	910. BD*(2) C 4- O44	0.36	0.22	0.008
164. LP (2)C153	913. BD*(1) C10-Ru51	0.27	0.35	0.009
164. LP (2)C153	914. BD*(1) C10- O48	0.08	0.23	0.004
164. LP (2)C153	915. BD*(2) C10- O48	0.06	0.23	0.003
165. LP (3)C153	176. RY*(9) C 1	0.10	3.59	0.019
165. LP (3)C153	185. RY*(3) C 2	0.06	2.19	0.011
165. LP (3)C153	187. RY*(5) C 2	0.12	2.33	0.016
165. LP (3)C153	188. RY*(6) C 2	0.63	4.05	0.049
165. LP (3)C153	189. RY*(7) C 2	0.09	5.25	0.021
165. LP (3)C153	190. RY*(8) C 2	0.06	9.17	0.023
165. LP (3)C153	192. RY*(10) C 2	0.08	3.68	0.017
165. LP (3)C153	207. RY*(10) C 3	0.07	9.02	0.025

165. LP (3)C153	213. RY*(1) C 4	0.99	2.66	0.050
165. LP (3)C153	214. RY*(2) C 4	0.16	1.87	0.017
165. LP (3)C153	215. RY*(3) C 4	0.12	1.99	0.015
165. LP (3)C153	219. RY*(7) C 4	1.19	7.02	0.089
165. LP (3)C153	220. RY*(8) C 4	0.37	4.47	0.040
165. LP (3)C153	221. RY*(9) C 4	0.08	3.34	0.016
165. LP (3)C153	223. RY*(11) C 4	0.06	3.48	0.015
165. LP (3)C153	224. RY*(12) C 4	0.10	3.76	0.019
165. LP (3)C153	226. RY*(14) C 4	0.06	46.01	0.053
165. LP (3)C153	260. RY*(3) C 7	0.10	2.37	0.015
165. LP (3)C153	261. RY*(4) C 7	0.07	1.89	0.011
165. LP (3)C153	264. RY*(7) C 7	0.45	4.43	0.043
165. LP (3)C153	267. RY*(10) C 7	0.09	4.00	0.019
165. LP (3)C153	288. RY*(1) C 9	0.29	1.84	0.023
165. LP (3)C153	289. RY*(2) C 9	0.05	0.95	0.007
165. LP (3)C153	290. RY*(3) C 9	0.18	2.21	0.019
165. LP (3)C153	291. RY*(4) C 9	0.11	1.57	0.013
165. LP (3)C153	292. RY*(5) C 9	0.08	2.36	0.014
165. LP (3)C153	293. RY*(6) C 9	0.45	4.29	0.043
165. LP (3)C153	295. RY*(8) C 9	0.05	4.63	0.015
165. LP (3)C153	297. RY*(10) C 9	0.05	4.43	0.015
165. LP (3)C153	303. RY*(1) C10	0.60	2.47	0.037
165. LP (3)C153	305. RY*(3) C10	0.10	3.01	0.017
165. LP (3)C153	309. RY*(7) C10	0.38	7.08	0.050
165. LP (3)C153	310. RY*(8) C10	0.25	4.38	0.032
165. LP (3)C153	311. RY*(9) C10	0.09	4.30	0.019
165. LP (3)C153	313. RY*(11) C10	0.11	2.19	0.015
165. LP (3)C153	315. RY*(13) C10	0.12	3.19	0.019
165. LP (3)C153	318. RY*(1) C11	0.39	1.64	0.024
165. LP (3)C153	319. RY*(2) C11	0.10	1.15	0.010
165. LP (3)C153	321. RY*(4) C11	0.28	2.66	0.027
165. LP (3)C153	323. RY*(6) C11	0.08	2.81	0.014
165. LP (3)C153	326. RY*(9) C11	0.21	14.38	0.053
165. LP (3)C153	329. RY*(12) C11	0.32	3.55	0.033
165. LP (3)C153	330. RY*(13) C11	0.25	3.88	0.031
165. LP (3)C153	378. RY*(1) C15	0.07	2.05	0.011
165. LP (3)C153	379. RY*(2) C15	0.11	0.90	0.010
165. LP (3)C153	380. RY*(3) C15	0.11	2.15	0.015
165. LP (3)C153	381. RY*(4) C15	0.11	1.42	0.012
165. LP (3)C153	383. RY*(6) C15	0.87	3.87	0.057
165. LP (3)C153	384. RY*(7) C15	0.14	8.58	0.034
165. LP (3)C153	444. RY*(7) C19	0.06	6.66	0.019
165. LP (3)C153	450. RY*(13) C19	0.05	3.05	0.012
165. LP (3)C153	560. RY*(3) H27	0.20	1.36	0.016
165. LP (3)C153	561. RY*(4) H27	0.08	2.19	0.013
165. LP (3)C153	565. RY*(3) H28	0.09	2.06	0.014
165. LP (3)C153	575. RY*(3) H30	0.07	2.22	0.012
165. LP (3)C153	588. RY*(1) H33	0.08	1.77	0.011
165. LP (3)C153	590. RY*(3) H33	0.08	1.35	0.010
165. LP (3)C153	595. RY*(3) H34	0.21	1.83	0.019
165. LP (3)C153	630. RY*(3) H41	0.21	1.63	0.018
165. LP (3)C153	635. RY*(3) H42	0.06	1.47	0.009
165. LP (3)C153	645. RY*(3) O44	0.16	2.16	0.018
165. LP (3)C153	646. RY*(4) O44	0.86	1.12	0.030
165. LP (3)C153	647. RY*(5) O44	0.29	2.80	0.028
165. LP (3)C153	648. RY*(6) O44	0.15	3.26	0.021
165. LP (3)C153	650. RY*(8) O44	0.06	4.03	0.015
165. LP (3)C153	653. RY*(11) O44	0.09	10.50	0.031
165. LP (3)C153	705. RY*(3) O48	0.23	2.39	0.023
165. LP (3)C153	706. RY*(4) O48	0.56	1.12	0.024
165. LP (3)C153	707. RY*(5) O48	0.17	2.49	0.020
165. LP (3)C153	708. RY*(6) O48	0.17	2.29	0.019
165. LP (3)C153	713. RY*(11) O48	0.08	9.81	0.027
165. LP (3)C153	718. RY*(1) N49	0.30	2.31	0.026
165. LP (3)C153	721. RY*(4) N49	0.14	4.95	0.025
165. LP (3)C153	726. RY*(9) N49	0.23	4.91	0.033
165. LP (3)C153	748. RY*(1)Ru51	4.42	18.45	0.278
165. LP (3)C153	749. RY*(2)Ru51	0.14	1.29	0.013
165. LP (3)C153	750. RY*(3)Ru51	3.11	8.65	0.160
165. LP (3)C153	751. RY*(4)Ru51	0.32	1.65	0.022
165. LP (3)C153	752. RY*(5)Ru51	1.21	4.56	0.072
165. LP (3)C153	753. RY*(6)Ru51	0.61	3.51	0.045
165. LP (3)C153	754. RY*(7)Ru51	0.58	4.60	0.050
165. LP (3)C153	755. RY*(8)Ru51	3.40	6.54	0.145
165. LP (3)C153	756. RY*(9)Ru51	0.31	3.01	0.030
165. LP (3)C153	757. RY*(10)Ru51	3.27	21.64	0.259
165. LP (3)C153	758. RY*(11)Ru51	0.07	7.23	0.022
165. LP (3)C153	759. RY*(12)Ru51	1.82	15.14	0.162
165. LP (3)C153	760. RY*(13)Ru51	1.37	5.18	0.082
165. LP (3)C153	761. RY*(14)Ru51	0.57	7.93	0.066
165. LP (3)C153	762. RY*(15)Ru51	3.23	14.62	0.212
165. LP (3)C153	763. RY*(16)Ru51	3.98	13.20	0.223
165. LP (3)C153	764. RY*(17)Ru51	1.50	10.93	0.125
165. LP (3)C153	765. RY*(18)Ru51	0.89	7.10	0.077
165. LP (3)C153	766. RY*(19)Ru51	0.63	7.24	0.066
165. LP (3)C153	767. RY*(20)Ru51	3.74	17.60	0.250
165. LP (3)C153	768. RY*(21)Ru51	1.76	17.25	0.170
165. LP (3)C153	770. RY*(23)Ru51	1.38	16.55	0.147
165. LP (3)C153	772. RY*(25)Ru51	1.67	9406.45	3.869
165. LP (3)C153	773. RY*(26)Ru51	1.03	37514.00	6.061
165. LP (3)C153	776. RY*(29)Ru51	3.74	77.83	0.526
165. LP (3)C153	777. RY*(30)Ru51	3.19	26.11	0.281
165. LP (3)C153	780. RY*(33)Ru51	3.30	324.72	1.008
165. LP (3)C153	785. RY*(38)Ru51	2.43	596.56	1.174
165. LP (3)C153	786. RY*(39)Ru51	0.41	18.28	0.084
165. LP (3)C153	787. RY*(40)Ru51	0.24	54.29	0.112
165. LP (3)C153	788. RY*(41)Ru51	0.66	89.33	0.237
165. LP (3)C153	789. RY*(42)Ru51	1.60	533.16	0.899
165. LP (3)C153	790. RY*(43)Ru51	0.05	18.62	0.031
165. LP (3)C153	791. RY*(44)Ru51	0.06	54.42	0.057
165. LP (3)C153	890. BD*(1) C 2- N49	0.15	0.83	0.011
165. LP (3)C153	892. BD*(1) C 7- N49	0.13	0.81	0.010
165. LP (3)C153	893. BD*(2) C 7- N49	0.19	0.35	0.008
165. LP (3)C153	897. BD*(1) C 9- C11	0.06	0.89	0.007
165. LP (3)C153	900. BD*(1) C11- C15	0.37	0.90	0.018
165. LP (3)C153	901. BD*(2) C11- C15	1.11	0.42	0.019
165. LP (3)C153	902. BD*(1) C11-Ru51	0.09	0.42	0.006
165. LP (3)C153	909. BD*(1) C 4- O44	0.06	0.38	0.004
165. LP (3)C153	911. BD*(3) C 4- O44	0.12	0.99	0.011
165. LP (3)C153	912. BD*(1) C 4-Ru51	71.07	0.47	0.164
165. LP (3)C153	913. BD*(1) C10-Ru51	0.38	0.51	0.012
165. LP (3)C153	914. BD*(1) C10- O48	0.38	0.38	0.011
165. LP (3)C153	915. BD*(2) C10- O48	0.12	0.39	0.006
165. LP (3)C153	916. BD*(3) C10- O48	1.10	0.99	0.032
166. LP (4)C153	169. RY*(2) C 1	0.08	0.81	0.008
166. LP (4)C153	176. RY*(9) C 1	0.07	3.46	0.015

166. LP (4)C153	178. RY*(11) C 1	0.08	2.85	0.015
166. LP (4)C153	185. RY*(3) C 2	0.28	2.06	0.023
166. LP (4)C153	187. RY*(5) C 2	0.14	2.20	0.017
166. LP (4)C153	188. RY*(6) C 2	1.67	3.93	0.079
166. LP (4)C153	189. RY*(7) C 2	0.13	5.12	0.026
166. LP (4)C153	190. RY*(8) C 2	0.11	9.04	0.031
166. LP (4)C153	191. RY*(9) C 2	0.05	3.90	0.014
166. LP (4)C153	192. RY*(10) C 2	0.22	3.55	0.027
166. LP (4)C153	193. RY*(11) C 2	0.10	4.60	0.021
166. LP (4)C153	207. RY*(10) C 3	0.06	8.89	0.023
166. LP (4)C153	213. RY*(1) C 4	1.32	2.53	0.056
166. LP (4)C153	214. RY*(2) C 4	0.16	1.75	0.016
166. LP (4)C153	215. RY*(3) C 4	0.15	1.87	0.016
166. LP (4)C153	219. RY*(7) C 4	1.59	6.89	0.102
166. LP (4)C153	220. RY*(8) C 4	0.10	4.35	0.021
166. LP (4)C153	222. RY*(10) C 4	0.09	1.95	0.013
166. LP (4)C153	223. RY*(11) C 4	0.06	3.35	0.013
166. LP (4)C153	224. RY*(12) C 4	0.11	3.63	0.020
166. LP (4)C153	225. RY*(13) C 4	0.12	2.82	0.018
166. LP (4)C153	260. RY*(3) C 7	0.14	2.24	0.017
166. LP (4)C153	264. RY*(7) C 7	0.52	4.31	0.046
166. LP (4)C153	267. RY*(10) C 7	0.12	3.88	0.021
166. LP (4)C153	288. RY*(1) C 9	0.26	1.71	0.021
166. LP (4)C153	290. RY*(3) C 9	0.18	2.08	0.019
166. LP (4)C153	291. RY*(4) C 9	0.22	1.44	0.017
166. LP (4)C153	292. RY*(5) C 9	0.07	2.23	0.012
166. LP (4)C153	293. RY*(6) C 9	0.31	4.16	0.035
166. LP (4)C153	297. RY*(10) C 9	0.06	4.30	0.016
166. LP (4)C153	303. RY*(1) C10	0.75	2.35	0.041
166. LP (4)C153	305. RY*(3) C10	0.09	2.88	0.016
166. LP (4)C153	309. RY*(7) C10	0.43	6.95	0.053
166. LP (4)C153	310. RY*(8) C10	0.26	4.25	0.032
166. LP (4)C153	311. RY*(9) C10	0.06	4.17	0.015
166. LP (4)C153	313. RY*(11) C10	0.10	2.06	0.014
166. LP (4)C153	315. RY*(13) C10	0.15	3.07	0.021
166. LP (4)C153	318. RY*(1) C11	0.64	1.51	0.030
166. LP (4)C153	319. RY*(2) C11	0.38	1.02	0.019
166. LP (4)C153	320. RY*(3) C11	0.20	1.29	0.016
166. LP (4)C153	321. RY*(4) C11	0.26	2.53	0.025
166. LP (4)C153	323. RY*(6) C11	0.13	2.69	0.018
166. LP (4)C153	324. RY*(7) C11	0.16	3.13	0.022
166. LP (4)C153	326. RY*(9) C11	0.05	14.26	0.026
166. LP (4)C153	328. RY*(11) C11	0.06	3.63	0.014
166. LP (4)C153	329. RY*(12) C11	0.26	3.42	0.029
166. LP (4)C153	330. RY*(13) C11	0.14	3.76	0.022
166. LP (4)C153	358. RY*(11) C13	0.05	6.31	0.017
166. LP (4)C153	378. RY*(1) C15	0.12	1.93	0.015
166. LP (4)C153	379. RY*(2) C15	0.17	0.77	0.011
166. LP (4)C153	380. RY*(3) C15	0.18	2.03	0.019
166. LP (4)C153	381. RY*(4) C15	0.13	1.30	0.013
166. LP (4)C153	383. RY*(6) C15	1.23	3.74	0.066
166. LP (4)C153	384. RY*(7) C15	0.29	8.45	0.049
166. LP (4)C153	414. RY*(7) C17	0.05	6.30	0.018
166. LP (4)C153	419. RY*(12) C17	0.06	5.72	0.018
166. LP (4)C153	444. RY*(7) C19	0.08	6.53	0.022
166. LP (4)C153	447. RY*(10) C19	0.05	3.64	0.014
166. LP (4)C153	450. RY*(13) C19	0.06	2.92	0.013
166. LP (4)C153	558. RY*(1) H27	0.33	1.64	0.023
166. LP (4)C153	560. RY*(3) H27	0.29	1.23	0.019
166. LP (4)C153	561. RY*(4) H27	0.20	2.06	0.020
166. LP (4)C153	565. RY*(3) H28	0.11	1.94	0.014
166. LP (4)C153	575. RY*(3) H30	0.08	2.09	0.012
166. LP (4)C153	588. RY*(1) H33	0.18	1.65	0.017
166. LP (4)C153	589. RY*(2) H33	0.08	2.19	0.013
166. LP (4)C153	590. RY*(3) H33	0.06	1.22	0.009
166. LP (4)C153	592. RY*(5) H33	0.05	4.39	0.015
166. LP (4)C153	595. RY*(3) H34	0.23	1.70	0.019
166. LP (4)C153	630. RY*(3) H41	0.22	1.50	0.018
166. LP (4)C153	634. RY*(2) H42	0.06	1.88	0.011
166. LP (4)C153	635. RY*(3) H42	0.20	1.35	0.016
166. LP (4)C153	636. RY*(4) H42	0.07	1.85	0.011
166. LP (4)C153	645. RY*(3) O44	0.16	2.03	0.018
166. LP (4)C153	646. RY*(4) O44	1.05	0.99	0.032
166. LP (4)C153	647. RY*(5) O44	0.33	2.67	0.029
166. LP (4)C153	648. RY*(6) O44	0.21	3.13	0.025
166. LP (4)C153	650. RY*(8) O44	0.12	3.90	0.021
166. LP (4)C153	653. RY*(11) O44	0.10	10.37	0.031
166. LP (4)C153	705. RY*(3) O48	0.20	2.26	0.021
166. LP (4)C153	706. RY*(4) O48	0.64	0.99	0.025
166. LP (4)C153	707. RY*(5) O48	0.20	2.37	0.021
166. LP (4)C153	708. RY*(6) O48	0.14	2.16	0.017
166. LP (4)C153	713. RY*(11) O48	0.08	9.68	0.027
166. LP (4)C153	718. RY*(1) N49	0.37	2.19	0.028
166. LP (4)C153	719. RY*(2) N49	0.12	1.12	0.011
166. LP (4)C153	726. RY*(9) N49	0.15	4.78	0.026
166. LP (4)C153	748. RY*(1)Ru51	4.58	18.33	0.282
166. LP (4)C153	750. RY*(3)Ru51	3.57	8.53	0.170
166. LP (4)C153	751. RY*(4)Ru51	0.19	1.52	0.017
166. LP (4)C153	752. RY*(5)Ru51	1.73	4.43	0.086
166. LP (4)C153	753. RY*(6)Ru51	0.39	3.38	0.035
166. LP (4)C153	754. RY*(7)Ru51	1.39	4.47	0.077
166. LP (4)C153	755. RY*(8)Ru51	2.54	6.41	0.125
166. LP (4)C153	756. RY*(9)Ru51	0.82	2.88	0.047
166. LP (4)C153	757. RY*(10)Ru51	3.21	21.52	0.257
166. LP (4)C153	758. RY*(11)Ru51	0.08	7.10	0.023
166. LP (4)C153	759. RY*(12)Ru51	1.83	15.01	0.162
166. LP (4)C153	760. RY*(13)Ru51	2.33	5.05	0.106
166. LP (4)C153	761. RY*(14)Ru51	0.59	7.80	0.067
166. LP (4)C153	762. RY*(15)Ru51	3.03	14.49	0.205
166. LP (4)C153	763. RY*(16)Ru51	1.82	13.07	0.151
166. LP (4)C153	764. RY*(17)Ru51	1.14	10.80	0.108
166. LP (4)C153	765. RY*(18)Ru51	0.18	6.97	0.034
166. LP (4)C153	766. RY*(19)Ru51	1.30	7.12	0.094
166. LP (4)C153	767. RY*(20)Ru51	3.10	17.47	0.227
166. LP (4)C153	768. RY*(21)Ru51	2.11	17.12	0.186
166. LP (4)C153	770. RY*(23)Ru51	0.94	16.42	0.121
166. LP (4)C153	772. RY*(25)Ru51	1.95	9406.32	4.186
166. LP (4)C153	773. RY*(26)Ru51	1.15	37513.88	6.412
166. LP (4)C153	774. RY*(27)Ru51	0.22	49.48	0.101
166. LP (4)C153	775. RY*(28)Ru51	0.15	186.34	0.164
166. LP (4)C153	776. RY*(29)Ru51	3.98	77.70	0.543
166. LP (4)C153	777. RY*(30)Ru51	3.05	25.98	0.275
166. LP (4)C153	780. RY*(33)Ru51	3.48	324.60	1.039
166. LP (4)C153	781. RY*(34)Ru51	0.09	50.45	0.066
166. LP (4)C153	784. RY*(37)Ru51	0.05	186.45	0.098
166. LP (4)C153	785. RY*(38)Ru51	2.73	596.44	1.247

