Electronic Supplementary Information for Dalton Transactions

The dehydrogenation of ammonia-borane catalysed by dicarbonylruthenacyclic complexes

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Electronic Supporting Information

• Extended crystallographic data for compound 7

Crystal data

$C_{23}H_{23}ClN_2O_2Ru$	Dx = 1.492 Mg m^{-3}
Mr = 495.95	
Monoclinic, $P2_1/c$	Mo Kα radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 9007 reflections
a = 17.6291 (5) Å	θ = 2.6–29.0°
b = 11.5208 (3) Å	μ = 0.85 mm−1
c = 24.1776 (6) Å	T = 173 (2) K
β = 115.955 (2)°	
V = 4415.2 (2) Å3	Prism, yellow
Z = 8	0.40 × 0.30 × 0.15 mm
F000 = 2016	

Data collection

Bruker APEX-II CCD diffractometer	33642 measured reflections
Radiation source: fine-focus sealed tube	11736 independent reflections
Monochromator: graphite	9823 reflections with $I > 2\sigma(I)$
	R_{int} = 0.020
T = 173(2) K	θ_{max} = 29.0°
P = ? kPa	θ_{min} = 1.3°
φ and ω scans	h = −24/24
Absorption correction: multi-scan sadabs	k = −15/13
T_{min} = 0.727, T_{max} = 0.883	l = −32/24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
R[$F^2 > 2\sigma(F^2)$] = 0.030	H-atom parameters constrained
wR(F^2) = 0.065	$w = 1/[\sigma2(Fo^2) + (0.0084P)^2 + 5.7412P]$

	where P = $(Fo^2 + 2Fc^2)/3$
S = 1.15	$(\Delta/\sigma)max = 0.001$
11736 reflections	$\Delta\rho max = 0.69$ e Å^{-3}
531 parameters	$\Delta\rho min = -0.61$ e Å^{-3}
	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.521615 (10)	−0.644658 (15)	−0.146951 (7)	0.02021 (4)
Cl1	0.63202 (3)	−0.79448 (5)	−0.12321 (3)	0.03101 (12)
O1	0.55903 (14)	−0.6083 (2)	−0.01454 (8)	0.0559 (6)
O2	0.64476 (12)	−0.45991 (18)	−0.14067 (10)	0.0459 (5)
N1	0.48032 (10)	−0.65600 (15)	−0.24377 (7)	0.0189 (3)
N2	0.43206 (10)	−0.78348 (16)	−0.15892 (8)	0.0208 (3)
C1	0.51628 (13)	−0.72037 (19)	−0.27259 (10)	0.0240 (4)
H1	0.5634	−0.7677	−0.2485	0.029*
C2	0.48707 (13)	−0.72002 (19)	−0.33585 (10)	0.0250 (4)
H2	0.5143	−0.7660	−0.3544	0.030*
C3	0.41747 (13)	−0.65190 (19)	−0.37233 (9)	0.0230 (4)
C4	0.38011 (13)	−0.58814 (18)	−0.34239 (9)	0.0224 (4)
H4	0.3317	−0.5424	−0.3658	0.027*
C5	0.41241 (12)	−0.58993 (17)	−0.27834 (9)	0.0195 (4)
C6	0.37991 (12)	−0.51973 (18)	−0.24274 (9)	0.0194 (4)
C7	0.31143 (13)	−0.44449 (19)	−0.27007 (10)	0.0241 (4)
H7	0.2817	−0.4407	−0.3136	0.029*
C8	0.28651 (14)	−0.3754 (2)	−0.23419 (10)	0.0263 (4)
H8	0.2401	−0.3240	−0.2533	0.032*
C9	0.32887 (13)	−0.38045 (19)	−0.17036 (10)	0.0243 (4)
C10	0.39551 (13)	−0.45858 (18)	−0.14317 (10)	0.0223 (4)
H10	0.4229	−0.4645	−0.0996	0.027*
C11	0.42329 (12)	−0.52841 (18)	−0.17789 (9)	0.0203 (4)
C12	0.38739 (15)	−0.6467 (2)	−0.44201 (10)	0.0292 (5)