166. LP (4)C153	786. RY*(39)Ru51	0.06	18.15	0.031
166. LP (4)C153	788. RY*(41)Ru51	0.73	89.21	0.249
166. LP (4)C153	789. RY*(42)Ru51	1.89	533.04	0.982
166. LP (4)C153	790. RY*(43)Ru51	0.06	18.50	0.033
166. LP (4)C153	794. RY*(47)Ru51	0.08	19.70	0.038
166. LP (4)C153	901. BD*(2) C11- C15	0.44	0.29	0.010
166. LP (4)C153	909. BD*(1) C 4- O44	0.18	0.26	0.006
166. LP (4)C153	911. BD*(3) C 4- O44	0.08	0.86	0.008
166. LP (4)C153	912. BD*(1) C 4-Ru51	2.56	0.34	0.027
166. LP (4)C153	913. BD*(1) C10-Ru51	0.18	0.38	0.008
166. LP (4)C153	914. BD*(1) C10- O48	0.09	0.26	0.004
166. LP (4)C153	915. BD*(2) C10- O48	0.06	0.26	0.004
166. LP (4)C153	916. BD*(3) C10- O48	0.19	0.86	0.012
from unit 4 to unit 2				
142. CR (1)C153	881. BD*(1) C 8-Ru52	0.84	100.56	0.285
143. CR (2)C153	167. LP*(1) C16	0.16	9.72	0.047
143. CR (2)C153	881. BD*(1) C 8-Ru52	6.22	9.87	0.243
143. CR (2)C153	926. BD*(1) C16-Ru52	0.14	9.81	0.035
144. CR (3)C153	881. BD*(1) C 8-Ru52	0.16	7.00	0.033
145. CR (4)C153	881. BD*(1) C 8-Ru52	0.32	7.01	0.047
146. CR (5)C153	881. BD*(1) C 8-Ru52	0.12	7.00	0.028
163. LP (1)C153	167. LP*(1) C16	0.58	0.64	0.023
163. LP (1)C153	570. RY*(3) H29	0.07	2.14	0.011
163. LP (1)C153	796. RY*(1)Ru52	0.17	0.57	0.009
163. LP (1)C153	797. RY*(2)Ru52	0.41	1.19	0.020
163. LP (1)C153	798. RY*(3)Ru52	0.14	1.43	0.013
163. LP (1)C153	799. RY*(4)Ru52	0.21	2.44	0.020
163. LP (1)C153	803. RY*(8)Ru52	0.09	1.80	0.012
163. LP (1)C153	805. RY*(10)Ru52	22.04	0.08	0.037
163. LP (1)C153	807. RY*(12)Ru52	0.24	7.78	0.038
163. LP (1)C153	808. RY*(13)Ru52	0.23	3.13	0.024
163. LP (1)C153	809. RY*(14)Ru52	0.06	5.96	0.017
163. LP (1)C153	812. RY*(17)Ru52	0.50	4.63	0.043
163. LP (1)C153	814. RY*(19)Ru52	0.07	5.91	0.018
163. LP (1)C153	819. RY*(24)Ru52	0.10	29464.06	1.527
163. LP (1)C153	820. RY*(25)Ru52	0.23	765.79	0.373
163. LP (1)C153	821. RY*(26)Ru52	0.19	12900.05	1.390
163. LP (1)C153	826. RY*(31)Ru52	0.06	18.68	0.029
163. LP (1)C153	830. RY*(35)Ru52	0.07	18.83	0.033
163. LP (1)C153	833. RY*(38)Ru52	0.22	3362.14	0.763
163. LP (1)C153	834. RY*(39)Ru52	0.08	18.64	0.035
163. LP (1)C153	836. RY*(41)Ru52	0.14	777.42	0.298
163. LP (1)C153	837. RY*(42)Ru52	0.08	3155.16	0.441
163. LP (1)C153	881. BD*(1) C 8-Ru52	12.31	0.79	0.096
163. LP (1)C153	883. BD*(1) C 6- O46	0.09	0.72	0.007
163. LP (1)C153	885. BD*(3) C 6- O46	0.06	1.31	0.008
163. LP (1)C153	926. BD*(1) C16-Ru52	0.21	0.73	0.012
163. LP (1)C153	928. BD*(1) C16- C18	0.12	1.23	0.011
164. LP (2)C153	796. RY*(1)Ru52	0.10	0.09	0.003
164. LP (2)C153	798. RY*(3)Ru52	0.27	0.94	0.014
164. LP (2)C153	803. RY*(8)Ru52	0.05	1.32	0.008
164. LP (2)C153	809. RY*(14)Ru52	0.17	5.48	0.028
164. LP (2)C153	810. RY*(15)Ru52	0.13	6.32	0.026
164. LP (2)C153	834. RY*(39)Ru52	0.07	18.15	0.032
164. LP (2)C153	838. RY*(43)Ru52	0.09	18.86	0.036
164. LP (2)C153	865. BD*(1) C12- N50	0.07	0.67	0.006
164. LP (2)C153	879. BD*(2) C 8- O47	0.38	0.22	0.009
164. LP (2)C153	882. BD*(1) C 6-Ru52	0.31	0.34	0.010
164. LP (2)C153	884. BD*(2) C 6- O46	0.08	0.22	0.004
164. LP (2)C153	927. BD*(1) C16- C22	0.10	0.73	0.008
164. LP (2)C153	928. BD*(1) C16- C18	0.08	0.74	0.007
165. LP (3)C153	167. LP*(1) C16	0.28	0.31	0.010
165. LP (3)C153	243. RY*(1) C 6	0.13	1.88	0.015
165. LP (3)C153	277. RY*(5) C 8	0.05	2.28	0.011
165. LP (3)C153	280. RY*(8) C 8	0.07	4.40	0.017
165. LP (3)C153	285. RY*(13) C 8	0.06	3.01	0.014
165. LP (3)C153	338. RY*(6) C12	0.06	3.17	0.013
165. LP (3)C153	364. RY*(2) C14	0.09	0.97	0.009
165. LP (3)C153	428. RY*(6) C18	0.06	2.80	0.013
165. LP (3)C153	568. RY*(1) H29	0.13	1.66	0.014
165. LP (3)C153	569. RY*(2) H29	0.06	2.31	0.012
165. LP (3)C153	570. RY*(3) H29	0.65	1.81	0.034
165. LP (3)C153	676. RY*(4) O46	0.10	0.89	0.009
165. LP (3)C153	733. RY*(1) N50	0.10	1.96	0.013
165. LP (3)C153	797. RY*(2)Ru52	0.31	0.86	0.016
165. LP (3)C153	798. RY*(3)Ru52	0.50	1.10	0.023
165. LP (3)C153	799. RY*(4)Ru52	1.26	2.11	0.050
165. LP (3)C153	801. RY*(6)Ru52	0.41	1.51	0.024
165. LP (3)C153	803. RY*(8)Ru52	0.22	1.48	0.017
165. LP (3)C153	806. RY*(11)Ru52	0.05	6.83	0.018
165. LP (3)C153	807. RY*(12)Ru52	0.17	7.45	0.034
165. LP (3)C153	808. RY*(13)Ru52	0.07	2.80	0.013
165. LP (3)C153	810. RY*(15)Ru52	0.15	6.47	0.030
165. LP (3)C153	812. RY*(17)Ru52	0.20	4.30	0.029
165. LP (3)C153	816. RY*(21)Ru52	0.07	13.75	0.029
165. LP (3)C153	818. RY*(23)Ru52	0.05	6.94	0.019
165. LP (3)C153	826. RY*(31)Ru52	0.16	18.35	0.053
165. LP (3)C153	827. RY*(32)Ru52	0.06	54.29	0.055
165. LP (3)C153	828. RY*(33)Ru52	0.06	155.73	0.097
165. LP (3)C153	834. RY*(39)Ru52	0.09	18.31	0.039
165. LP (3)C153	838. RY*(43)Ru52	0.06	19.02	0.032
165. LP (3)C153	878. BD*(1) C 8- O47	0.10	0.38	0.006
165. LP (3)C153	881. BD*(1) C 8-Ru52	27.65	0.46	0.101
165. LP (3)C153	884. BD*(2) C 6- O46	0.21	0.38	0.008
165. LP (3)C153	885. BD*(3) C 6- O46	0.16	0.98	0.012
165. LP (3)C153	921. BD*(1) C20- N50	0.07	0.81	0.007
165. LP (3)C153	922. BD*(2) C20- N50	0.08	0.35	0.005
165. LP (3)C153	928. BD*(1) C16- C18	0.11	0.90	0.010
166. LP (4)C153	167. LP*(1) C16	2.91	0.18	0.024
166. LP (4)C153	243. RY*(1) C 6	0.61	1.76	0.032
166. LP (4)C153	246. RY*(4) C 6	0.08	1.87	0.012
166. LP (4)C153	249. RY*(7) C 6	0.16	6.53	0.031
166. LP (4)C153	253. RY*(11) C 6	0.12	2.11	0.016
166. LP (4)C153	254. RY*(12) C 6	0.05	2.93	0.012
166. LP (4)C153	273. RY*(1) C 8	1.41	1.62	0.047
166. LP (4)C153	279. RY*(7) C 8	0.82	4.61	0.060
166. LP (4)C153	280. RY*(8) C 8	0.08	4.27	0.018
166. LP (4)C153	284. RY*(12) C 8	0.14	2.99	0.020
166. LP (4)C153	286. RY*(14) C 8	0.18	45.87	0.088
166. LP (4)C153	287. RY*(15) C 8	0.10	26.88	0.051
166. LP (4)C153	335. RY*(3) C12	0.20	1.97	0.019
166. LP (4)C153	336. RY*(4) C12	0.05	1.58	0.009
166. LP (4)C153	338. RY*(6) C12	1.28	3.05	0.061
166. LP (4)C153	339. RY*(7) C12	0.15	8.93	0.036
166. LP (4)C153	340. RY*(8) C12	0.05	4.48	0.015

166. LP (4)C153	341. RY*(9) C12	0.24	5.05	0.034
166. LP (4)C153	342. RY*(10) C12	0.09	2.65	0.015
166. LP (4)C153	364. RY*(2) C14	0.11	0.85	0.009
166. LP (4)C153	373. RY*(11) C14	0.08	2.95	0.015
166. LP (4)C153	393. RY*(1) C16	0.56	1.31	0.026
166. LP (4)C153	394. RY*(2) C16	0.39	0.88	0.018
166. LP (4)C153	395. RY*(3) C16	0.23	1.24	0.016
166. LP (4)C153	404. RY*(12) C16	0.11	3.17	0.018
166. LP (4)C153	425. RY*(3) C18	0.14	1.92	0.016
166. LP (4)C153	426. RY*(4) C18	0.06	1.25	0.009
166. LP (4)C153	428. RY*(6) C18	0.69	2.67	0.042
166. LP (4)C153	429. RY*(7) C18	0.16	8.14	0.035
166. LP (4)C153	454. RY*(2) C20	0.07	0.87	0.007
166. LP (4)C153	459. RY*(7) C20	0.18	3.62	0.025
166. LP (4)C153	462. RY*(10) C20	0.08	3.80	0.017
166. LP (4)C153	487. RY*(5) C22	0.20	3.88	0.027
166. LP (4)C153	522. RY*(10) C24	0.08	3.90	0.017
166. LP (4)C153	568. RY*(1) H29	0.40	1.53	0.024
166. LP (4)C153	569. RY*(2) H29	0.10	2.19	0.014
166. LP (4)C153	570. RY*(3) H29	0.46	1.69	0.027
166. LP (4)C153	571. RY*(4) H29	0.22	1.90	0.020
166. LP (4)C153	572. RY*(5) H29	0.10	3.69	0.019
166. LP (4)C153	580. RY*(3) H31	0.11	1.37	0.012
166. LP (4)C153	610. RY*(3) H37	0.17	1.32	0.014
166. LP (4)C153	615. RY*(3) H38	0.05	1.88	0.009
166. LP (4)C153	625. RY*(3) H40	0.13	1.57	0.014
166. LP (4)C153	675. RY*(3) O46	0.09	2.12	0.013
166. LP (4)C153	676. RY*(4) O46	0.63	0.76	0.021
166. LP (4)C153	677. RY*(5) O46	0.10	2.21	0.015
166. LP (4)C153	680. RY*(8) O46	0.11	2.16	0.015
166. LP (4)C153	690. RY*(3) O47	0.07	1.96	0.011
166. LP (4)C153	691. RY*(4) O47	0.79	0.71	0.023
166. LP (4)C153	692. RY*(5) O47	0.20	2.45	0.022
166. LP (4)C153	733. RY*(1) N50	0.64	1.83	0.033
166. LP (4)C153	735. RY*(3) N50	0.22	2.39	0.022
166. LP (4)C153	796. RY*(1)Ru52	149.24	0.12	0.130
166. LP (4)C153	797. RY*(2)Ru52	20.21	0.73	0.119
166. LP (4)C153	798. RY*(3)Ru52	5.36	0.97	0.070
166. LP (4)C153	799. RY*(4)Ru52	1.24	1.99	0.048
166. LP (4)C153	800. RY*(5)Ru52	1.12	3.28	0.059
166. LP (4)C153	801. RY*(6)Ru52	1.49	1.39	0.044
166. LP (4)C153	803. RY*(8)Ru52	5.04	1.35	0.081
166. LP (4)C153	806. RY*(11)Ru52	0.07	6.70	0.021
166. LP (4)C153	807. RY*(12)Ru52	1.71	7.32	0.109
166. LP (4)C153	808. RY*(13)Ru52	0.36	2.68	0.030
166. LP (4)C153	809. RY*(14)Ru52	0.79	5.51	0.064
166. LP (4)C153	810. RY*(15)Ru52	0.63	6.35	0.062
166. LP (4)C153	811. RY*(16)Ru52	0.15	6.28	0.030
166. LP (4)C153	812. RY*(17)Ru52	5.50	4.17	0.148
166. LP (4)C153	814. RY*(19)Ru52	0.97	5.45	0.071
166. LP (4)C153	816. RY*(21)Ru52	0.23	13.63	0.055
166. LP (4)C153	817. RY*(22)Ru52	0.37	9.44	0.058
166. LP (4)C153	818. RY*(23)Ru52	2.44	6.81	0.126
166. LP (4)C153	819. RY*(24)Ru52	1.94	29463.61	7.387
166. LP (4)C153	820. RY*(25)Ru52	4.25	765.33	1.761
166. LP (4)C153	821. RY*(26)Ru52	3.54	12899.60	6.602
166. LP (4)C153	822. RY*(27)Ru52	0.26	49.50	0.112
166. LP (4)C153	823. RY*(28)Ru52	0.16	186.38	0.170
166. LP (4)C153	826. RY*(31)Ru52	0.15	18.22	0.052
166. LP (4)C153	827. RY*(32)Ru52	0.09	54.17	0.070
166. LP (4)C153	829. RY*(34)Ru52	0.06	49.93	0.055
166. LP (4)C153	830. RY*(35)Ru52	0.15	18.37	0.051
166. LP (4)C153	831. RY*(36)Ru52	0.08	54.13	0.066
166. LP (4)C153	833. RY*(38)Ru52	4.16	3361.68	3.652
166. LP (4)C153	835. RY*(40)Ru52	0.11	54.19	0.076
166. LP (4)C153	836. RY*(41)Ru52	2.53	776.97	1.371
166. LP (4)C153	837. RY*(42)Ru52	1.60	3154.71	2.194
166. LP (4)C153	865. BD*(1) C12- N50	0.21	0.70	0.012
166. LP (4)C153	881. BD*(1) C 8-Ru52	54.45	0.33	0.121
166. LP (4)C153	882. BD*(1) C 6-Ru52	0.12	0.37	0.006
166. LP (4)C153	883. BD*(1) C 6- O46	0.42	0.27	0.010
166. LP (4)C153	884. BD*(2) C 6- O46	0.35	0.25	0.009
166. LP (4)C153	885. BD*(3) C 6- O46	0.48	0.86	0.020
166. LP (4)C153	922. BD*(2) C20- N50	0.22	0.22	0.007
166. LP (4)C153	923. BD*(1) C20- C23	0.09	0.73	0.008
166. LP (4)C153	925. BD*(1) C22- C25	0.07	0.75	0.007
166. LP (4)C153	926. BD*(1) C16-Ru52	0.88	0.27	0.014
166. LP (4)C153	928. BD*(1) C16- C18	0.28	0.77	0.014
from unit 4 to unit 3				
163. LP (1)C153	640. RY*(3) H43	0.18	2.81	0.020
165. LP (3)C153	638. RY*(1) H43	0.35	1.90	0.025
165. LP (3)C153	640. RY*(3) H43	1.07	2.48	0.050
165. LP (3)C153	642. RY*(5) H43	0.09	2.84	0.015
165. LP (3)C153	660. RY*(3) O45	0.10	2.52	0.015
165. LP (3)C153	662. RY*(5) O45	0.41	2.63	0.032
165. LP (3)C153	667. RY*(10) O45	0.07	5.25	0.018
165. LP (3)C153	668. RY*(11) O45	0.05	5.52	0.017
165. LP (3)C153	934. BD*(1) H43- O45	0.09	0.85	0.008
166. LP (4)C153	638. RY*(1) H43	1.49	1.78	0.050
166. LP (4)C153	641. RY*(4) H43	0.23	2.88	0.025
166. LP (4)C153	642. RY*(5) H43	0.37	2.71	0.031
166. LP (4)C153	658. RY*(1) O45	0.28	2.63	0.026
166. LP (4)C153	659. RY*(2) O45	0.50	1.78	0.029
166. LP (4)C153	661. RY*(4) O45	0.22	4.15	0.030
166. LP (4)C153	662. RY*(5) O45	0.53	2.51	0.036
166. LP (4)C153	663. RY*(6) O45	0.05	2.90	0.012
166. LP (4)C153	664. RY*(7) O45	0.11	2.49	0.016
166. LP (4)C153	666. RY*(9) O45	0.09	2.61	0.015
166. LP (4)C153	668. RY*(11) O45	0.39	5.39	0.045
166. LP (4)C153	671. RY*(14) O45	0.06	4.91	0.017
166. LP (4)C153	934. BD*(1) H43- O45	0.07	0.72	0.007
within unit 4				
165. LP (3)C153	847. RY*(4)C153	2.74	2.80	0.085
165. LP (3)C153	850. RY*(7)C153	1.55	4.07	0.077
165. LP (3)C153	852. RY*(9)C153	0.57	2.10	0.034
165. LP (3)C153	853. RY*(10)C153	1.26	4.96	0.077
166. LP (4)C153	845. RY*(2)C153	0.55	1.21	0.025
166. LP (4)C153	846. RY*(3)C153	3.27	6.31	0.140
166. LP (4)C153	847. RY*(4)C153	1.83	2.67	0.068
166. LP (4)C153	848. RY*(5)C153	3.87	6.77	0.158
166. LP (4)C153	849. RY*(6)C153	0.96	1.55	0.038
166. LP (4)C153	853. RY*(10)C153	0.78	4.83	0.060

NATURAL BOND ORBITALS (Summary):

NBO	Occupancy	Energy	Principal Delocalizations (geminal,vicinal,remote)
Molecular unit 1 (C13H8NO2Ru)			
1. BD (1) C 1- C 2	1.98282	-0.66149	805(r),875(v),718(v),199(v) 886(g),776(r),748(r),755(r) 780(r),777(r),767(r),913(r) 890(g),759(r),847(r),848(r) 825(r),846(r),638(r),640(r) 815(r),570(r),853(r)
2. BD (2) C 1- C 2	1.63590	-0.25227	874(v),893(v),200(v),719(v) 888(g),805(r),884(r)
3. BD (1) C 1- C 3	1.98475	-0.65640	877(v),891(v),805(r),230(v) 873(g),887(g)
4. BD (1) C 1- H 42	1.97639	-0.48911	890(v),873(v),198(v),183(v) 796(r),797(r)
5. BD (1) C 2- H 27	1.97198	-0.47982	805(r),892(v),886(v),718(v) 755(r),168(v),759(r),748(r) 757(r),767(r),776(r),825(r) 780(r),764(r),777(r),785(r) 847(r),848(r),815(r),846(r) 640(r),884(r),638(r),570(r) 824(r),833(r),799(r),820(r) 661(r),821(r),811(r),845(r) 836(r),659(r)
6. BD (1) C 2- N 49	1.98610	-0.77398	805(r),913(r),759(r),755(r) 894(v),757(r),767(r),776(r) 780(r),748(r),260(v),764(r) 785(r),777(r),889(v),762(r) 760(r),721(g),772(r),789(r) 188(g),750(r),761(r),197(g) 170(v),848(r),887(g),258(v) 773(r),293(r),763(r),892(g) 196(g),189(g),825(r),219(r) 754(r),720(g),847(r),846(r) 851(r),640(r),853(r),570(r) 638(r),661(r),815(r),796(r) 856(r),852(r),813(r),665(r) 338(r),799(r),659(r),797(r) 854(r),811(r),845(r),569(r) 833(r),662(r)
7. BD (1) C 3- C 5	1.98395	-0.66314	894(v),805(r),889(v),876(g) 170(v),886(g),258(v)
8. BD (2) C 3- C 5	1.66321	-0.25308	893(v),888(v),169(v),263(v)
9. BD (1) C 3- H 41	1.97843	-0.49266	876(v),887(v),228(v),168(v) 805(r)
10. BD (1) C 4- O 44	1.99744	-0.38779	796(r),825(r),797(r),815(r) 833(r),814(r),824(r),820(r) 821(r),801(r),840(r)
11. BD (2) C 4- O 44	1.99744	-0.38616	
12. BD (3) C 4- O 44	1.99514	-1.07776	748(v),750(v),776(v),767(v) 780(v),805(r),213(g),752(v) 755(v),777(v),785(v),763(v) 762(v),757(v),764(v),772(v) 789(v),219(g),759(v),770(v) 760(v),773(v),766(v),847(r) 848(r),383(r),765(v),188(r) 646(g),640(r),788(v),846(r) 303(r),761(v),768(v),638(r) 220(g),570(r),706(r),754(v) 293(r),264(r),796(r),645(g) 718(r),309(r),825(r),318(r) 853(r),215(g),214(g),329(r) 662(r),310(r),321(r),319(r) 774(v),707(r),384(r),769(v) 792(v),330(r),221(g),705(r) 815(r),726(r),595(r),315(r) 288(r),224(g),630(r),647(g) 227(g),568(r),338(r),793(v) 642(r),189(r),326(r),749(v) 799(r),721(r),775(v),668(r) 856(r),658(r),813(r),641(r) 669(r),851(r),667(r),364(r) 845(r),804(r),797(r),660(r) 811(r),661(r),569(r),800(r) 659(r),854(r),285(r),663(r) 734(r),665(r),373(r),735(r) 666(r),341(r),855(r),849(r) 812(r),844(r),344(r),393(r) 809(r),816(r),833(r),255(r) 396(r)
13. BD (1) C 4-Ru 51	1.91955	-0.53020	902(g),913(g),718(r),805(r) 305(v),912(g),304(v),796(r) 213(g),914(v),645(v),916(v) 318(v),219(g),759(g),660(r) 915(v),754(g),847(r),706(r) 756(g),848(r),750(g),911(g) 892(r),900(v),767(g),777(g) 658(r),317(v),748(g),768(g) 890(r),757(g),846(r),901(v) 897(v),764(g),640(r),799(r) 667(r),570(r),663(r),666(r) 642(r),825(r),845(r),849(r) 638(r),672(r),853(r),338(r) 881(r),364(r),668(r),926(r) 659(r),664(r),641(r),801(r) 661(r),669(r),860(r),856(r) 800(r),816(r),815(r),834(r) 858(r)
14. BD (1) C 5- C 7	1.97942	-0.65297	805(r),875(v),897(v),199(v) 894(g),873(g),290(v),718(v) 913(r),892(g),848(r),847(r)
15. BD (1) C 5- H 28	1.97434	-0.49079	892(v),886(v),258(v),198(v) 805(r)
20. BD (1) C 7- C 9	1.97250	-0.60140	890(v),900(v),898(v),873(v) 897(g),318(v),876(g),718(v) 348(v),895(g),228(v),754(r) 354(v),805(r),847(r),848(r) 845(r),853(r)
21. BD (1) C 7- N 49	1.98200	-0.75815	913(r),185(v),895(v),891(v) 877(v),759(r),750(r),272(g) 754(r),876(g),825(r),720(g) 762(r),749(r),796(r),271(g) 776(r),767(r),780(r),265(g)

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                                                894(g),777(r),757(r),233(v)
                                                288(v),291(v),755(r),785(r)
                                                748(r),764(r),268(g),235(v)
                                                805(r),847(r),848(r),853(r)
                                                797(r),824(r),815(r),638(r)
                                                570(r),846(r),845(r),833(r)
                                                820(r),818(r),568(r),662(r)
                                                821(r),798(r)
22. BD ( 2) C  7- N 49        1.72309    -0.29832  888(v),896(v),874(v),805(r)
                                                184(v),229(v),289(v),796(r)
                                                825(r),853(r),850(r),861(r)
                                                860(r),858(r),852(r),846(r)
                                                803(r),798(r),818(r)
27. BD ( 1) C  9- C 11        1.97155    -0.60703  876(v),908(v),899(v),895(g)
                                                380(v),750(v),767(v),757(v)
                                                754(v),776(v),759(v),780(v)
                                                894(g),302(g),351(v),796(r)
                                                296(g),748(v),749(v),777(v)
                                                258(v),318(g),301(g),762(v)
                                                761(v),293(g),785(v),755(v)
                                                805(r),350(v),763(v),378(v)
                                                290(g),764(v),772(v),760(v)
                                                355(v),789(v),900(g),354(v)
                                                781(v),848(r),847(r),853(r)
                                                640(r),797(r),825(r),846(r)
                                                570(r),638(r),851(r),668(r)
                                                845(r),568(r),856(r),852(r)
                                                658(r)
28. BD ( 1) C  9- C 13        1.97418    -0.62243  902(v),892(v),905(v),897(g)
                                                410(v),260(v),898(g),894(g)
                                                320(v)
29. BD ( 2) C  9- C 13        1.62982    -0.22035  893(v),901(v),904(v),409(v)
                                                319(v),289(g),262(v),796(r)
30. BD ( 1) C 10- O 48        1.99651    -0.39227  805(r),853(r),847(r),861(r)
31. BD ( 2) C 10- O 48        1.99560    -0.39770  805(r),796(r),334(r),853(r)
                                                640(r),336(r),570(r),847(r)
                                                797(r),864(r),347(r),364(r)
                                                856(r)
32. BD ( 3) C 10- O 48        1.99463    -1.06911  748(v),750(v),776(v),767(v)
                                                780(v),757(v),752(v),785(v)
                                                303(g),777(v),755(v),764(v)
                                                762(v),772(v),789(v),770(v)
                                                763(v),766(v),760(v),768(v)
                                                309(g),773(v),759(v),847(r)
                                                753(v),848(r),219(r),805(r)
                                                383(r),846(r),213(r),796(r)
                                                765(v),788(v),640(r),188(r)
                                                638(r),646(r),305(g),705(g)
                                                310(g),570(r),706(g),761(v)
                                                853(r),318(r),751(v),264(r)
                                                293(r),647(r),329(r),319(r)
                                                662(r),797(r),718(r),384(r)
                                                781(v),288(r),568(r),595(r)
                                                317(g),825(r),330(r),316(g)
                                                338(r),321(r),380(r),726(r)
                                                642(r),630(r),668(r),856(r)
                                                660(r),641(r),845(r),813(r)
                                                799(r),658(r),569(r),814(r)
                                                800(r),336(r),851(r),364(r)
                                                667(r),669(r),661(r),734(r)
                                                824(r),804(r),341(r),665(r)
                                                344(r),844(r),666(r),285(r)
                                                854(r),855(r),663(r),279(r)
                                                255(r),373(r),798(r),809(r)
                                                818(r),740(r),852(r),735(r)
                                                393(r),745(r),273(r),580(r)
                                                834(r),343(r),334(r),253(r)
                                                664(r),811(r),671(r),457(r)
33. BD ( 1) C 10-Ru 51        1.92613    -0.53610  902(g),912(g),805(r),705(v)
                                                318(v),910(v),660(r),897(v)
                                                215(v),911(v),303(g),913(g)
                                                658(r),796(r),850(r),721(r)
                                                916(g),309(g),588(r),715(v)
                                                288(r),849(r),846(r),334(r)
                                                848(r),661(r),659(r),881(r)
                                                804(r),801(r),860(r),803(r)
                                                799(r),926(r),664(r),847(r)
                                                861(r),858(r),669(r),667(r)
                                                845(r),672(r),662(r),853(r)
                                                336(r),812(r),641(r),817(r)
                                                639(r),798(r),825(r),864(r)
                                                882(r),863(r),670(r),840(r)
                                                663(r)
34. BD ( 1) C 11- C 15        1.97955    -0.61437  805(r),748(v),750(v),752(v)
                                                767(v),776(v),780(v),757(v)
                                                777(v),894(v),785(v),759(v)
                                                763(v),762(v),768(v),321(g)
                                                772(v),847(r),789(v),383(g)
                                                764(v),906(v),760(v),288(v)
                                                755(v),766(v),758(v),773(v)
                                                219(r),753(v),754(v),440(v)
                                                290(v),213(r),907(g),303(r)
                                                318(g),848(r),853(r),788(v)
                                                326(g),264(r),646(r),770(v)
                                                761(v),796(r),846(r),384(g)
                                                380(g),908(g),570(r),638(r)
                                                320(g),188(r),592(v),640(r)
                                                391(g),897(g),381(g),392(g)
                                                588(v),706(r),589(v),441(v)
                                                662(r),799(r),856(r),338(r)
                                                669(r),568(r),845(r),851(r)
                                                659(r),813(r),660(r),661(r)
                                                364(r),642(r),569(r),815(r)
                                                825(r),861(r),855(r),665(r)
                                                852(r),253(r),804(r)
35. BD ( 2) C 11- C 15        1.60134    -0.21004  904(v),896(v),289(v),439(v)
                                                912(v),796(r),319(g),853(r)
                                                797(r),861(r),860(r),850(r)
36. BD ( 1) C 11-Ru 51        1.85393    -0.36055  913(g),912(g),895(v),907(v)
                                                718(r),305(v),902(g),909(v)
                                                915(v),890(r),916(v),805(r)
                                                908(v),378(v),304(v),288(v)
                                                876(r),661(r),914(v),894(v)
                                                911(v),380(v),658(r),672(r)
                                                849(r),670(r),660(r),850(r)
                                                926(r),845(r),852(r),853(r)
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				802(r),659(r),860(r),861(r)
				639(r),394(r)
41. BD (1) C 13- C 17	1.98340	-0.63110	894(v),906(v),895(g),440(v)	
				903(g),288(v),805(r)
42. BD (1) C 13- H 30	1.97486	-0.46918	897(v),903(v),288(v),408(v)	
				805(r)
45. BD (1) C 15- C 19	1.97849	-0.62129	805(r),902(v),905(v),900(g)	
				318(v),410(v),903(g),748(r)
				750(r),776(r),780(r),847(r)
				848(r),640(r),846(r),570(r)
				796(r),853(r),638(r)
46. BD (1) C 15- H 33	1.97496	-0.44868	897(v),903(v),318(v),438(v)	
				444(v),847(r),848(r),805(r)
				846(r),825(r),660(r)
50. BD (1) C 17- C 19	1.98463	-0.62317	899(v),908(v),350(v),898(g)	
				805(r),907(g),381(v)
51. BD (2) C 17- C 19	1.64105	-0.22032	896(v),901(v),379(v),349(v)	
				352(v)
52. BD (1) C 17- H 34	1.97742	-0.46239	895(v),907(v),348(v),438(v)	
56. BD (1) C 19- H 35	1.97665	-0.45949	900(v),898(v),408(v),378(v)	
				805(r)
73. CR (1) C 1	1.99935	-9.79348	199(v),186(v),890(v)	
74. CR (1) C 2	1.99935	-9.82635	892(v),168(v),170(v)	
75. CR (1) C 3	1.99938	-9.80296	170(v),230(v),876(v)	
76. CR (1) C 4	1.99944	-9.90041	646(v)	
77. CR (1) C 5	1.99929	-9.79437	199(v),260(v),894(v),892(v)	
79. CR (1) C 7	1.99926	-9.83495	890(v),897(v),895(v),228(v)	
				288(v),720(v)
81. CR (1) C 9	1.99918	-9.77502	320(v),876(v),902(v),350(v)	
				258(v),348(v),892(v)
82. CR (1) C 10	1.99946	-9.89518	706(v)	
83. CR (1) C 11	1.99907	-9.78103	380(v),290(v),895(v),894(v)	
				907(v),902(g),288(v)
85. CR (1) C 13	1.99930	-9.77276	410(v),897(v),290(v),894(v)	
87. CR (1) C 15	1.99930	-9.75985	902(v),440(v),320(v),321(v)	
89. CR (1) C 17	1.99937	-9.76624	350(v),440(v),895(v),907(v)	
91. CR (1) C 19	1.99937	-9.76959	900(v),410(v),380(v),381(v)	
99. CR (1) O 44	1.99979	-18.58421	213(v),912(v)	
103. CR (1) O 48	1.99980	-18.58778	303(v),913(v)	
104. CR (1) N 49	1.99947	-13.88722	913(r),258(v),260(v),185(v)	
				183(v)
106. CR (1)Ru 51	2.00000	-826.14408		
107. CR (2)Ru 51	2.00000	-113.66637	789(g),785(g),780(g),776(g)	
				916(v),911(v),788(g)
108. CR (3)Ru 51	1.99999	-21.94861	789(g),785(g),780(g),916(v)	
				911(v),776(g),788(g),900(v)
				748(g),757(g),767(g),777(g)
				902(g),750(g),890(r),762(g)
				892(r),759(g),755(g),897(v)
				764(g),763(g),770(g),848(r)
				847(r),846(r),853(r),882(r)
				640(r),805(r)
109. CR (4)Ru 51	1.98720	-4.60970	916(v),911(v),900(v),303(v)	
				213(v),902(g),789(g),890(r)
				892(r),785(g),780(g),776(g)
				897(v),748(g),757(g),767(g)
				777(g),762(g),750(g),759(g)
				755(g),763(g),764(g),788(g)
				760(g),770(g),318(v),752(g)
				915(v),309(v),772(g),848(r)
				846(r),847(r),805(r),640(r)
				882(r),853(r),638(r),926(r)
				570(r),661(r)
110. CR (5)Ru 51	2.00000	-91.91771		
111. CR (6)Ru 51	2.00000	-28.68760		
112. CR (7)Ru 51	1.99366	-1.84234	913(g),902(g),916(v),900(v)	
				890(r)
113. CR (8)Ru 51	2.00000	-91.91809		
114. CR (9)Ru 51	2.00000	-28.68812		
115. CR (10)Ru 51	1.99491	-1.84645	912(g),902(g),913(g),915(v)	
				911(v),909(v),934(r)
116. CR (11)Ru 51	2.00000	-91.91778		
117. CR (12)Ru 51	2.00000	-28.68776		
118. CR (13)Ru 51	1.99208	-1.84416	912(g),913(g),911(v),902(g)	
				916(v),914(v)
119. CR (14)Ru 51	2.00000	-10.09618		
120. CR (15)Ru 51	2.00000	-10.09583		
121. CR (16)Ru 51	2.00000	-10.09692		
122. CR (17)Ru 51	2.00000	-10.09520		
123. CR (18)Ru 51	2.00000	-10.09482		
148. LP (1) O 44	1.97801	-0.68602	213(v),805(r),912(v),215(v)	
				220(v),219(v),847(r),848(r)
				640(r),846(r)
154. LP (1) O 48	1.97768	-0.68008	303(v),913(v),310(v),805(r)	
				796(r),848(r),846(r),847(r)
155. LP (1) N 49	1.65970	-0.37281	913(r),876(v),887(v),796(r)	
				891(v),183(v),258(v),894(v)
				900(r),757(r),902(r),748(r)
				767(r),755(r),260(v),911(r)
				776(r),750(r),764(r),780(r)
				185(v),777(r),910(r),762(r)
				785(r),305(r),797(r),895(r)
				825(r),848(r),847(r),846(r)
				570(r),640(r),638(r),853(r)
				824(r),805(r),851(r),338(r)
				662(r),882(r),798(r),845(r)
				803(r),815(r)
157. LP (1)Ru 51	1.76340	-0.20477	796(r),915(v),914(v),909(v)	
				805(r),825(r),797(r),901(v)
				720(r),815(r),659(r),306(v)
				216(v),824(r),801(r),320(v)
				833(r),820(r),900(v),319(v)
				821(r),836(r),814(r),810(r)
				798(r),819(r),818(r),847(r)
				926(r),837(r),799(r),811(r)
				804(r),668(r),840(r),733(r)
				812(r),800(r),845(r),273(r)
				841(r),676(r),570(r),813(r)
				691(r),817(r),638(r),852(r)
				428(r),807(r)
158. LP (2)Ru 51	1.71227	-0.20911	909(v),796(r),915(v),901(v)	
				914(v),797(r),216(v),319(v)
				825(r),902(g),306(v),720(r)
				815(r),658(r),845(r),320(v)
				804(r),840(r),659(r),799(r)
				833(r),934(r),817(r),820(r)

				798(r),841(r),821(r),801(r)
				882(r),805(r),848(r),814(r)
				800(r),846(r),836(r),824(r)
				852(r),819(r),810(r),802(r)
				860(r),273(r),837(r),811(r)
				393(r),858(r),861(r),733(r)
				668(r),803(r),850(r),806(r)
				926(r),816(r),243(r),676(r)
159.	LP (3)Ru 51	1.66503	-0.22008	910(v),914(v),915(v),893(r)
				304(v),719(r),214(v),796(r)
				909(v),844(r),803(r),934(r)
				802(r)
168.	RY*(1) C 1	0.00291	1.65991	
169.	RY*(2) C 1	0.00212	0.54161	
170.	RY*(3) C 1	0.00109	1.84990	
171.	RY*(4) C 1	0.00059	1.23904	
172.	RY*(5) C 1	0.00034	1.81619	
173.	RY*(6) C 1	0.00012	7.80076	
174.	RY*(7) C 1	0.00010	3.73384	
175.	RY*(8) C 1	0.00006	2.37374	
176.	RY*(9) C 1	0.00004	3.19237	
177.	RY*(10) C 1	0.00001	4.52707	
178.	RY*(11) C 1	0.00002	2.57955	
179.	RY*(12) C 1	0.00001	8.41022	
180.	RY*(13) C 1	0.00001	2.13361	
181.	RY*(14) C 1	0.00000	24.78095	
182.	RY*(15) C 1	0.00000	39.42229	
183.	RY*(1) C 2	0.00601	1.49816	
184.	RY*(2) C 2	0.00498	0.63948	
185.	RY*(3) C 2	0.00230	1.78834	
186.	RY*(4) C 2	0.00127	1.42942	
187.	RY*(5) C 2	0.00058	1.92744	
188.	RY*(6) C 2	0.00036	3.65314	
189.	RY*(7) C 2	0.00015	4.84951	
190.	RY*(8) C 2	0.00012	8.77224	
191.	RY*(9) C 2	0.00009	3.62780	
192.	RY*(10) C 2	0.00009	3.27897	
193.	RY*(11) C 2	0.00005	4.33120	
194.	RY*(12) C 2	0.00002	2.67539	
195.	RY*(13) C 2	0.00002	3.20310	
196.	RY*(14) C 2	0.00000	39.99577	
197.	RY*(15) C 2	0.00000	26.15495	
198.	RY*(1) C 3	0.00252	1.73202	
199.	RY*(2) C 3	0.00153	1.71042	
200.	RY*(3) C 3	0.00098	0.52425	
201.	RY*(4) C 3	0.00079	1.17762	
202.	RY*(5) C 3	0.00052	1.82087	
203.	RY*(6) C 3	0.00010	3.11635	
204.	RY*(7) C 3	0.00005	6.86842	
205.	RY*(8) C 3	0.00003	3.78718	
206.	RY*(9) C 3	0.00002	2.00420	
207.	RY*(10) C 3	0.00001	8.61734	
208.	RY*(11) C 3	0.00001	2.94857	
209.	RY*(12) C 3	0.00002	4.96196	
210.	RY*(13) C 3	0.00000	2.33290	
211.	RY*(14) C 3	0.00000	29.13652	
212.	RY*(15) C 3	0.00000	36.18911	
213.	RY*(1) C 4	0.01427	2.25688	
214.	RY*(2) C 4	0.00422	1.47512	
215.	RY*(3) C 4	0.00410	1.59405	
216.	RY*(4) C 4	0.00317	1.78830	
217.	RY*(5) C 4	0.00198	1.97148	
218.	RY*(6) C 4	0.00160	1.97943	
219.	RY*(7) C 4	0.00022	6.62171	
220.	RY*(8) C 4	0.00013	4.07361	
221.	RY*(9) C 4	0.00010	2.93740	
222.	RY*(10) C 4	0.00008	1.67778	
223.	RY*(11) C 4	0.00005	3.07996	
224.	RY*(12) C 4	0.00003	3.36217	
225.	RY*(13) C 4	0.00002	2.55104	
226.	RY*(14) C 4	0.00000	45.60743	
227.	RY*(15) C 4	0.00000	26.60998	
228.	RY*(1) C 5	0.00308	1.52671	
229.	RY*(2) C 5	0.00178	0.46640	
230.	RY*(3) C 5	0.00090	1.64969	
231.	RY*(4) C 5	0.00052	1.60067	
232.	RY*(5) C 5	0.00037	1.81186	
233.	RY*(6) C 5	0.00015	6.27186	
234.	RY*(7) C 5	0.00011	4.60520	
235.	RY*(8) C 5	0.00008	3.17626	
236.	RY*(9) C 5	0.00006	1.74545	
237.	RY*(10) C 5	0.00002	3.18140	
238.	RY*(11) C 5	0.00002	4.74429	
239.	RY*(12) C 5	0.00002	6.56242	
240.	RY*(13) C 5	0.00000	2.31304	
241.	RY*(14) C 5	0.00000	30.21627	
242.	RY*(15) C 5	0.00000	36.68473	
258.	RY*(1) C 7	0.00833	1.55010	
259.	RY*(2) C 7	0.00512	0.60429	
260.	RY*(3) C 7	0.00343	1.96976	
261.	RY*(4) C 7	0.00110	1.48678	
262.	RY*(5) C 7	0.00101	1.77824	
263.	RY*(6) C 7	0.00055	1.81766	
264.	RY*(7) C 7	0.00053	4.03623	
265.	RY*(8) C 7	0.00019	11.60429	
266.	RY*(9) C 7	0.00019	3.83340	
267.	RY*(10) C 7	0.00012	3.60615	
268.	RY*(11) C 7	0.00010	5.51055	
269.	RY*(12) C 7	0.00003	3.00913	
270.	RY*(13) C 7	0.00002	3.53409	
271.	RY*(14) C 7	0.00000	41.95976	
272.	RY*(15) C 7	0.00000	23.88850	
288.	RY*(1) C 9	0.00790	1.43894	
289.	RY*(2) C 9	0.00432	0.54768	
290.	RY*(3) C 9	0.00276	1.80836	
291.	RY*(4) C 9	0.00105	1.16655	
292.	RY*(5) C 9	0.00052	1.95867	
293.	RY*(6) C 9	0.00050	3.88835	
294.	RY*(7) C 9	0.00043	1.82907	
295.	RY*(8) C 9	0.00021	4.22880	
296.	RY*(9) C 9	0.00014	13.72900	
297.	RY*(10) C 9	0.00012	4.03184	
298.	RY*(11) C 9	0.00008	3.81585	
299.	RY*(12) C 9	0.00004	2.80766	
300.	RY*(13) C 9	0.00002	2.97936	
301.	RY*(14) C 9	0.00000	41.62670	

302.	RY*(15) C 9	0.00000	25.75011
303.	RY*(1) C 10	0.01427	2.07618
304.	RY*(2) C 10	0.00540	0.90908
305.	RY*(3) C 10	0.00407	2.61220
306.	RY*(4) C 10	0.00283	1.77949
307.	RY*(5) C 10	0.00203	1.68199
308.	RY*(6) C 10	0.00151	2.30908
309.	RY*(7) C 10	0.00026	6.67801
310.	RY*(8) C 10	0.00011	3.98263
311.	RY*(9) C 10	0.00009	3.90191
312.	RY*(10) C 10	0.00009	2.06995
313.	RY*(11) C 10	0.00007	1.78658
314.	RY*(12) C 10	0.00004	2.74645
315.	RY*(13) C 10	0.00003	2.79435
316.	RY*(14) C 10	0.00000	45.55271
317.	RY*(15) C 10	0.00000	25.41748
318.	RY*(1) C 11	0.00834	1.23876
319.	RY*(2) C 11	0.00744	0.74680
320.	RY*(3) C 11	0.00588	1.01445
321.	RY*(4) C 11	0.00249	2.26017
322.	RY*(5) C 11	0.00050	1.98037
323.	RY*(6) C 11	0.00044	2.41428
324.	RY*(7) C 11	0.00037	2.85968
325.	RY*(8) C 11	0.00030	4.63621
326.	RY*(9) C 11	0.00024	13.98357
327.	RY*(10) C 11	0.00013	4.12641
328.	RY*(11) C 11	0.00013	3.35717
329.	RY*(12) C 11	0.00007	3.14662
330.	RY*(13) C 11	0.00002	3.48581
331.	RY*(14) C 11	0.00000	39.85164
332.	RY*(15) C 11	0.00000	26.53757
348.	RY*(1) C 13	0.00322	1.53942
349.	RY*(2) C 13	0.00237	0.53113
350.	RY*(3) C 13	0.00100	1.73248
351.	RY*(4) C 13	0.00069	1.53820
352.	RY*(5) C 13	0.00049	1.78780
353.	RY*(6) C 13	0.00012	3.68252
354.	RY*(7) C 13	0.00012	7.24406
355.	RY*(8) C 13	0.00007	2.80206
356.	RY*(9) C 13	0.00003	2.88043
357.	RY*(10) C 13	0.00002	3.44014
358.	RY*(11) C 13	0.00002	6.04004
359.	RY*(12) C 13	0.00003	2.59930
360.	RY*(13) C 13	0.00000	37.01188
361.	RY*(14) C 13	0.00000	2.07021
362.	RY*(15) C 13	0.00000	31.76723
378.	RY*(1) C 15	0.00502	1.65279
379.	RY*(2) C 15	0.00310	0.50163
380.	RY*(3) C 15	0.00160	1.75490
381.	RY*(4) C 15	0.00094	1.02411
382.	RY*(5) C 15	0.00030	1.80435
383.	RY*(6) C 15	0.00022	3.46828
384.	RY*(7) C 15	0.00013	8.18227
385.	RY*(8) C 15	0.00007	2.69610
386.	RY*(9) C 15	0.00007	4.72076
387.	RY*(10) C 15	0.00005	4.27254
388.	RY*(11) C 15	0.00003	5.36334
389.	RY*(12) C 15	0.00001	2.48520
390.	RY*(13) C 15	0.00002	3.31431
391.	RY*(14) C 15	0.00000	26.86682
392.	RY*(15) C 15	0.00000	40.20264
408.	RY*(1) C 17	0.00258	1.70594
409.	RY*(2) C 17	0.00225	0.49150
410.	RY*(3) C 17	0.00138	1.90889
411.	RY*(4) C 17	0.00093	1.17447
412.	RY*(5) C 17	0.00043	1.83487
413.	RY*(6) C 17	0.00010	3.50431
414.	RY*(7) C 17	0.00006	6.02774
415.	RY*(8) C 17	0.00001	3.47642
416.	RY*(9) C 17	0.00001	3.14384
417.	RY*(10) C 17	0.00001	3.38787
418.	RY*(11) C 17	0.00001	3.28343
419.	RY*(12) C 17	0.00001	5.45121
420.	RY*(13) C 17	0.00000	31.31780
421.	RY*(14) C 17	0.00000	37.22835
422.	RY*(15) C 17	0.00001	1.93082
438.	RY*(1) C 19	0.00314	1.58434
439.	RY*(2) C 19	0.00182	0.51959
440.	RY*(3) C 19	0.00121	1.87747
441.	RY*(4) C 19	0.00062	1.38023
442.	RY*(5) C 19	0.00053	1.85237
443.	RY*(6) C 19	0.00011	3.86854
444.	RY*(7) C 19	0.00009	6.25760
445.	RY*(8) C 19	0.00004	2.41814
446.	RY*(9) C 19	0.00001	7.57950
447.	RY*(10) C 19	0.00001	3.36332
448.	RY*(11) C 19	0.00000	36.48825
449.	RY*(12) C 19	0.00000	3.28250
450.	RY*(13) C 19	0.00001	2.64648
451.	RY*(14) C 19	0.00000	31.07028
452.	RY*(15) C 19	0.00001	2.00781
558.	RY*(1) H 27	0.00138	1.36728
559.	RY*(2) H 27	0.00056	1.98015
560.	RY*(3) H 27	0.00021	0.95889
561.	RY*(4) H 27	0.00007	1.79020
562.	RY*(5) H 27	0.00005	3.42944
563.	RY*(1) H 28	0.00043	1.70360
564.	RY*(2) H 28	0.00038	0.91762
565.	RY*(3) H 28	0.00033	1.66620
566.	RY*(4) H 28	0.00009	1.43103
567.	RY*(5) H 28	0.00002	4.37429
573.	RY*(1) H 30	0.00055	1.00443
574.	RY*(2) H 30	0.00051	1.40051
575.	RY*(3) H 30	0.00033	1.82239
576.	RY*(4) H 30	0.00011	1.57189
577.	RY*(5) H 30	0.00002	4.31092
588.	RY*(1) H 33	0.00117	1.37625
589.	RY*(2) H 33	0.00053	1.91953
590.	RY*(3) H 33	0.00034	0.94984
591.	RY*(4) H 33	0.00011	1.46391
592.	RY*(5) H 33	0.00003	4.12028
593.	RY*(1) H 34	0.00062	0.88562
594.	RY*(2) H 34	0.00046	1.47368
595.	RY*(3) H 34	0.00033	1.42971
596.	RY*(4) H 34	0.00005	1.44248
597.	RY*(5) H 34	0.00001	4.65246

598.	RY*(1) H 35	0.00051	0.88969	
599.	RY*(2) H 35	0.00037	1.83859	
600.	RY*(3) H 35	0.00028	0.99311	
601.	RY*(4) H 35	0.00005	1.50527	
602.	RY*(5) H 35	0.00001	4.81933	
628.	RY*(1) H 41	0.00041	1.61036	
629.	RY*(2) H 41	0.00035	0.86123	
630.	RY*(3) H 41	0.00031	1.22798	
631.	RY*(4) H 41	0.00005	1.40238	
632.	RY*(5) H 41	0.00001	4.84313	
633.	RY*(1) H 42	0.00048	0.91033	
634.	RY*(2) H 42	0.00036	1.60265	
635.	RY*(3) H 42	0.00024	1.07316	
636.	RY*(4) H 42	0.00004	1.57287	
637.	RY*(5) H 42	0.00002	4.47891	
643.	RY*(1) O 44	0.00268	0.68966	
644.	RY*(2) O 44	0.00195	0.70477	
645.	RY*(3) O 44	0.00097	1.76239	
646.	RY*(4) O 44	0.00020	0.71922	
647.	RY*(5) O 44	0.00005	2.40125	
648.	RY*(6) O 44	0.00002	2.86244	
649.	RY*(7) O 44	0.00002	4.05375	
650.	RY*(8) O 44	0.00002	3.63166	
651.	RY*(9) O 44	0.00000	100.20330	
652.	RY*(10) O 44	0.00000	3.26874	
653.	RY*(11) O 44	0.00000	10.09673	
654.	RY*(12) O 44	0.00001	1.24746	
655.	RY*(13) O 44	0.00000	4.51001	
656.	RY*(14) O 44	0.00000	64.38029	
657.	RY*(15) O 44	0.00000	2.98603	
703.	RY*(1) O 48	0.00289	0.72577	
704.	RY*(2) O 48	0.00205	0.76649	
705.	RY*(3) O 48	0.00134	1.98973	
706.	RY*(4) O 48	0.00022	0.71722	
707.	RY*(5) O 48	0.00006	2.09505	
708.	RY*(6) O 48	0.00003	1.89145	
709.	RY*(7) O 48	0.00004	1.51051	
710.	RY*(8) O 48	0.00002	1.59029	
711.	RY*(9) O 48	0.00001	1.39242	
712.	RY*(10) O 48	0.00000	4.89454	
713.	RY*(11) O 48	0.00000	9.41259	
714.	RY*(12) O 48	0.00001	5.21945	
715.	RY*(13) O 48	0.00000	69.88343	
716.	RY*(14) O 48	0.00000	4.88563	
717.	RY*(15) O 48	0.00000	96.89437	
718.	RY*(1) N 49	0.01012	1.91451	
719.	RY*(2) N 49	0.00673	0.84609	
720.	RY*(3) N 49	0.00501	2.11671	
721.	RY*(4) N 49	0.00202	4.55053	
722.	RY*(5) N 49	0.00049	1.80225	
723.	RY*(6) N 49	0.00031	1.78041	
724.	RY*(7) N 49	0.00032	3.08037	
725.	RY*(8) N 49	0.00014	13.98916	
726.	RY*(9) N 49	0.00012	4.50809	
727.	RY*(10) N 49	0.00008	3.30465	
728.	RY*(11) N 49	0.00004	4.75358	
729.	RY*(12) N 49	0.00005	4.49848	
730.	RY*(13) N 49	0.00002	5.14107	
731.	RY*(14) N 49	0.00000	48.25327	
732.	RY*(15) N 49	0.00000	27.23159	
748.	RY*(1)Ru 51	0.00794	18.05599	
749.	RY*(2)Ru 51	0.00722	0.89188	
750.	RY*(3)Ru 51	0.00563	8.25581	
751.	RY*(4)Ru 51	0.00456	1.25173	
752.	RY*(5)Ru 51	0.00420	4.15971	
753.	RY*(6)Ru 51	0.00393	3.10814	
754.	RY*(7)Ru 51	0.00310	4.19837	
755.	RY*(8)Ru 51	0.00270	6.13832	
756.	RY*(9)Ru 51	0.00220	2.60828	
757.	RY*(10)Ru 51	0.00126	21.24419	
758.	RY*(11)Ru 51	0.00077	6.83220	
759.	RY*(12)Ru 51	0.00053	14.73701	
760.	RY*(13)Ru 51	0.00036	4.77796	
761.	RY*(14)Ru 51	0.00029	7.53022	
762.	RY*(15)Ru 51	0.00022	14.21945	
763.	RY*(16)Ru 51	0.00018	12.79787	
764.	RY*(17)Ru 51	0.00016	10.53205	
765.	RY*(18)Ru 51	0.00011	6.69917	
766.	RY*(19)Ru 51	0.00007	6.84368	
767.	RY*(20)Ru 51	0.00003	17.20237	
768.	RY*(21)Ru 51	0.00001	16.85227	
769.	RY*(22)Ru 51	0.00002	8.91019	
770.	RY*(23)Ru 51	0.00001	16.15258	
771.	RY*(24)Ru 51	0.00000	2234.43985	
772.	RY*(25)Ru 51	0.00000	9406.04790	
773.	RY*(26)Ru 51	0.00000	37513.60496	
774.	RY*(27)Ru 51	0.00000	49.21263	
775.	RY*(28)Ru 51	0.00000	186.07030	
776.	RY*(29)Ru 51	0.00001	77.42677	
777.	RY*(30)Ru 51	0.00000	25.71184	
778.	RY*(31)Ru 51	0.00000	18.63520	
779.	RY*(32)Ru 51	0.00000	53.83398	
780.	RY*(33)Ru 51	0.00000	324.32589	
781.	RY*(34)Ru 51	0.00000	50.18125	
782.	RY*(35)Ru 51	0.00000	18.44450	
783.	RY*(36)Ru 51	0.00000	53.88333	
784.	RY*(37)Ru 51	0.00000	186.18134	
785.	RY*(38)Ru 51	0.00000	596.16282	
786.	RY*(39)Ru 51	0.00000	17.87961	
787.	RY*(40)Ru 51	0.00000	53.88814	
788.	RY*(41)Ru 51	0.00000	88.93320	
789.	RY*(42)Ru 51	0.00000	532.76526	
790.	RY*(43)Ru 51	0.00000	18.22289	
791.	RY*(44)Ru 51	0.00000	54.01708	
792.	RY*(45)Ru 51	0.00000	50.95141	
793.	RY*(46)Ru 51	0.00000	186.02991	
794.	RY*(47)Ru 51	0.00000	19.42641	
795.	RY*(48)Ru 51	0.00000	53.87513	
873.	BD*(1) C 3- C 5	0.01279	0.46023	
874.	BD*(2) C 3- C 5	0.28773	-0.02354	888(v),893(v),229(g),200(g)
875.	BD*(1) C 3- H 41	0.01463	0.36995	
876.	BD*(1) C 5- C 7	0.03150	0.46145	
877.	BD*(1) C 5- H 28	0.01528	0.37204	
886.	BD*(1) C 1- C 3	0.01480	0.44297	
887.	BD*(1) C 1- C 2	0.02264	0.46419	
888.	BD*(2) C 1- C 2	0.28685	-0.02269	874(v),893(v),884(r),169(g)

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                                                    184(g),879(r)
889. BD*( 1) C  1- H 42        0.01334     0.37442
890. BD*( 1) C  2- N 49        0.02376     0.43498
891. BD*( 1) C  2- H 27        0.02499     0.37370
892. BD*( 1) C  7- N 49        0.03586     0.41587
893. BD*( 2) C  7- N 49        0.50057    -0.04382  874(v),888(v),896(v),259(g)
                                                    719(g),229(v),805(r),184(v)
                                                    289(v),796(r),825(r),803(r)
                                                    815(r)
894. BD*( 1) C  7- C  9        0.03027     0.41508
895. BD*( 1) C  9- C 13        0.02953     0.48149
896. BD*( 2) C  9- C 13        0.41082     0.00582  904(v),901(v),893(v),349(g)
                                                    289(g)
897. BD*( 1) C  9- C 11        0.03382     0.49138
898. BD*( 1) C 13- C 17        0.01320     0.48556
899. BD*( 1) C 13- H 30        0.01659     0.38805
900. BD*( 1) C 11- C 15        0.02089     0.50429
901. BD*( 2) C 11- C 15        0.30039     0.02120  896(v),904(v),379(g),912(v)
                                                    319(g),796(r),797(r),881(r)
                                                    846(r),848(r)
902. BD*( 1) C 11-Ru 51        0.28627     0.01989  912(g),913(g),926(r),915(v)
                                                    909(v),796(r),718(r),305(v)
                                                    895(v),908(v),907(v),757(g)
                                                    797(r),777(g),914(v),759(g)
                                                    661(r),672(r),658(r),825(r)
                                                    638(r),882(r),670(r),853(r)
                                                    878(r),934(r),659(r),847(r)
                                                    849(r),570(r),798(r),640(r)
                                                    802(r),850(r),851(r),852(r)
                                                    815(r),338(r),364(r),848(r)
                                                    833(r),820(r),883(r),821(r)
                                                    814(r),824(r)
903. BD*( 1) C 17- C 19        0.01534     0.46900
904. BD*( 2) C 17- C 19        0.35553     0.00381  896(v),901(v),409(g),439(g)
905. BD*( 1) C 17- H 34        0.01446     0.39437
906. BD*( 1) C 19- H 35        0.01454     0.39506
907. BD*( 1) C 15- C 19        0.02223     0.47858
908. BD*( 1) C 15- H 33        0.01908     0.40107
909. BD*( 1) C  4- O 44        0.24641    -0.01388  914(r),915(r),902(v),643(g)
                                                    217(g),796(r),218(g),797(r)
                                                    825(r),926(r),801(r),815(r)
910. BD*( 2) C  4- O 44        0.18514    -0.01995  914(r),644(g),915(r),218(g)
911. BD*( 3) C  4- O 44        0.01434     0.59076
912. BD*( 1) C  4-Ru 51        0.34326     0.07019  913(g),902(g),881(r),796(r)
                                                    911(g),901(v),805(r),305(v)
                                                    915(v),797(r),914(v),849(r)
                                                    882(r),825(r),766(g),718(r)
                                                    769(g),801(r),660(r),815(r)
                                                    803(r),798(r),824(r),658(r)
                                                    394(r),669(r),934(r),812(r)
                                                    733(r),810(r),667(r),861(r)
                                                    663(r),820(r),850(r),833(r)
                                                    676(r),640(r),821(r),638(r)
                                                    659(r)
913. BD*( 1) C 10-Ru 51        0.32707     0.11050  912(g),902(g),882(r),916(g)
                                                    805(r),753(g),309(g),796(r)
                                                    910(v),732(r),759(g),660(r)
                                                    789(g),772(g),881(r),785(g)
                                                    803(r),849(r),847(r),846(r)
                                                    926(r),797(r),850(r),658(r)
                                                    825(r),669(r),801(r),638(r)
                                                    934(r),848(r),798(r),804(r)
                                                    667(r),662(r),570(r),812(r)
                                                    659(r),568(r),824(r),860(r)
                                                    845(r),640(r),852(r),861(r)
914. BD*( 1) C 10- O 48        0.20527    -0.01403  909(r),910(r),915(g),704(g)
                                                    308(g),304(g),916(g),703(g)
                                                    307(g),912(v),805(r),926(r)
                                                    796(r),853(r),861(r),850(r)
                                                    860(r)
915. BD*( 2) C 10- O 48        0.23397    -0.00929  909(r),307(g),902(v),914(g)
                                                    910(r),916(g),703(g),912(v)
                                                    304(g),704(g),864(r),805(r)
                                                    853(r),640(r),796(r),803(r)
                                                    850(r)
916. BD*( 3) C 10- O 48        0.01837     0.59117
         -------------------------------
               Total Lewis  147.83322  ( 96.8961%)
          Valence non-Lewis    4.44154  (  2.9112%)
          Rydberg non-Lewis    0.29397  (  0.1927%)
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              Total unit  1  152.56873  (100.0000%)
             Charge unit  1    0.43127

Molecular unit  2  (C13H8NO2Ru)
 16. BD ( 1) C  6- O 46        1.99654    -0.40277  825(v),805(v),798(v),848(r)
 17. BD ( 2) C  6- O 46        1.99612    -0.38941  796(v),184(r),853(r),186(r)
                                                    720(r)
 18. BD ( 3) C  6- O 46        1.99465    -1.09120  825(v),805(v),815(v),833(v)
                                                    820(v),821(v),824(v),803(v)
                                                    836(v),819(v),837(v),807(v)
                                                    796(v),243(g),818(v),817(v)
                                                    800(v),257(g),802(v),245(g)
                                                    828(v),811(v),799(v),249(g)
                                                    797(v),804(v),810(v),256(g)
                                                    829(v),251(g),809(v),733(r)
                                                    840(v),279(r),832(v),848(r)
                                                    640(r),188(r),853(r),846(r)
                                                    560(r),766(r),184(r),748(r)
                                                    847(r),638(r),852(r),661(r)
                                                    668(r),754(r),190(r),761(r)
                                                    850(r),169(r),861(r),776(r)
                                                    750(r),185(r),642(r)
 19. BD ( 1) C  6-Ru 52        1.92504    -0.53561  805(g),796(g),825(g),797(g)
                                                    926(g),881(g),824(g),812(g)
                                                    798(g),801(g),803(g),815(g)
                                                    810(g),927(v),879(v),660(r)
                                                    274(v),828(g),880(v),675(v)
                                                    814(g),279(v),393(v),846(r)
                                                    818(g),676(v),848(r),733(r)
                                                    882(g),811(g),428(r),847(r)
                                                    257(g),273(v),885(g),849(r)
                                                    850(r),661(r),560(r),659(r)
                                                    558(r),184(r),845(r),662(r)
                                                    669(r),658(r),756(r),751(r)
                                                    860(r),912(r),858(r),902(r)
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			638(r),188(r),861(r),934(r)
			672(r),318(r),755(r),757(r)
			664(r),667(r),758(r),792(r)
			559(r),671(r),186(r),190(r)
			670(r)
23. BD (1) C 8- O 47	1.99736	-0.38931	796(v),755(r),757(r),756(r)
			776(r),780(r),764(r),748(r)
			777(r),770(r),767(r),785(r)
			792(r),847(r),759(r),769(r)
24. BD (2) C 8- O 47	1.99750	-0.38766	798(v),796(v)
25. BD (3) C 8- O 47	1.99516	-1.09960	805(v),825(v),815(v),824(v)
			833(v),820(v),821(v),818(v)
			836(v),819(v),837(v),796(v)
			800(v),817(v),273(g),812(v)
			803(v),807(v),280(g),840(v)
			816(v),847(r),287(g),828(v)
			797(v),798(v),841(v),286(g)
			808(v),281(g),640(r),560(r)
			757(r),853(r),848(r),846(r)
			856(r),755(r),659(r),767(r)
			766(r),765(r),852(r),753(r)
			760(r),764(r),763(r),780(r)
			777(r),752(r),850(r),861(r)
			785(r),188(r),750(r),776(r)
			660(r),169(r)
26. BD (1) C 8-Ru 52	1.91979	-0.53786	805(g),796(g),825(g),797(g)
			815(g),824(g),882(g),926(g)
			803(g),798(g),812(g),811(g)
			810(g),818(g),801(g),799(g)
			245(v),814(g),885(v),828(g)
			883(v),733(r),691(v),249(v)
			884(v),243(v),804(g),881(g)
			428(r),244(v),338(r),167(v)
			250(v),660(r),921(r),394(v)
			928(v),690(v),404(v),560(r)
			807(g),820(g),865(r),927(v)
			809(g),247(v),287(g),286(g)
			847(r),661(r),669(r),640(r)
			558(r),846(r),853(r),848(r)
			667(r),755(r),638(r),765(r)
			861(r),757(r),672(r),766(r)
			856(r),668(r),662(r),760(r)
			671(r),751(r),658(r),767(r)
			758(r),860(r),852(r),184(r)
			188(r),850(r),764(r),720(r)
			774(r),659(r)
37. BD (1) C 12- C 14	1.98338	-0.67171	805(r),825(r),919(v),733(v)
			796(r),815(r),469(v),867(g)
			882(r),865(g),797(r),818(r)
			847(r)
38. BD (2) C 12- C 14	1.64997	-0.26079	918(v),922(v),470(v),734(v)
			864(g),915(r)
39. BD (1) C 12- H 29	1.97414	-0.49940	805(r),921(v),825(r),867(v)
			733(v),796(r),363(v),797(r)
			818(r),815(r),824(r),798(r)
			799(r),767(r),757(r),755(r)
			750(r),748(r),776(r),780(r)
			777(r),847(r),764(r),915(r)
			785(r),760(r),640(r),762(r)
			759(r),752(r),772(r),789(r)
			763(r),770(r),303(r),848(r)
			219(r),773(r),638(r),661(r)
			213(r),753(r),768(r),660(r)
40. BD (1) C 12- N 50	1.98629	-0.78518	805(r),825(r),882(r),924(v)
			797(r),818(r),801(r),798(r)
			868(v),815(r),833(r),455(v)
			820(r),821(r),824(r),863(g)
			347(g),736(g),365(v),836(r)
			369(v),346(g),803(r),799(r)
			921(g),819(r),453(v),811(r)
			847(r),659(r),934(r),757(r)
			767(r),852(r),755(r),780(r)
			776(r),750(r),753(r),762(r)
			560(r),777(r),748(r),785(r)
43. BD (1) C 14- C 21	1.98417	-0.66167	866(v),920(v),805(r),500(v)
			863(g),917(g)
44. BD (1) C 14- H 31	1.97619	-0.49612	865(v),917(v),468(v),805(r)
			333(v)
47. BD (1) C 16- C 18	1.97959	-0.62183	805(v),825(v),803(v),815(v)
			924(v),824(v),796(v),833(v)
			820(v),797(v),821(v),930(v)
			836(v),931(g),515(v),806(v)
			819(v),812(v),817(v),837(v)
			396(g),733(r),437(g),487(v)
			818(v),483(v),933(g),927(g)
			822(v),435(g),840(v),802(v)
			640(r),848(r),659(r),846(r)
			560(r),658(r),642(r)
48. BD (1) C 16- C 22	1.97140	-0.61125	805(v),796(v),825(v),923(v)
			933(v),871(v),925(g),818(v)
			824(v),815(v),924(g),425(v)
			496(g),531(v),497(g),798(v)
			530(v),491(g),833(v),820(v)
			395(g),453(v),533(v),821(v)
			429(v),802(v),928(g),801(v)
			846(r),848(r),188(r)
49. BD (1) C 16-Ru 52	1.85838	-0.36774	805(g),796(g),797(g),825(g)
			882(g),881(g),798(g),824(g)
			815(g),803(g),925(v),931(v)
			799(g),811(g),812(g),818(g)
			245(v),810(g),801(g),828(g)
			885(v),814(g),865(r),733(r)
			878(v),243(v),926(g),425(v)
			846(r),848(r),884(v),847(r)
			249(v),880(v),274(v),933(v)
			279(v),338(r),273(v),807(g)
			691(r),640(r),809(g),250(v)
			560(r),404(g),658(r),924(v)
			804(g),923(r),428(v),845(r)
			808(g),423(v),659(r),660(r)
			672(r),661(r),849(r),558(r)
			670(r),668(r),753(r),663(r)
			639(r),666(r),664(r),642(r)
			850(r),188(r),641(r),902(r)
			665(r),720(r),860(r),853(r)
			184(r),662(r),858(r),757(r)

53. BD (1) C 18- C 24	1.97863	-0.62434	805(r),926(v),872(v),825(r) 928(g),545(v),929(g),393(v) 815(r)
54. BD (2) C 18- C 24	1.65806	-0.21947	167(v),870(v),544(v),394(v) 424(g)
55. BD (1) C 18- H 32	1.97499	-0.45115	805(r),927(v),929(v),393(v) 825(r),513(v)
57. BD (1) C 20- C 22	1.97250	-0.60600	805(r),865(v),928(v),869(v) 917(v),796(r),825(r),927(g) 923(g),528(v),925(g),498(v) 393(v),733(v),802(r)
58. BD (1) C 20- C 23	1.97966	-0.65700	805(r),919(v),927(v),469(v) 825(r),924(g),485(v),917(g) 796(r),882(r)
59. BD (1) C 20- N 50	1.98126	-0.76235	805(r),796(r),882(r),825(r) 925(v),866(v),335(v),920(v) 735(g),467(g),923(g),818(r) 815(r),466(g),824(r),924(g) 505(v),461(g),503(v),846(r) 748(r),776(r),755(r),780(r) 848(r),638(r),188(r),777(r) 785(r),767(r),757(r),750(r) 759(r),764(r),763(r),772(r) 789(r)
60. BD (2) C 20- N 50	1.71962	-0.30257	147(v),864(v),918(v),334(v) 499(v),797(r),484(v),734(g) 805(r),853(r),850(r),861(r) 860(r),750(r),767(r),748(r) 852(r),776(r),777(r),858(r) 766(r),780(r),762(r),785(r) 759(r)
61. BD (1) C 21- C 23	1.98409	-0.66890	805(r),924(v),868(v),923(g) 365(v),867(g),453(v)
62. BD (2) C 21- C 23	1.66342	-0.25801	922(v),864(v),364(v),458(v)
63. BD (1) C 21- H 37	1.97829	-0.49755	923(v),863(v),498(v),363(v)
64. BD (1) C 22- C 25	1.97412	-0.62449	805(r),926(v),921(v),872(v) 927(g),545(v),455(v),869(g) 924(g),825(r),395(v)
65. BD (1) C 23- H 38	1.97410	-0.49499	921(v),867(v),453(v),805(r) 468(v)
66. BD (1) C 24- C 26	1.98460	-0.62510	805(r),871(v),933(v),530(v) 869(g),931(g),426(v)
67. BD (1) C 24- H 36	1.97665	-0.46147	928(v),869(v),805(r),423(v) 543(v)
68. BD (1) C 25- C 26	1.98339	-0.63379	924(v),930(v),805(r),925(g) 515(v),929(g),483(v)
69. BD (2) C 25- C 26	1.69282	-0.22632	147(v),932(v),514(v),484(v)
70. BD (1) C 25- H 39	1.97485	-0.47183	927(v),929(v),483(v),543(v) 805(r)
71. BD (1) C 26- H 40	1.97737	-0.46429	925(v),931(v),528(v),513(v)
78. CR (1) C 6	1.99945	-9.89695	676(v)
80. CR (1) C 8	1.99944	-9.90184	691(v)
84. CR (1) C 12	1.99935	-9.83915	921(v),365(v),363(v)
86. CR (1) C 14	1.99935	-9.79966	469(v),336(v),865(v),335(v)
88. CR (1) C 16	1.99908	-9.78226	425(v),485(v),925(v),924(v) 931(v),926(g),483(v)
90. CR (1) C 18	1.99930	-9.76181	395(v),926(v),515(v),929(v)
92. CR (1) C 20	1.99926	-9.84023	865(v),927(v),925(v),498(v) 483(v),735(v)
93. CR (1) C 21	1.99938	-9.80787	500(v),365(v),923(v)
94. CR (1) C 22	1.99918	-9.77704	923(v),395(v),926(v),530(v) 453(v),393(v),921(v),528(v)
95. CR (1) C 23	1.99929	-9.79887	469(v),455(v),924(v),921(v)
96. CR (1) C 24	1.99937	-9.77170	928(v),545(v),425(v),426(v)
97. CR (1) C 25	1.99930	-9.77514	545(v),485(v),927(v),924(v)
98. CR (1) C 26	1.99937	-9.76826	530(v),515(v),925(v)
101. CR (1) O 46	1.99980	-18.58851	243(v),882(v)
102. CR (1) O 47	1.99979	-18.58577	273(v),881(v)
105. CR (1) N 50	1.99947	-13.89392	882(r),335(v),453(v),455(v) 333(v)
124. CR (1)Ru 52	2.00000	-825.13895	
125. CR (2)Ru 52	2.00000	-114.72811	828(g),824(g),836(g),820(g) 885(v),880(v)
126. CR (3)Ru 52	1.99999	-21.89627	824(g),828(g),885(v),880(v) 836(g),805(g),820(g),797(g) 815(g),833(g),796(g),928(v) 810(g),926(g),812(g),865(r) 818(g),927(v),921(r),803(g) 811(g),825(g),807(g),848(r) 846(r),847(r),853(r),913(r)
127. CR (4)Ru 52	1.98735	-4.61241	885(v),880(v),928(v),243(v) 926(g),865(r),273(v),921(r) 927(v),828(g),833(g),805(g) 821(g),913(r),902(r)
128. CR (5)Ru 52	2.00000	-91.94240	
129. CR (6)Ru 52	2.00000	-28.66704	
130. CR (7)Ru 52	1.99242	-1.84537	882(g),881(g),885(v),880(v) 879(v),934(r)
131. CR (8)Ru 52	2.00000	-91.94220	
132. CR (9)Ru 52	2.00000	-28.66665	
133. CR (10)Ru 52	1.99491	-1.84707	825(g),881(g),926(g),805(g) 882(g),884(v),880(v),878(v) 934(r)
134. CR (11)Ru 52	2.00000	-91.94148	
135. CR (12)Ru 52	2.00000	-28.66563	
136. CR (13)Ru 52	1.99309	-1.84194	926(g),881(g),882(g),883(v) 880(v)
137. CR (14)Ru 52	2.00000	-10.09767	
138. CR (15)Ru 52	2.00000	-10.09661	
139. CR (16)Ru 52	2.00000	-10.09741	
140. CR (17)Ru 52	2.00000	-10.09690	
141. CR (18)Ru 52	2.00000	-10.09523	
147. LP (1) C 22	1.05144	-0.10580	167(v),922(v),870(v),529(v) 484(g),394(v),457(v),932(r)
152. LP (1) O 46	1.97792	-0.68287	805(r),243(v),882(v),796(r) 251(v),250(v),825(r)
153. LP (1) O 47	1.97818	-0.68793	273(v),805(r),881(v),825(r) 274(v),280(v),796(r)
156. LP (1) N 50	1.67087	-0.38031	882(r),805(r),796(r),825(r) 923(v),863(v),797(r),866(v) 453(v),333(v),824(r),926(r) 815(r),924(v),928(r),798(r) 818(r),801(r),879(r),811(r) 273(r),459(v),338(v),455(v) 880(r),820(r),833(r),807(r) 925(r),821(r),846(r),848(r)

				853(r),560(r),748(r),188(r)
				776(r),766(r),638(r),913(r)
				659(r),750(r),558(r),780(r)
				658(r)
160.	LP (1)Ru	52	1.77295	-0.20548 796(g),883(v),884(v),167(v)
				878(v),735(r),246(v),805(g)
				395(v),659(r),928(v),755(r)
				394(v),467(r),865(r),757(r)
				921(r),776(r),780(r),767(r)
				748(r),777(r),661(r),756(r)
				764(r),785(r),668(r),848(r)
				759(r),750(r),846(r),772(r)
				789(r),658(r),760(r),770(r)
				934(r),660(r),763(r),188(r)
				768(r),561(r),773(r),765(r)
				762(r),761(r),792(r),219(r)
				383(r),646(r),213(r),856(r)
				788(r),706(r),847(r),793(r)
				293(r),769(r),752(r),664(r)
				303(r),640(r),663(r),638(r)
				329(r)
161.	LP (2)Ru	52	1.71317	-0.20834 878(v),167(v),805(g),796(g)
				884(v),276(v),883(v),797(g)
				394(v),755(r),879(v),776(r)
				756(r),757(r),780(r),246(v)
				777(r),926(g),764(r),767(r)
				785(r),770(r),748(r),658(r)
				759(r),792(r),853(r),772(r)
				789(r),750(r),769(r),761(r)
				640(r),760(r),660(r),763(r)
				793(r),768(r),852(r),659(r)
				845(r),773(r),219(r),847(r)
				762(r),646(r),188(r),851(r)
				383(r),788(r),638(r),303(r)
				213(r),309(r),765(r),861(r)
				860(r),305(r),913(r),293(r)
				856(r),264(r),753(r),647(r)
				329(r),313(r),850(r),667(r)
				641(r),706(r),858(r),225(r)
				846(r),848(r),721(r),708(r)
				639(r),752(r),310(r),758(r)
				855(r),224(r),630(r),318(r)
				664(r),916(r),781(r)
162.	LP (3)Ru	52	1.66584	-0.22141 879(v),884(v),883(v),922(r)
				244(v),275(v),734(r),878(v)
				818(g),797(g),844(r),756(r)
				749(r),852(r)
167.	LP*(1) C	16	0.89449	-0.09213 147(v),932(v),424(v),394(g)
				881(v),484(v),922(r),805(v)
				870(r),488(v),853(r),861(r)
				850(r),860(r),852(r),912(r)
				858(r),776(r),777(r),780(r)
				769(r),785(r),755(r),761(r)
243.	RY*(1) C	6	0.01383	1.48453
244.	RY*(2) C	6	0.00533	0.86942
245.	RY*(3) C	6	0.00381	2.60103
246.	RY*(4) C	6	0.00295	1.60178
247.	RY*(5) C	6	0.00172	1.82233
248.	RY*(6) C	6	0.00149	2.33185
249.	RY*(7) C	6	0.00025	6.25755
250.	RY*(8) C	6	0.00010	3.87153
251.	RY*(9) C	6	0.00008	3.03832
252.	RY*(10) C	6	0.00009	2.62505
253.	RY*(11) C	6	0.00006	1.84138
254.	RY*(12) C	6	0.00003	2.65495
255.	RY*(13) C	6	0.00004	2.67899
256.	RY*(14) C	6	0.00000	45.39379
257.	RY*(15) C	6	0.00000	25.46942
273.	RY*(1) C	8	0.01434	1.35250
274.	RY*(2) C	8	0.00419	1.95777
275.	RY*(3) C	8	0.00407	0.97821
276.	RY*(4) C	8	0.00310	1.84838
277.	RY*(5) C	8	0.00188	1.88385
278.	RY*(6) C	8	0.00166	1.97527
279.	RY*(7) C	8	0.00022	4.33382
280.	RY*(8) C	8	0.00013	3.99823
281.	RY*(9) C	8	0.00009	2.77955
282.	RY*(10) C	8	0.00009	1.76165
283.	RY*(11) C	8	0.00005	3.43689
284.	RY*(12) C	8	0.00003	2.71411
285.	RY*(13) C	8	0.00003	2.61230
286.	RY*(14) C	8	0.00000	45.59659
287.	RY*(15) C	8	0.00000	26.60683
333.	RY*(1) C	12	0.00634	1.50011
334.	RY*(2) C	12	0.00511	0.65209
335.	RY*(3) C	12	0.00238	1.69969
336.	RY*(4) C	12	0.00135	1.30573
337.	RY*(5) C	12	0.00063	1.78196
338.	RY*(6) C	12	0.00031	2.77545
339.	RY*(7) C	12	0.00013	8.65339
340.	RY*(8) C	12	0.00011	4.20700
341.	RY*(9) C	12	0.00009	4.77582
342.	RY*(10) C	12	0.00009	2.37572
343.	RY*(11) C	12	0.00005	4.66817
344.	RY*(12) C	12	0.00002	2.62326
345.	RY*(13) C	12	0.00002	3.36097
346.	RY*(14) C	12	0.00000	40.06670
347.	RY*(15) C	12	0.00000	26.15028
363.	RY*(1) C	14	0.00281	1.67942
364.	RY*(2) C	14	0.00220	0.57431
365.	RY*(3) C	14	0.00111	1.85650
366.	RY*(4) C	14	0.00061	1.15245
367.	RY*(5) C	14	0.00035	1.81208
368.	RY*(6) C	14	0.00012	7.87718
369.	RY*(7) C	14	0.00010	3.73266
370.	RY*(8) C	14	0.00007	2.17842
371.	RY*(9) C	14	0.00004	3.14489
372.	RY*(10) C	14	0.00001	4.30678
373.	RY*(11) C	14	0.00002	2.67554
374.	RY*(12) C	14	0.00001	3.62810
375.	RY*(13) C	14	0.00000	25.00240
376.	RY*(14) C	14	0.00000	39.46694
377.	RY*(15) C	14	0.00001	6.59923
393.	RY*(1) C	16	0.00830	1.03860
394.	RY*(2) C	16	0.00746	0.60861
395.	RY*(3) C	16	0.00567	0.97188

396. RY*(4) C 16	0.00236	2.15356
397. RY*(5) C 16	0.00045	2.16911
398. RY*(6) C 16	0.00043	2.50405
399. RY*(7) C 16	0.00036	2.52957
400. RY*(8) C 16	0.00030	4.33261
401. RY*(9) C 16	0.00024	13.75692
402. RY*(10) C 16	0.00012	3.53994
403. RY*(11) C 16	0.00013	3.97440
404. RY*(12) C 16	0.00007	2.89469
405. RY*(13) C 16	0.00003	3.26697
406. RY*(14) C 16	0.00000	26.53375
407. RY*(15) C 16	0.00000	39.77919
423. RY*(1) C 18	0.00484	1.62135
424. RY*(2) C 18	0.00292	0.47080
425. RY*(3) C 18	0.00161	1.65062
426. RY*(4) C 18	0.00094	0.97893
427. RY*(5) C 18	0.00033	1.80517
428. RY*(6) C 18	0.00021	2.39840
429. RY*(7) C 18	0.00013	7.86698
430. RY*(8) C 18	0.00007	3.67284
431. RY*(9) C 18	0.00007	3.77453
432. RY*(10) C 18	0.00004	4.72609
433. RY*(11) C 18	0.00003	4.66849
434. RY*(12) C 18	0.00002	3.16630
435. RY*(13) C 18	0.00000	40.55771
436. RY*(14) C 18	0.00001	2.33264
437. RY*(15) C 18	0.00000	26.77984
453. RY*(1) C 20	0.00833	1.52168
454. RY*(2) C 20	0.00511	0.60142
455. RY*(3) C 20	0.00338	1.92095
456. RY*(4) C 20	0.00109	1.51588
457. RY*(5) C 20	0.00103	1.73007
458. RY*(6) C 20	0.00055	1.97699
459. RY*(7) C 20	0.00055	3.35197
460. RY*(8) C 20	0.00020	6.55845
461. RY*(9) C 20	0.00018	8.90968
462. RY*(10) C 20	0.00012	3.53233
463. RY*(11) C 20	0.00010	5.44512
464. RY*(12) C 20	0.00003	2.97276
465. RY*(13) C 20	0.00002	3.44541
466. RY*(14) C 20	0.00000	41.91461
467. RY*(15) C 20	0.00000	23.94290
468. RY*(1) C 21	0.00249	1.74387
469. RY*(2) C 21	0.00153	1.71945
470. RY*(3) C 21	0.00100	0.52900
471. RY*(4) C 21	0.00076	1.17551
472. RY*(5) C 21	0.00051	1.81067
473. RY*(6) C 21	0.00009	3.05722
474. RY*(7) C 21	0.00005	6.91659
475. RY*(8) C 21	0.00003	3.89026
476. RY*(9) C 21	0.00001	5.54769
477. RY*(10) C 21	0.00001	4.79608
478. RY*(11) C 21	0.00001	2.89046
479. RY*(12) C 21	0.00002	3.32838
480. RY*(13) C 21	0.00000	35.97075
481. RY*(14) C 21	0.00000	30.57715
482. RY*(15) C 21	0.00000	2.61863
483. RY*(1) C 22	0.00799	1.32833
484. RY*(2) C 22	0.00436	0.52822
485. RY*(3) C 22	0.00274	1.72767
486. RY*(4) C 22	0.00104	1.09615
487. RY*(5) C 22	0.00051	3.60851
488. RY*(6) C 22	0.00044	1.80119
489. RY*(7) C 22	0.00041	1.83784
490. RY*(8) C 22	0.00021	3.96077
491. RY*(9) C 22	0.00014	13.58449
492. RY*(10) C 22	0.00012	4.19138
493. RY*(11) C 22	0.00008	3.84726
494. RY*(12) C 22	0.00004	2.80446
495. RY*(13) C 22	0.00002	2.97114
496. RY*(14) C 22	0.00000	25.55774
497. RY*(15) C 22	0.00000	41.74951
498. RY*(1) C 23	0.00304	1.52141
499. RY*(2) C 23	0.00178	0.45940
500. RY*(3) C 23	0.00090	1.64585

(1) Analytical Frequencies

```
============================================================
=== CALCULATE ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ===
============================================================

                  -------------------------------------------------

                  This Analytical Second Derivatives Progam
                           was written for ADF by

                               Stephen K. Wolff

                         Scientific Computing & Modelling

                               Vrije University
                             Theoretical Chemistry
                               De Boelelaan 1083
                               1081 HV Amsterdam
                                The Netherlands

                  -------------------------------------------------
                               Date last modified:
                                    JUNE 2006


                                   References:
                                   ===========

                   Attila Berces, Ross M. Dickson, Liangyou Fan
                   Heiko Jacobsen, David Swerhone, Tom Ziegler,
                   Computer Physics Communications 100 (1997) 247.

                   Heiko Jacobsen, Attila Berces
```

```
   David Swerhone, Tom Ziegler,
   Computer Physics Communications 100 (1997) 263.

   Stephen K. Wolff
   Int. J. Quantum Chem. 104 (2005) 645.

  -----------------------------------------------

<><><><><><><><><><><><><><><><><><><><><><><><><>

  SECOND DERIVATIVES INFORMATION:
  -------------------------------

  === PRINT

    EIGS,  lprint_eigbas =  F
    U1,    lprint_u1     =  F
    PARTS, lprint_parts  =  F

  === DEBUG

    ALL        =  F
    B1         =  F
    DENSITIES  =  F
    FIT        =  F
    HESSIAN    =  F
    NUMBERS    =  F
    SYMMETRY   =  F
    U1         =  F

  === CPKS

    MAX_CPKS_ITERATIONS    =    20
    U1_ACCURACY PARAMETER  =     5.00
    U1 ACCURACY            =     0.0000100

<><><><><><><><><><><><><><><><><><><><><><><><><>
```

Number of elements of the density matrix on this node (used, total):   110446   436645

List of All Frequencies:

Intensities
===========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
19.543396	0.000000	0.000000
24.708185	41.454678	0.256739
29.956414	149.349202	1.121426
34.334230	43.252524	0.372235
41.785282	1.316679	0.013791
59.727368	6.361891	0.095244
63.006077	2.320333	0.036645
68.406642	5.044096	0.086489
73.323142	4.477301	0.082288
83.848440	45.265688	0.951354
85.616706	6.526972	0.140071
88.840392	3.174013	0.070680
91.200764	27.219689	0.622243
93.705992	43.004140	1.010080
100.696657	62.253143	1.571283
107.994957	6.234802	0.168773
114.367145	15.936527	0.456849
123.348358	3.649308	0.112829
129.621138	6.776412	0.220168
180.961776	12.299711	0.557904
182.986214	4.229080	0.193973
189.602080	1.575466	0.074874
202.157481	18.796257	0.952444
218.282884	17.574005	0.961543
239.926618	33.964145	2.042571
248.667615	33.835153	2.108946
251.022802	153.338484	9.648114
253.636264	60.880104	3.870480
262.814571	4.372046	0.288013
268.019960	23.757495	1.596048
284.125315	20.228845	1.440652
286.669315	4.042982	0.290510
326.693063	360.519391	29.522057
364.374559	242.636193	22.160609
365.564672	18.955368	1.736899
376.471843	1132.546331	106.872643
409.577989	87.261143	8.958506
415.069798	49.372097	5.136660
419.058230	108.023402	11.346719
423.668468	10.567088	1.122172
430.797352	176.823073	19.093697
466.681306	8.437757	0.987019
467.800756	13.944298	1.635067
469.542689	12.863722	1.513979
473.661901	16.657576	1.977690
480.716443	12.012565	1.447447
482.291259	6.077769	0.734737
514.490496	78.314025	10.099386
515.393515	11.042619	1.426557
519.929496	96.203102	12.537519
522.968252	83.128963	10.896970
543.023714	37.126288	5.053339
545.349004	41.870124	5.723436
552.718931	7.198719	0.997327
557.741704	7.260112	1.014973
595.269410	100.416484	14.982926
596.815755	91.752392	13.725739
626.802349	33.384159	5.245044
627.094422	31.390534	4.934120
633.988422	199.762954	31.744928
635.322096	21.857863	3.480805
643.131107	16.037999	2.585400
644.094388	21.291088	3.437363
661.019698	4.696720	0.778193

661.467741	20.416933	3.385145
712.670415	32.064975	5.727930
714.407389	31.229450	5.592273
721.940685	139.653227	25.271473
723.302966	100.636745	18.245463
736.039749	377.429292	69.632974
741.925291	369.572827	68.728723
756.846182	1.266304	0.240228
756.953665	2.973468	0.564171
778.456525	12.015067	2.344437
783.745629	26.704186	5.246051
784.230975	43.915050	8.632477
843.365824	2.542464	0.537463
844.243031	3.649757	0.772342
855.401785	4.772057	1.023184
863.888324	6.716052	1.454286
920.572915	0.478578	0.110430
920.727556	0.188586	0.043523
931.117337	3.851339	0.898865
960.855396	0.910193	0.219215
961.210179	0.349496	0.084205
966.206642	6.529215	1.581281
970.032506	0.278060	0.067609
982.174082	18.629925	4.586460
1001.047760	21.743155	5.455762
1003.265426	20.784709	5.226824
1007.522492	102.839040	25.971129
1008.530594	89.414568	22.603486
1018.519587	22.615236	5.773625
1019.392150	10.070199	2.573104
1044.588303	5.978481	1.565359
1048.669094	5.900318	1.550929
1052.404964	53.775955	14.185645
1053.101567	35.067504	9.256636
1097.552277	5.383339	1.481000
1100.308542	9.865009	2.720759
1116.261171	2.027324	0.567240
1118.075117	1.032162	0.289266
1150.236809	17.520519	5.051406
1151.247882	12.547785	3.620879
1157.445264	20.432828	5.927984
1158.275342	20.722765	6.016412
1234.979821	6.511505	2.015669
1235.477726	30.654966	9.493226
1266.328413	54.582545	17.325198
1269.095902	49.465778	15.735384
1287.020236	9.171854	2.958834
1288.897435	5.648968	1.825011
1299.513603	71.177426	23.184684
1299.794663	28.079632	9.148381
1311.286606	7.062372	2.321273
1314.535278	17.024419	5.609480
1411.029525	59.952693	21.204247
1412.752003	44.339367	15.701223
1427.656057	9.804737	3.508630
1428.565164	8.204466	2.937842
1441.256469	22.625313	8.173610
1444.204525	34.369657	12.441764
1465.325316	209.656419	77.005241
1467.795792	192.776714	70.924826
1540.689492	26.090493	10.075706
1541.006631	28.705914	11.088019
1555.044216	78.560054	30.621227
1555.675837	72.071272	28.103432
1570.960989	103.003655	40.559828
1572.184960	117.224778	46.195655
1592.958240	133.879925	53.456180
1594.496934	139.281103	55.666505
1928.911602	1256.616488	607.565562
1933.743433	1367.650659	662.906231
1990.120240	1710.920101	853.467751
1995.907752	1085.555613	543.088507
3081.741886	1.798427	1.389207
3082.993255	1.589595	1.228392
3090.679949	9.935450	7.696967
3091.328450	9.020422	6.989564
3096.912544	28.321130	21.984550
3101.935435	3.238378	2.517899
3102.452862	10.800536	8.399019
3104.096646	12.281479	9.555732
3104.764752	12.276533	9.553940
3114.263083	5.236620	4.087751
3116.507780	44.475035	34.742621
3117.480568	42.624889	33.307734
3130.181373	4.489158	3.522188
3133.793341	5.269367	4.139109
3136.459276	8.034499	6.316501
3139.292938	4.058779	3.193783
3698.479042	13.333560	12.360822

```
============================
Statistical Thermal Analysis  ***  ideal gas assumed  ***
============================

Pressure:                 1.000000 atm.
Temperature:            298.150000 K


Moments of Inertia (and direction vectors)
========================================

      13056.8254      23531.1792      26602.5978
-------------------------------------------------
         -0.5685          0.6364          0.5214
         -0.7474         -0.6643         -0.0040
          0.3438         -0.3919          0.8533


The rotational contribution to the molecular entropy includes
a term, dependent on the symmetry number sigma. The results
reported below were computed using sigma = 1, determined
from the point group symmetry of the input geometry (NOSYM).
If this is not the correct symmetry, please contact SCM to
```

report a bug.

Temp		Transl	Rotat	Vibrat	Total
298.15	Entropy (cal/mole-K):	45.414	37.345	126.614	209.373
	Internal Energy (Kcal/mole):	0.889	0.889	245.087	246.864
	Constant Volume Heat Capacity (cal/mole-K):	2.981	2.981	121.056	127.018

****

==========
*** DONE CALCULATING ANALYTICAL SECOND DERIVATIVES OF THE ENERGY ***
==========

==========
SCAN POTENTIAL ENERGY SURFACE ALONG A RANGE OF NORMAL MODES *** with IR intensities ***
==========

RANGE OF FREQUENCIES: from -1000.000 to 0.000

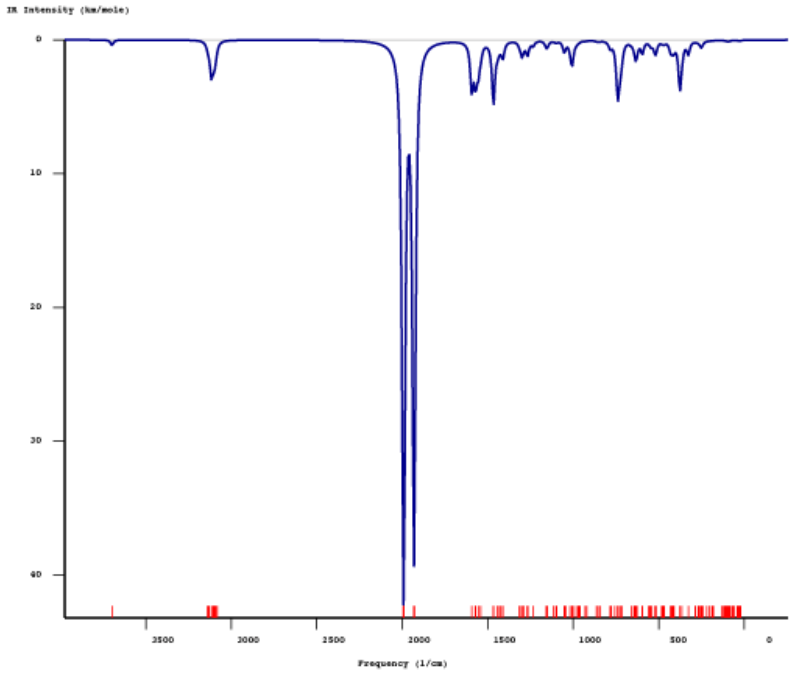
==========
Vibration symmetry: *** A ***
==========

Total number of frequencies of this symmetry: 153
Frequencies, cm^(-1):

19.543	24.708	29.956	34.334	41.785	59.727	63.006	68.407
73.323	83.848	85.617	88.840	91.201	93.706	100.697	107.995
114.367	123.348	129.621	180.962	182.986	189.602	202.157	218.283
239.927	248.668	251.023	253.636	262.815	268.020	284.125	286.669
326.693	364.375	365.565	376.472	409.578	415.070	419.058	423.668
430.797	466.681	467.801	469.543	473.662	480.716	482.291	514.490
515.394	519.929	522.968	543.024	545.349	552.719	557.742	595.269
596.816	626.802	627.094	633.988	635.322	643.131	644.094	661.020
661.468	712.670	714.407	721.941	723.303	736.040	741.925	756.846
756.954	778.457	783.746	784.231	843.366	844.243	855.402	863.888
920.573	920.728	931.117	960.855	961.210	966.207	970.033	982.174
1001.048	1003.265	1007.522	1008.531	1018.520	1019.392	1044.588	1048.669
1052.405	1053.102	1097.552	1100.309	1116.261	1118.075	1150.237	1151.248
1157.445	1158.275	1234.980	1235.478	1266.328	1269.096	1287.020	1288.897
1299.514	1299.795	1311.287	1314.535	1411.030	1412.752	1427.656	1428.565
1441.256	1444.205	1465.325	1467.796	1540.689	1541.007	1555.044	1555.676
1570.961	1572.185	1592.958	1594.497	1928.912	1933.743	1990.120	1995.908
3081.742	3082.993	3090.680	3091.328	3096.913	3101.935	3102.453	3104.097
3104.765	3114.263	3116.508	3117.481	3130.181	3133.793	3136.459	3139.293
3698.479							

Number of frequencies in the requested range: 0

(2) Computed IR spectrum



d) *ax-ax*-3c geometry optimization using dispersion corrected Becke-Perdew functional BP-D and the TZP(ZORA) basis set.

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2008.01   September 22, 2008  *
*  ------------------------------------                                     *
*                                          Build 200809251856               *
*                                                                           *
*                                                                           *
*                               =================                           *
*                               |               |                           *
*                               |     A D F     |                           *
*                               |               |                           *
*                               =================                           *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*************************  pentium_linux_ifc / hpmpi  **************************

 ADF 2008.01  RunTime: Sep29-2008 11:48:56

 Temporary files are created in /tmp/kid_0.MRnoCk

 axial-OH


 ============================
 A T T A C H E D   F I L E S
 ============================



 ================================
 M O D E L   P A R A M E T E R S
 ================================

 DENSITY FUNCTIONAL POTENTIAL (scf)
    LDA:                          VWN
    Gradient Corrections:         Becke88 Perdew86                    == Not Default ==

 SPIN  (restricted / unrestr.)
    Molecule:                     Restricted
    Fragments:                    Restricted

 OTHER ASPECTS
    Relativistic Corrections:     scalar (ZORA,SAPA)                   *** SPECIAL ***
    Core Treatment:               Frozen Orbital(s)

    Electric Field:               ---

    Hyperfine or Zeeman Interaction:   ---

    Empirical Dispersion Correction included with factor    1.05000

    Van der Waals Radii used in dispersion are scaled by    1.10000


Geometry CYCLE 20
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ------------------------------------------
     1 C    -0.000033 -0.000037 -0.000039
     2 H    -0.000033  0.000008 -0.000030
     3 O     0.000070 -0.000095  0.000061
     4 C    -0.000050 -0.000011  0.000035
     5 C     0.000035  0.000031 -0.000026
     6 Cl    0.000238  0.000095  0.000039
     7 C     0.000091  0.000074 -0.000167
     8 N     0.000038 -0.000036 -0.000038
     9 O    -0.000162  0.000121 -0.000043
    10 C    -0.000006  0.000020  0.000075
    11 O     0.000080  0.000009  0.000206
    12 H    -0.000015  0.000004  0.000034
    13 C     0.000005 -0.000028 -0.000044
    14 C     0.000009  0.000036 -0.000029
    15 C    -0.000025 -0.000098 -0.000183
    16 Ru    0.000034 -0.000128  0.000289
    17 H    -0.000028 -0.000002 -0.000009
    18 Ru    0.000256  0.000241  0.000327
    19 C     0.000024 -0.000021  0.000048
    20 C    -0.000121 -0.000574  0.000000
    21 C    -0.000009 -0.000129  0.000015
    22 C     0.000025  0.000000  0.000000
    23 O    -0.000646  0.000082 -0.000276
    24 H     0.000005  0.000036 -0.000049
    25 H     0.000012  0.000014 -0.000023
    26 C     0.000038  0.000063 -0.000106
    27 O     0.000128  0.000209 -0.000129
    28 N    -0.000182  0.000074  0.000111
    29 H     0.000033  0.000040 -0.000064
    30 C     0.000000 -0.000039 -0.000077
    31 C     0.000007  0.000127 -0.000005
    32 H     0.000047  0.000078 -0.000040
    33 C     0.000034  0.000047 -0.000008
    34 C    -0.000035 -0.000006 -0.000029
    35 C    -0.000043  0.000027 -0.000004
```

```
    36 C    -0.000027  0.000030  0.000081
    37 H     0.000039 -0.000052  0.000049
    38 C    -0.000073 -0.000087 -0.000015
    39 C    -0.000050 -0.000041  0.000005
    40 H     0.000002 -0.000037  0.000035
    41 C    -0.000048 -0.000038  0.000042
    42 C    -0.000011 -0.000003 -0.000014
    43 C    -0.000008 -0.000054 -0.000019
    44 H    -0.000040 -0.000031 -0.000013
    45 H    -0.000012  0.000013  0.000005
    46 C     0.000061 -0.000016 -0.000022
    47 H     0.000001  0.000053 -0.000023
    48 C     0.000037  0.000014 -0.000007
    49 H     0.000042 -0.000007  0.000026
    50 H     0.000008 -0.000017  0.000036
    51 H    -0.000029  0.000044 -0.000017
    52 H    -0.000003  0.000012  0.000008
    53 H     0.000292 -0.000015  0.000022
 ----------------------------------------

------------------------------------
Geometry Convergence after Step  20
------------------------------------
current energy                              -13.40385505 Hartree
abs of energy change              0.00001380     0.00100000    T
constrained gradient max          0.00064628     0.00100000    T
constrained gradient rms          0.00010746     0.00066667    T
gradient max                      0.00064628
gradient rms                      0.00010746
cart. step max                    0.00789063     0.01000000    T
cart. step rms                    0.00255033     0.00666667    T


 Number of elements of the density matrix on this node (used, total):     54137    436645


 ======================================================
 Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
 ======================================================

 General Accuracy Parameter :                          4.50

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
    Nr. of used Symmetry Operators                     1

    Points in the Atomic Spheres                   34100
    Points in the Atomic Polyhedra                341667
    Points in the Outer Region                     30039
    ----------------------------------------------------
    Total                                         405806

    Sum of Weights                                159644.737003

 Total nr. of points:     405806
 Nr. of blocks:             3171
 Block length:               128
 Nr. of dummy points:         82


 Test of Precision of the Numerical Integration Grid
 ===================================================

 Integral of the Total Core Density:                   0.00000000000000

============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

                                        hartree             eV         kcal/mol          kJ/mol
                                ---------------------  -----------  ----------  -----------

Pauli Repulsion
  Kinetic (Delta T^0):           155.940740394113561     4243.3634     97854.30     409422.36
  Delta V^Pauli Coulomb:        -81.358429163581349    -2213.8755    -51053.19    -213606.53
  Delta V^Pauli LDA-XC:         -19.263983398197382     -524.1997    -12088.33     -50577.58
  Delta V^Pauli GGA-Exchange:     1.121596797437739       30.5202       703.81       2944.75
  Delta V^Pauli GGA-Correlation:  -0.315335931120833       -8.5807      -197.88       -827.91
                                ---------------------  -----------  ----------  -----------
  Total Pauli Repulsion:         56.124588698651735     1527.2278     35218.71     147355.09
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  56.124588698651735     1527.2278     35218.71     147355.09
  Electrostatic Interaction:       -11.959020744807901     -325.4215     -7504.40     -31398.40
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                ---------------------  -----------  ----------  -----------
```

Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	44.165567953843833	1201.8063	27714.32	115956.68
Orbital Interactions				
A:	-57.453395408670453	-1563.3864	-36052.55	-150843.87
Total Orbital Interactions:	-57.458310816425708	-1563.5202	-36055.64	-150856.77
Alternative Decomposition Orb.Int.				
Kinetic:	-143.252166157953354	-3898.0898	-89892.10	-376108.51
Coulomb:	79.025462496355416	2150.3922	49589.23	207481.32
XC:	6.768392845172219	184.1773	4247.23	17770.41
Total Orbital Interactions:	-57.458310816425723	-1563.5202	-36055.64	-150856.77
Residu (E=Steric+OrbInt+Res):	0.000007489838925	0.0002	0.00	0.02
Dispersion Energy:	-0.111119996685867	-3.0237	-69.73	-291.75
Total Bonding Energy:	-13.403855369428817	-364.7375	-8411.05	-35191.82

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	-11.959020744807901	-325.4215	-7504.40	-31398.40
Kinetic Energy:	12.688574236160207	345.2737	7962.20	33313.85
Coulomb (Steric+OrbInt) Energy:	-2.332959177387011	-63.4830	-1463.95	-6125.18
XC Energy:	-11.689329686708255	-318.0828	-7335.17	-30690.33
Dispersion Energy:	-0.111119996685867	-3.0237	-69.73	-291.75
Total Bonding Energy:	-13.403855369428827	-364.7375	-8411.05	-35191.82

Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree): -0.0134530474
2. Electrostatic (Fit correction): 0.0000000000

Scaled ZORA energy correction, not included in bonding energy (hartree): -523.7497653635
WARNING: This scaled ZORA energy correction should only be used to compare two calculations in which the only difference in the calculation is the electron configuration. Then the difference in energy of this term should be added to the difference in energy of the two electron configurations. This term should not be used otherwise. In practice it is useful only for core excitation energy calculations.

FRAGMENT ENERGY TERMS *** (summed over all fragments) ***

The energy terms below are (parts of) the Total Energy of the fragments from which the molecule is built.

Exchange and Correlation				
Exchange LDA:	-441.223520222119191	-12006.3029	-276871.97	-1158432.19
Exchange GGA:	-37.432103212619360	-1018.5794	-23489.00	-98277.97
Correlation LDA:	-23.634037647907569	-643.1149	-14830.58	-62051.16
Correlation GGA:	11.032317242403911	300.2046	6922.88	28965.34
Total XC:	-491.257343840242243	-13367.7925	-308268.67	-1289795.97

BOND-ORDER ANALYSIS

		DIST. [A]	BOND-ORDERS (THRESHOLD = 0.010)				
			MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
C	1 - C 4	1.3911	1.4222	1.4313	1.4887	1.4787	1.5263
C	1 - C 5	1.3992	1.3590	1.4026	1.4609	1.4257	1.5182
C	1 - N 8	2.3994	0.0189	0.0244	0.0258	-0.0169	0.0272
C	1 - C 10	2.4076	0.0083	0.0098	0.0102	-0.0246	0.0107
C	1 - H 12	3.3992	0.0011	0.0145	0.0152	0.0483	0.0143
C	1 - C 14	2.7787	0.0594	0.0939	0.0971	0.1249	0.0976
C	1 - Ru 16	4.4496	0.0040	0.0109	0.0120	0.1236	0.0116
C	1 - C 21	4.9780	0.0143	0.0137	0.0140	-0.0095	0.0146
C	1 - C 26	5.1874	0.0132	0.0131	0.0136	-0.0178	0.0142
C	1 - C 36	7.0231	0.0114	0.0126	0.0132	-0.0181	0.0137
C	1 - H 52	1.0888	1.0285	0.9227	0.9700	0.9852	0.9044
H	2 - C 4	1.0893	1.0132	0.8960	0.9361	0.9233	0.8526
H	2 - C 5	3.4035	-0.0005	0.0132	0.0138	0.0382	0.0128
H	2 - Cl 6	2.5547	0.0404	0.0252	0.0309	0.1147	0.0342
H	2 - C 14	3.3074	0.0045	0.0153	0.0160	-0.0119	0.0142
O	3 - Cl 6	4.2711	0.0046	0.0088	0.0113	-0.0997	0.0138
O	3 - C 7	1.1639	2.0415	2.1885	2.3668	2.3773	2.4102
O	3 - Ru 16	3.0431	0.2151	0.2487	0.2888	0.4137	0.2848
O	3 - C 20	3.5591	0.0078	0.0186	0.0201	0.0615	0.0205
O	3 - C 21	3.7336	-0.0013	0.0093	0.0101	-0.0187	0.0107
O	3 - O 23	5.1492	0.0051	0.0127	0.0158	-0.1611	0.0188
C	4 - C 5	2.3960	0.0273	0.0137	0.0142	0.0120	0.0145
C	4 - Cl 6	3.3344	-0.0024	0.0189	0.0231	0.0134	0.0275
C	4 - N 8	1.3470	1.3763	1.3974	1.4737	1.4603	1.5205
C	4 - C 10	2.7406	0.0631	0.1074	0.1116	0.1083	0.1143
C	4 - C 14	2.3515	0.0301	0.0143	0.0148	0.0172	0.0145
C	4 - Ru 16	3.1419	-0.0028	0.0152	0.0167	0.0257	0.0158
C	4 - C 19	3.6430	0.0071	0.0136	0.0141	0.0136	0.0142

C	4 - H	51	3.3934	0.0032	0.0143	0.0150	0.0177	0.0137
C	5 - N	8	2.7786	0.0388	0.0940	0.0993	0.0694	0.1038
C	5 - C	10	1.3904	1.4113	1.4660	1.5260	1.4931	1.5835
C	5 - C	14	2.4212	0.0417	0.0124	0.0128	0.0322	0.0127
C	5 - C	19	3.7953	0.0075	0.0167	0.0173	0.0132	0.0177
C	5 - H	51	1.0909	1.0272	0.9239	0.9688	0.9751	0.8984
Cl	6 - C	7	3.4035	0.0043	0.0231	0.0278	0.1171	0.0325
Cl	6 - O	9	4.2632	0.0049	0.0091	0.0116	-0.1037	0.0141
Cl	6 - O	11	4.2869	0.0049	0.0092	0.0118	-0.0997	0.0144
Cl	6 - C	13	3.3653	0.0080	0.0259	0.0312	0.1206	0.0364
Cl	6 - C	15	3.4083	0.0047	0.0241	0.0290	0.1173	0.0338
Cl	6 - Ru	16	2.5884	0.4365	0.2589	0.3325	0.5660	0.3753
Cl	6 - H	17	2.5533	0.0379	0.0257	0.0315	0.1159	0.0349
Cl	6 - Ru	18	2.5760	0.4417	0.2654	0.3413	0.5741	0.3852
Cl	6 - C	20	3.3871	0.0092	0.0251	0.0302	0.1098	0.0353
Cl	6 - C	21	4.6109	0.0541	0.1067	0.1287	0.0605	0.1548
Cl	6 - C	22	3.3298	0.0008	0.0194	0.0236	0.0141	0.0281
Cl	6 - O	23	3.0814	-0.0098	0.0105	0.0144	-0.3344	0.0188
Cl	6 - O	27	4.3034	0.0046	0.0086	0.0111	-0.1075	0.0135
Cl	6 - C	33	4.5896	0.0542	0.1080	0.1303	0.0594	0.1567
C	7 - N	8	2.9260	0.0265	0.0278	0.0289	0.0718	0.0291
C	7 - Ru	16	1.8793	1.0809	1.0869	1.1811	1.0211	1.0829
C	7 - C	20	2.6425	0.0880	0.0737	0.0742	0.0387	0.0704
C	7 - C	21	2.8439	0.0622	0.0474	0.0478	0.0714	0.0473
C	7 - O	23	3.9872	0.0601	0.1332	0.1564	0.2834	0.1777
C	7 - O	27	3.5279	0.0086	0.0187	0.0202	0.0695	0.0207
N	8 - C	10	2.3969	0.0152	0.0161	0.0170	-0.0227	0.0179
N	8 - H	12	3.3776	0.0132	0.0136	0.0145	0.0521	0.0137
N	8 - C	14	1.3661	1.2918	1.3060	1.3700	1.3898	1.3870
N	8 - Ru	16	2.1613	0.2515	0.3294	0.3687	0.4818	0.3583
N	8 - C	19	2.3853	0.0146	0.0208	0.0219	0.0150	0.0227
N	8 - C	20	4.0215	0.0437	0.1182	0.1228	0.1603	0.1236
N	8 - C	21	2.6856	0.0293	0.0302	0.0315	0.0045	0.0329
N	8 - O	23	2.7658	0.0024	0.0123	0.0149	-0.1500	0.0176
N	8 - C	26	3.7008	0.0193	0.0315	0.0332	-0.0028	0.0348
N	8 - C	36	4.9650	0.0108	0.0125	0.0132	-0.0224	0.0138
N	8 - H	52	3.3735	0.0123	0.0141	0.0150	0.0555	0.0141
O	9 - C	13	1.1650	2.0076	2.1748	2.3545	2.3651	2.4015
O	9 - C	15	3.5285	0.0084	0.0181	0.0196	0.0671	0.0200
O	9 - Ru	18	3.0395	0.2258	0.2504	0.2915	0.4215	0.2879
O	9 - O	23	3.8121	0.0042	0.0073	0.0092	-0.1738	0.0109
C	10 - H	12	1.0878	1.0180	0.9218	0.9637	0.9770	0.9032
C	10 - C	14	1.4050	1.3710	1.3466	1.3923	1.4098	1.3979
C	10 - Ru	16	4.3415	0.0049	0.0104	0.0114	0.1156	0.0110
C	10 - C	19	2.5439	0.0100	0.0101	0.0105	0.0049	0.0107
C	10 - C	21	3.7866	0.0240	0.0331	0.0339	0.0119	0.0352
C	10 - C	26	3.0262	0.0197	0.0173	0.0180	-0.0114	0.0187
C	10 - C	36	5.2169	0.0115	0.0123	0.0128	-0.0164	0.0133
C	10 - H	52	3.4078	0.0022	0.0143	0.0150	0.0482	0.0139
O	11 - C	13	3.5618	0.0077	0.0176	0.0191	0.0656	0.0194
O	11 - C	15	1.1642	2.0403	2.1861	2.3642	2.3745	2.4086
O	11 - Ru	18	3.0429	0.2150	0.2505	0.2914	0.4169	0.2873
O	11 - O	23	5.1620	0.0045	0.0119	0.0149	-0.1628	0.0177
O	11 - C	33	3.7490	-0.0010	0.0095	0.0103	-0.0199	0.0109
C	13 - C	15	2.6424	0.0894	0.0720	0.0724	0.0331	0.0685
C	13 - Ru	18	1.8766	1.0643	1.0909	1.1877	1.0267	1.0886
C	13 - O	23	2.8926	0.0172	0.0266	0.0313	0.1743	0.0355
C	13 - N	28	4.0248	0.0429	0.1186	0.1234	0.1670	0.1240
C	13 - C	33	2.8711	0.0755	0.0405	0.0409	0.0657	0.0405
C	14 - Ru	16	2.9910	-0.0006	0.0176	0.0193	-0.0671	0.0179
C	14 - C	19	1.4605	1.1697	1.1004	1.1333	1.1347	1.1172
C	14 - C	21	2.4583	0.0415	0.0119	0.0121	0.0300	0.0120
C	14 - C	26	2.5148	0.0240	0.0110	0.0113	0.0353	0.0114
C	14 - C	31	3.7409	0.0103	0.0126	0.0130	0.0395	0.0130
C	14 - C	34	3.7847	0.0110	0.0163	0.0169	0.0439	0.0170
C	14 - H	51	3.4118	0.0046	0.0145	0.0151	-0.0119	0.0135
C	15 - Ru	18	1.8789	1.0839	1.0932	1.1900	1.0307	1.0912
C	15 - O	23	3.9983	0.0569	0.1313	0.1542	0.2801	0.1753
C	15 - N	28	2.9066	0.0272	0.0280	0.0291	0.0733	0.0293
C	15 - C	33	2.8599	0.0638	0.0470	0.0474	0.0718	0.0469
Ru	16 - Ru	18	3.5002	0.0239	0.0114	0.0133	-0.3245	0.0119
Ru	16 - C	19	2.9442	-0.0068	0.0262	0.0288	0.0457	0.0273
Ru	16 - C	20	1.8714	1.1042	1.1103	1.2055	1.0575	1.1083
Ru	16 - C	21	2.0591	0.6389	0.7510	0.8172	0.8588	0.7812
Ru	16 - O	23	2.1152	0.3667	0.3318	0.4161	0.7887	0.4573
Ru	16 - C	26	4.2940	0.0114	0.0171	0.0189	0.1124	0.0181
Ru	16 - O	27	3.0349	0.2304	0.2582	0.3002	0.4337	0.2969
Ru	16 - C	31	3.1235	0.0054	0.0270	0.0298	0.1331	0.0287
Ru	16 - C	34	4.8864	0.0133	0.0115	0.0127	0.1187	0.0122
Ru	16 - C	36	4.4123	0.0121	0.0204	0.0224	0.1153	0.0216
H	17 - C	22	1.0893	1.0126	0.8949	0.9352	0.9220	0.8510
H	17 - C	38	3.3076	0.0046	0.0154	0.0160	-0.0097	0.0142
H	17 - C	39	3.4039	-0.0001	0.0132	0.0138	0.0382	0.0128
Ru	18 - C	22	3.1353	-0.0046	0.0167	0.0184	0.0271	0.0174
Ru	18 - O	23	2.1200	0.3377	0.3234	0.4062	0.7805	0.4463
Ru	18 - N	28	2.1569	0.2634	0.3340	0.3747	0.4925	0.3645
Ru	18 - C	30	4.4450	0.0042	0.0109	0.0121	0.1220	0.0117
Ru	18 - C	33	2.0568	0.6292	0.7492	0.8170	0.8615	0.7814
Ru	18 - C	35	3.1202	0.0020	0.0267	0.0295	0.1279	0.0284
Ru	18 - C	38	2.9950	0.0011	0.0185	0.0203	-0.0588	0.0189
Ru	18 - C	41	2.9461	-0.0031	0.0259	0.0286	0.0535	0.0270
Ru	18 - C	42	4.3454	0.0045	0.0102	0.0113	0.1174	0.0109
Ru	18 - C	43	4.4078	0.0122	0.0208	0.0229	0.1140	0.0220
Ru	18 - C	46	4.2963	0.0107	0.0168	0.0185	0.1142	0.0178
Ru	18 - C	48	4.8849	0.0129	0.0112	0.0123	0.1181	0.0119
C	19 - C	21	1.4223	1.3399	1.3146	1.3437	1.3373	1.3688
C	19 - C	26	1.4083	1.3435	1.3469	1.3958	1.3862	1.4284
C	19 - H	32	3.4195	0.0141	0.0142	0.0147	0.0196	0.0136
C	19 - C	34	2.4324	0.0343	0.0116	0.0120	0.0063	0.0123
C	19 - C	36	2.7968	0.0538	0.0933	0.0967	0.0914	0.0989
C	19 - H	37	3.4210	0.0065	0.0143	0.0149	0.0199	0.0138
C	20 - C	21	2.8453	0.0729	0.0428	0.0431	0.0643	0.0427
C	20 - O	23	2.9987	0.0163	0.0296	0.0347	0.1616	0.0396
C	20 - O	27	1.1670	1.9925	2.1547	2.3317	2.3396	2.3881
C	21 - O	23	2.8824	0.0007	0.0214	0.0252	-0.0681	0.0295
C	21 - H	24	3.4462	0.0063	0.0146	0.0150	0.0336	0.0140
C	21 - C	26	2.4577	0.0132	0.0125	0.0128	-0.0070	0.0132
C	21 - C	31	1.4055	1.4088	1.4165	1.4513	1.4210	1.5049
C	21 - C	34	2.8380	0.0418	0.0994	0.1020	0.0791	0.1058
C	21 - C	36	2.4439	0.0209	0.0125	0.0128	-0.0069	0.0133
C	21 - H	40	3.4268	0.0044	0.0145	0.0149	0.0354	0.0139
C	22 - N	28	1.3475	1.3755	1.3932	1.4699	1.4558	1.5184
C	22 - C	30	1.3903	1.4205	1.4313	1.4885	1.4789	1.5256
C	22 - C	38	2.3527	0.0294	0.0144	0.0149	0.0170	0.0147
C	22 - C	39	2.3956	0.0279	0.0141	0.0146	0.0125	0.0149
C	22 - C	41	3.6413	0.0069	0.0136	0.0140	0.0133	0.0141

C	22 - C	42	2.7417	0.0632	0.1065	0.1107	0.1073	0.1133
C	22 - H	45	3.3925	0.0033	0.0143	0.0150	0.0176	0.0137
O	23 - O	27	3.9457	0.0035	0.0075	0.0093	-0.1789	0.0111
O	23 - N	28	2.9207	0.0027	0.0086	0.0104	-0.1604	0.0123
O	23 - C	33	2.8630	0.0061	0.0239	0.0281	-0.0695	0.0330
O	23 - H	53	0.9778	1.1226	0.8467	1.0638	1.1536	1.0465
H	24 - C	26	1.0904	1.0266	0.9266	0.9632	0.9740	0.9094
H	24 - C	36	3.3992	0.0031	0.0147	0.0153	0.0401	0.0145
H	25 - N	28	3.3728	0.0120	0.0142	0.0151	0.0575	0.0142
H	25 - C	30	1.0887	1.0280	0.9221	0.9696	0.9844	0.9030
H	25 - C	42	3.4080	0.0022	0.0143	0.0150	0.0490	0.0140
C	26 - C	31	2.7958	0.0599	0.1086	0.1128	0.0828	0.1175
C	26 - C	34	1.3931	1.4085	1.4619	1.5213	1.4804	1.5846
C	26 - C	36	2.4133	0.0102	0.0096	0.0100	-0.0163	0.0104
C	26 - H	40	3.4037	0.0043	0.0145	0.0152	0.0426	0.0142
N	28 - C	30	2.3990	0.0187	0.0239	0.0253	-0.0184	0.0267
N	28 - C	33	2.6779	0.0235	0.0301	0.0313	0.0021	0.0328
N	28 - C	38	1.3673	1.2854	1.3024	1.3669	1.3850	1.3876
N	28 - C	39	2.7785	0.0388	0.0925	0.0978	0.0669	0.1023
N	28 - C	41	2.3829	0.0103	0.0216	0.0227	0.0124	0.0236
N	28 - C	42	2.3979	0.0138	0.0163	0.0172	-0.0248	0.0181
N	28 - C	43	4.9579	0.0108	0.0125	0.0132	-0.0231	0.0139
N	28 - C	46	3.7008	0.0191	0.0313	0.0330	-0.0052	0.0347
N	28 - H	47	3.3784	0.0131	0.0137	0.0146	0.0540	0.0138
H	29 - C	35	1.0904	1.0244	0.9217	0.9606	0.9728	0.9019
H	29 - C	41	3.4189	0.0139	0.0142	0.0148	0.0220	0.0136
H	29 - C	48	3.4123	0.0051	0.0143	0.0149	0.0453	0.0140
C	30 - C	33	4.9697	0.0147	0.0140	0.0144	-0.0098	0.0149
C	30 - C	38	2.7785	0.0569	0.0928	0.0960	0.1210	0.0966
C	30 - C	39	1.3989	1.3583	1.4021	1.4603	1.4259	1.5169
C	30 - C	42	2.4081	0.0091	0.0096	0.0100	-0.0249	0.0105
C	30 - C	43	7.0171	0.0115	0.0128	0.0133	-0.0169	0.0139
C	30 - C	46	5.1910	0.0129	0.0129	0.0134	-0.0182	0.0140
C	30 - H	47	3.3999	0.0015	0.0145	0.0152	0.0479	0.0142
C	31 - H	32	1.0904	1.0240	0.9224	0.9609	0.9741	0.9045
C	31 - C	34	2.4322	0.0164	0.0105	0.0109	-0.0222	0.0114
C	31 - C	36	1.4002	1.3951	1.4321	1.4872	1.4477	1.5485
C	31 - H	37	3.4216	0.0062	0.0143	0.0150	0.0452	0.0140
H	32 - C	34	3.4106	0.0053	0.0142	0.0149	0.0448	0.0140
C	33 - C	35	1.4059	1.4055	1.4096	1.4445	1.4147	1.4973
C	33 - C	38	2.4578	0.0347	0.0117	0.0119	0.0290	0.0119
C	33 - C	41	1.4237	1.3395	1.3152	1.3453	1.3366	1.3736
C	33 - C	42	3.7876	0.0246	0.0339	0.0348	0.0114	0.0362
C	33 - C	43	2.4433	0.0260	0.0135	0.0138	-0.0063	0.0143
C	33 - H	44	3.4261	0.0047	0.0146	0.0150	0.0366	0.0140
C	33 - C	46	2.4618	0.0097	0.0132	0.0135	-0.0076	0.0140
C	33 - C	48	2.8399	0.0411	0.0978	0.1005	0.0766	0.1043
C	33 - H	49	3.4499	0.0065	0.0146	0.0150	0.0344	0.0141
C	34 - C	36	1.4018	1.3708	1.4081	1.4648	1.4247	1.5258
C	34 - H	37	1.0905	1.0316	0.9288	0.9724	0.9859	0.9135
C	35 - C	38	3.7400	0.0097	0.0127	0.0131	0.0361	0.0131
C	35 - C	43	1.3989	1.4005	1.4386	1.4936	1.4567	1.5531
C	35 - C	46	2.7981	0.0611	0.1097	0.1140	0.0848	0.1186
C	35 - C	48	2.4332	0.0172	0.0100	0.0105	-0.0209	0.0109
C	35 - H	50	3.4217	0.0060	0.0142	0.0149	0.0438	0.0139
C	36 - H	40	1.0918	1.0304	0.9276	0.9691	0.9798	0.9072
C	38 - C	39	2.4209	0.0402	0.0121	0.0125	0.0301	0.0124
C	38 - C	41	1.4608	1.1760	1.1031	1.1365	1.1397	1.1240
C	38 - C	42	1.4050	1.3711	1.3472	1.3930	1.4090	1.4012
C	38 - H	45	3.4114	0.0044	0.0145	0.0151	-0.0098	0.0135
C	38 - C	46	2.5162	0.0229	0.0106	0.0110	0.0333	0.0110
C	38 - C	48	3.7836	0.0113	0.0166	0.0171	0.0417	0.0172
C	39 - C	41	3.7969	0.0075	0.0169	0.0175	0.0116	0.0179
C	39 - C	42	1.3908	1.4120	1.4645	1.5247	1.4913	1.5826
C	39 - H	45	1.0908	1.0270	0.9234	0.9685	0.9748	0.8975
C	41 - C	42	2.5473	0.0096	0.0105	0.0109	0.0027	0.0112
C	41 - C	43	2.7945	0.0515	0.0912	0.0945	0.0871	0.0968
C	41 - C	46	1.4096	1.3350	1.3399	1.3892	1.3769	1.4245
C	41 - C	48	2.4310	0.0342	0.0121	0.0125	0.0043	0.0129
C	41 - H	50	3.4202	0.0065	0.0144	0.0150	0.0224	0.0139
C	42 - C	43	5.2189	0.0117	0.0125	0.0130	-0.0161	0.0135
C	42 - C	46	3.0328	0.0186	0.0170	0.0177	-0.0128	0.0185
C	42 - H	47	1.0877	1.0183	0.9215	0.9638	0.9776	0.9031
C	43 - H	44	1.0917	1.0309	0.9270	0.9688	0.9791	0.9058
C	43 - C	46	2.4135	0.0103	0.0096	0.0100	-0.0163	0.0104
C	43 - C	48	1.4030	1.3631	1.4014	1.4578	1.4186	1.5178
C	43 - H	49	3.4004	0.0032	0.0148	0.0154	0.0397	0.0145
H	44 - C	46	3.4030	0.0043	0.0144	0.0151	0.0433	0.0141
C	46 - C	48	1.3919	1.4173	1.4685	1.5284	1.4868	1.5926
C	46 - H	49	1.0904	1.0261	0.9266	0.9634	0.9747	0.9099
C	48 - H	50	1.0903	1.0319	0.9284	0.9722	0.9858	0.9129
Sum :				73.0792	73.9538	78.3908	78.3908	78.3908

Atomic summation :

C	1	3.9597	3.9824	4.1557	4.1530	4.1881
H	2	1.0777	0.9785	1.0274	1.0416	0.9415
O	3	2.2935	2.5112	2.7405	2.7444	2.7876
C	4	3.9809	3.9571	4.1450	4.1088	4.1507
C	5	3.9288	3.9755	4.1483	4.1273	4.1963
Cl	6	1.1235	1.0200	1.2786	1.3640	1.4783
C	7	3.3824	3.6303	3.9353	3.8684	3.9012
N	8	3.2022	3.4885	3.6945	3.6985	3.7631
O	9	2.2779	2.5014	2.7326	2.7393	2.7830
C	10	3.9631	3.9866	4.1453	4.1392	4.1530
O	11	2.2927	2.5102	2.7401	2.7444	2.7881
H	12	1.0402	0.9803	1.0251	1.0359	0.9596
C	13	3.3674	3.6154	3.9102	3.8551	3.8625
C	14	4.1097	4.0031	4.1563	4.1497	4.1581
C	15	3.3890	3.6313	3.9387	3.8708	3.9049
Ru	16	4.3841	4.5883	5.1462	5.2190	4.9663
H	17	1.0777	0.9780	1.0272	1.0416	0.9407
Ru	18	4.3231	4.5723	5.1388	5.2110	4.9562
C	19	4.0341	4.0203	4.1437	4.1314	4.1859
C	20	3.3967	3.6262	3.9169	3.8557	3.8812
C	21	3.7929	3.9739	4.1391	4.0964	4.2175
C	22	3.9880	3.9561	4.1449	4.1077	4.1511
O	23	2.0014	1.9826	2.4571	2.6407	2.6084
H	24	1.0373	0.9870	1.0260	1.0345	0.9675
H	25	1.0453	0.9745	1.0250	1.0379	0.9538
C	26	3.9655	3.9923	4.1495	4.1427	4.1987
O	27	2.2743	2.4953	2.7255	2.7361	2.7858
N	28	3.1985	3.4832	3.6917	3.6983	3.7655
H	29	1.0705	0.9831	1.0253	1.0353	0.9615
C	30	3.9583	3.9818	4.1553	4.1518	4.1854

```
 C     31                          4.0108     3.9884     4.1281     4.1217     4.1911
 H     32                          1.0696     0.9842     1.0260     1.0352     0.9645
 C     33                          3.7823     3.9681     4.1371     4.0949     4.2193
 C     34                          3.9562     3.9859     4.1530     4.1454     4.2217
 C     35                          4.0113     3.9879     4.1280     4.1195     4.1859
 C     36                          3.9727     3.9855     4.1492     4.1347     4.2130
 H     37                          1.0435     0.9806     1.0266     1.0367     0.9633
 C     38                          4.1033     4.0036     4.1580     4.1486     4.1697
 C     39                          3.9335     3.9748     4.1484     4.1269     4.1955
 H     40                          1.0408     0.9799     1.0237     1.0349     0.9574
 C     41                          4.0280     4.0183     4.1439     4.1321     4.1956
 C     42                          3.9646     3.9861     4.1455     4.1404     4.1561
 C     43                          3.9732     3.9846     4.1481     4.1335     4.2081
 H     44                          1.0404     0.9793     1.0234     1.0350     0.9560
 H     45                          1.0365     0.9756     1.0234     1.0377     0.9469
 C     46                          3.9616     3.9920     4.1502     4.1438     4.2033
 H     47                          1.0420     0.9799     1.0251     1.0359     0.9593
 C     48                          3.9588     3.9855     4.1530     4.1450     4.2211
 H     49                          1.0390     0.9869     1.0262     1.0346     0.9679
 H     50                          1.0443     0.9802     1.0265     1.0368     0.9626
 H     51                          1.0361     0.9760     1.0235     1.0376     0.9477
 H     52                          1.0454     0.9749     1.0252     1.0377     0.9550
 H     53                          1.1281     0.8822     1.1040     1.0527     1.0792
-----------------------------------------------------------------------------------------

(*) Values from:
    - Mayer bond-order analysis
    - Gophinatan-Jug bond order analysis
    - Nalewajski-Mrozek bond order analysis
      a) N-M (1) - bond-orders calculated from two-electron valence indices
                   based on partitioning of tr(Delta_P^2] (3-index set)
      b) N-M (2) - bond-orders calculated from two-electron valence indices
                   based on partitioning of tr(Delta_P^2] (4-index set)
      c) N-M (3) - bond-orders calculated from valence indices
                   based on partitioning of tr(P*Delta_P]
     A. Michalak, R.L. DeKock, T. Ziegler, J. Comp. Chem., subm.
     and original articles by Nalewajski et al. )


========================
No memory problems found
========================

Maximum number of active allocate calls:        5837

*****************************************************************************

                           A D F   E X I T
NORMAL TERMINATION
```

e) *eq-eq*-3c geometry optimization using dispersion corrected Becke-Perdew functional BP-D and the TZP(ZORA) basis set.

```
*****************************************************************************
*                                                                           *
*  ------------------------------------                                     *
*   Amsterdam Density Functional  (ADF)         2008.01   September 22, 2008  *
*  ------------------------------------                                     *
*                                              Build 200810072116           *
*                                                                           *
*                                                                           *
*                              =================                            *
*                              |               |                            *
*                              |     A D F     |                            *
*                              |               |                            *
*                              =================                            *
*                                                                           *
*                                                                           *
*   Online information and documentation:  http://www.scm.com               *
*   E-mail:  support@scm.com   info@scm.com                                 *
*                                                                           *
*   Scientific publications using ADF results must be properly referenced   *
*   See the User Manuals (or the web site) for recommended citations        *
*   The terms and conditions of the End User License Agreement apply to     *
*   the use of ADF, http://www.scm.com/Sales/LicAgreement.html              *
*                                                                           *
*************************  pentium64_linux / hpmpi  ***************************

ADF 2008.01  RunTime: Oct23-2008 18:00:16

Temporary files are created in /tmp/kid_0.IEYURs

equatorial-OH


============================
A T T A C H E D   F I L E S
============================



==============================
M O D E L   P A R A M E T E R S
==============================

DENSITY FUNCTIONAL POTENTIAL (scf)
   LDA:                         VWN
   Gradient Corrections:        Becke88 Perdew86                    == Not Default ==

SPIN  (restricted / unrestr.)
   Molecule:                    Restricted
   Fragments:                   Restricted

OTHER ASPECTS
   Relativistic Corrections:    scalar (ZORA,SAPA)                   *** SPECIAL ***
   Core Treatment:              Frozen Orbital(s)

   Electric Field:              ---

   Hyperfine or Zeeman Interaction:   ---
```

```
   Empirical Dispersion Correction included with factor    1.05000

   Van der Waals Radii used in dispersion are scaled by    1.10000


 Fragment File(s)
 ----------------
 C:
        file : t21.C
        jobid: ADF 2008.01  RunTime: Oct23-2008 17:59:45
        title: Carbon (TZP)
 H:
        file : t21.H
        jobid: ADF 2008.01  RunTime: Oct23-2008 17:59:37
        title: Hydrogen (TZP)
 O:
        file : t21.O
        jobid: ADF 2008.01  RunTime: Oct23-2008 17:59:44
        title: Oxygen (TZP)
 N:
        file : t21.N
        jobid: ADF 2008.01  RunTime: Oct23-2008 17:59:38
        title: Nitrogen (TZP)
 Ru:
        file : t21.Ru
        jobid: ADF 2008.01  RunTime: Oct23-2008 17:59:42
        title: Ruthenium (TZP, all electron)
 Cl:
        file : t21.Cl
        jobid: ADF 2008.01  RunTime: Oct23-2008 17:59:40
        title: Chlorine (TZP)


                                  *******************************************
                                  *  R U N   T Y P E : GEOMETRY OPTIMIZATION  *
                                  *******************************************

Geometry CYCLE 28
 ==============

 Energy gradients wrt nuclear displacements
 ==========================================

     Atom      Cartesian (a.u./angstrom)
                  X         Y         Z
 ------------------------------------------
     1 C     0.000048  0.000007  0.000036
     2 H    -0.000009  0.000016  0.000004
     3 O     0.000170 -0.000189  0.000346
     4 C    -0.000005 -0.000071 -0.000119
     5 C     0.000003 -0.000067 -0.000094
     6 O     0.000020  0.000033 -0.000004
     7 C     0.000061  0.000757 -0.000001
     8 N    -0.000128 -0.000041  0.000169
     9 O    -0.000330 -0.000095 -0.000633
    10 C    -0.000014  0.000096  0.000063
    11 O     0.000163  0.000198 -0.000295
    12 H    -0.000014 -0.000002  0.000012
    13 C     0.000642  0.000074  0.000910
    14 C     0.000026 -0.000019 -0.000027
    15 C    -0.000317 -0.000381  0.000240
    16 Ru   -0.000702 -0.000933 -0.000897
    17 H     0.000032 -0.000024 -0.000034
    18 Ru   -0.000018  0.000169 -0.000020
    19 C    -0.000097  0.000064 -0.000010
    20 C     0.000206 -0.000106  0.000092
    21 C     0.000146 -0.000040  0.000109
    22 C     0.000040  0.000005 -0.000013
    23 Cl    0.000319  0.000346  0.000168
    24 H     0.000038  0.000001  0.000008
    25 H     0.000027 -0.000063  0.000034
    26 C     0.000032  0.000047 -0.000003
    27 O    -0.000150  0.000086  0.000014
    28 N    -0.000036  0.000050 -0.000061
    29 H    -0.000044  0.000021  0.000061
    30 C    -0.000010  0.000032  0.000031
    31 C    -0.000034 -0.000013 -0.000025
    32 H    -0.000075  0.000031 -0.000037
    33 C    -0.000008  0.000090  0.000226
    34 C    -0.000055 -0.000011 -0.000003
    35 C     0.000030 -0.000136  0.000036
    36 C     0.000073  0.000056  0.000058
    37 H     0.000053  0.000016  0.000014
    38 C    -0.000045 -0.000005  0.000008
    39 C     0.000007 -0.000062  0.000029
    40 H     0.000017 -0.000070 -0.000074
    41 C     0.000072 -0.000057  0.000026
    42 C    -0.000050  0.000118 -0.000040
    43 C    -0.000049  0.000106 -0.000121
    44 H    -0.000012 -0.000009  0.000011
    45 H     0.000010 -0.000001  0.000019
    46 C    -0.000043 -0.000064 -0.000049
    47 H    -0.000005  0.000005  0.000010
    48 C     0.000066 -0.000012 -0.000074
    49 H    -0.000035  0.000020 -0.000020
    50 H    -0.000012  0.000042 -0.000063
    51 H     0.000012 -0.000008  0.000001
    52 H    -0.000008  0.000003  0.000000
    53 H    -0.000010 -0.000008 -0.000021
 ------------------------------------------

--------------------------------------
Geometry Convergence after Step  28
--------------------------------------
current energy                          -13.39096581 Hartree
abs of energy change          0.00002338     0.00100000    T
constrained gradient max      0.00093326     0.00100000    T
constrained gradient rms      0.00019280     0.00066667    T
gradient max                  0.00093326
gradient rms                  0.00019280
cart. step max                0.00667614     0.01000000    T
cart. step rms                0.00205824     0.00666667    T
```

```
 Number of elements of the density matrix on this node (used, total):     54137    436645


 ================================================
 Numerical Integration : Voronoi Polyhedra (Te Velde)  ***  (parameters, tests)  ***
 ================================================

 General Accuracy Parameter :                          4.50

 Symmetry used in the points section:  NOSYM


 Summary of the Symmetry Unique Points:
 --------------------------------------
    Nr. of used Symmetry Operators                     1

    Points in the Atomic Spheres                   34100
    Points in the Atomic Polyhedra                338666
    Points in the Outer Region                     28404
    ------------------------------------------------------
    Total                                         401170

    Sum of Weights                                161993.403613

 Total nr. of points:     401170
 Nr. of blocks:             3135
 Block length:               128
 Nr. of dummy points:        110


 Test of Precision of the Numerical Integration Grid
 ===================================================

 Integral of the Total Core Density:                   0.00000000000000

============================
 B O N D I N G   E N E R G Y  ***  (decomposition)  ***
 ============================

*** WARNING ***

The bond energy is computed as an energy difference between molecule and
fragments. In particular when the fragments are single atoms, they are usually
computed as SPHERICALLY SYMMETRIC and SPIN-RESTRICTED. Obviously, this usually
does NOT represent the true atomic groundstate.

To obtain the 'real' bond energy, (atomic) correction terms must be applied
for the true (multiplet) fragment ground state. See ref: E.J.Baerends,
V.Branchadell, M.Sodupe, Chem.Phys.Lett.265 (1997) 481

General theoretical background on the bond energy decomposition scheme used
here (Morokuma-Ziegler) can be found in the review paper:
F.M. Bickelhaupt and E.J. Baerends,
"Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry"
In: Rev. Comput. Chem.; Lipkowitz, K. B. and Boyd, D. B., Eds.;
Wiley-VCH: New York, 2000, Vol. 15, 1-86.

Symbols used in the Bickelhaupt-Baerends (BB) paper are given below to make
the direct connection to that paper, where detailed explanations can be found
on the meaning of the various terms.

                                          hartree             eV          kcal/mol          kJ/mol
                                  ---------------------  -----------  ----------  -----------

Pauli Repulsion
  Kinetic (Delta T^0):             156.064729320830565     4246.7374     97932.11     409747.89
  Delta V^Pauli Coulomb:           -81.419251205861258    -2215.5306    -51091.36    -213766.21
  Delta V^Pauli LDA-XC:            -19.282718452177342     -524.7095    -12100.09     -50626.77
  Delta V^Pauli GGA-Exchange:        1.121852519327099       30.5272       703.97       2945.42
  Delta V^Pauli GGA-Correlation:    -0.315458276886922       -8.5841      -197.95       -828.24
                                  ---------------------  -----------  ----------  -----------
  Total Pauli Repulsion:           56.169153905232143     1528.4404     35246.68     147472.09
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  56.169153905232143     1528.4404     35246.68     147472.09
  Electrostatic Interaction:       -11.968775761993907     -325.6870     -7510.52     -31424.02
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  ---------------------  -----------  ----------  -----------
  Total Steric Interaction:         44.200378143238240     1202.7535     27736.16     116048.08
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -57.474525919437646    -1563.9614    -36065.81    -150899.35
                                  ---------------------  -----------  ----------  -----------
  Total Orbital Interactions:      -57.479805870986461    -1564.1051    -36069.13    -150913.21

Alternative Decomposition Orb.Int.
  Kinetic:                        -143.374884113043379    -3901.4291    -89969.11    -376430.70
  Coulomb:                          79.112243456420757     2152.7537     49643.69     207709.17
  XC:                                6.782834785636183      184.5703      4256.29      17808.33
                                  ---------------------  -----------  ----------  -----------
  Total Orbital Interactions:      -57.479805870986439    -1564.1051    -36069.13    -150913.21

  Residu (E=Steric+OrbInt+Res):     -0.000004462667838       -0.0001          0.00         -0.01
  Dispersion Energy:                -0.111533216971144       -3.0350        -69.99        -292.83

Total Bonding Energy:               -13.390965407387203      -364.3867      -8402.96      -35157.97


Summary of Bonding Energy (energy terms are taken from the energy decomposition above)
================================================================================

  Electrostatic Energy:             -11.968775761993907      -325.6870      -7510.52      -31424.02
  Kinetic Energy:                    12.689845207787187       345.3083       7963.00       33317.18
  Coulomb (Steric+OrbInt) Energy:    -2.307012212108333       -62.7770      -1447.67       -6057.06
  XC Energy:                        -11.693489424100983      -318.1960      -7337.78      -30701.25
  Dispersion Energy:                 -0.111533216971144        -3.0350        -69.99        -292.83
                                  ---------------------  -----------  ----------  -----------
  Total Bonding Energy:              -13.390965407387181      -364.3867      -8402.96      -35157.97
```

```
Correction terms (incorporated in energies above; only for test purposes):

1. Indication of fit-quality: 1st-order fit-correction used in the energy (hartree):  -0.0143236274
2. Electrostatic (Fit correction):   0.0000000000

Scaled ZORA energy correction, not included in bonding energy (hartree):         -920.9344468127
 WARNING: This scaled ZORA energy correction should only be used to compare two calculations
 in which the only difference in the calculation is the electron configuration.
 Then the difference in energy of this term should be added to the difference in energy of
 the two electron configurations.
 This term should not be used otherwise.
 In practice it is useful only for core excitation energy calculations.
```