C13	0.3731 (2)	−0.7699 (3)	−0.46815 (12)	0.0534 (8)
H13A	0.4267	−0.8123	−0.4510	0.080*
H13B	0.3509	−0.7664	−0.5130	0.080*
H13C	0.3326	−0.8100	−0.4572	0.080*
C14	0.4549 (2)	−0.5854 (4)	−0.45479 (13)	0.0621 (10)
H14A	0.4631	−0.5065	−0.4381	0.093*
H14B	0.4368	−0.5819	−0.4993	0.093*
H14C	0.5080	−0.6286	−0.4352	0.093*
C15	0.30464 (19)	−0.5795 (3)	−0.47447 (11)	0.0500 (8)
H15A	0.2612	−0.6155	−0.4651	0.075*
H15B	0.2865	−0.5811	−0.5190	0.075*
H15C	0.3132	−0.4989	−0.4601	0.075*
C16	0.30488 (16)	−0.2992 (2)	−0.13163 (12)	0.0347 (5)
H16A	0.3319	−0.2237	−0.1289	0.052*
H16B	0.3237	−0.3318	−0.0903	0.052*
H16C	0.2435	−0.2894	−0.1506	0.052*
C17	0.37519 (14)	−0.7754 (2)	−0.13612 (10)	0.0290 (5)
H17	0.3749	−0.7077	−0.1137	0.035*
C18	0.31710 (15)	−0.8618 (2)	−0.14405 (11)	0.0357 (6)
H18	0.2778	−0.8538	−0.1272	0.043*
C19	0.31680 (16)	−0.9598 (2)	−0.17676 (13)	0.0380 (6)
H19	0.2773	−1.0203	−0.1829	0.046*
C20	0.37512 (16)	−0.9683 (2)	−0.20043 (12)	0.0356 (5)
H20	0.3759	−1.0345	−0.2236	0.043*
C21	0.43219 (14)	−0.8794 (2)	−0.18992 (11)	0.0289 (5)
H21	0.4732	−0.8866	−0.2053	0.035*
C22	0.54644 (15)	−0.6243 (2)	−0.06371 (11)	0.0324 (5)
C23	0.59799 (14)	−0.5279 (2)	−0.14209 (10)	0.0278 (5)
Ru2	0.033023 (10)	−0.929850 (15)	−0.139715 (7)	0.01975 (4)
Cl2	0.13685 (3)	−0.77306 (5)	−0.12274 (3)	0.02872 (11)
O3	0.09266 (12)	−0.9770 (2)	−0.00484 (8)	0.0474 (5)
O4	0.15497 (13)	−1.10167 (18)	−0.14767 (11)	0.0510 (5)

N3	−0.01950 (11)	−0.91734 (15)	−0.23726 (8)	0.0211 (3)
N4	−0.05661 (11)	−0.79628 (16)	−0.14417 (8)	0.0242 (4)
C24	0.00996 (14)	−0.8500 (2)	−0.26916 (10)	0.0276 (5)
H24	0.0572	−0.8015	−0.2471	0.033*
C25	−0.02575 (15)	−0.8489 (2)	−0.33243 (11)	0.0318 (5)
H25	−0.0030	−0.8003	−0.3532	0.038*
C26	−0.09538 (15)	−0.9191 (2)	−0.36628 (10)	0.0275 (5)
C27	−0.12520 (14)	−0.98757 (19)	−0.33298 (10)	0.0257 (4)
H27	−0.1729	−1.0359	−0.3543	0.031*
C28	−0.08667 (13)	−0.98707 (18)	−0.26874 (9)	0.0214 (4)
C29	−0.11149 (13)	−1.05988 (18)	−0.22951 (10)	0.0215 (4)
C30	−0.17957 (14)	−1.1368 (2)	−0.25315 (10)	0.0269 (4)
H30	−0.2123	−1.1428	−0.2964	0.032*
C31	−0.19961 (14)	−1.2043 (2)	−0.21405 (11)	0.0301 (5)
H31	−0.2461	−1.2562	−0.2307	0.036*
C32	−0.15217 (15)	−1.1969 (2)	−0.15051 (11)	0.0284 (5)
C33	−0.08442 (14)	−1.11962 (19)	−0.12718 (10)	0.0250 (4)
H33	−0.0522	−1.1139	−0.0839	0.030*
C34	−0.06232 (13)	−1.05057 (18)	−0.16516 (10)	0.0213 (4)
C35	−0.13376 (17)	−0.9190 (2)	−0.43684 (11)	0.0364 (6)
C36	−0.1590 (2)	−0.7942 (3)	−0.46002 (12)	0.0505 (8)
H36A	−0.1972	−0.7634	−0.4439	0.076*
H36B	−0.1875	−0.7940	−0.5051	0.076*
H36C	−0.1084	−0.7456	−0.4458	0.076*
C37	−0.0674 (2)	−0.9649 (4)	−0.45625 (14)	0.0636 (10)
H37A	−0.0167	−0.9166	−0.4379	0.095*
H37B	−0.0901	−0.9624	−0.5012	0.095*
H37C	−0.0531	−1.0452	−0.4421	0.095*
C38	−0.21235 (19)	−0.9948 (3)	−0.46583 (12)	0.0489 (7)
H38A	−0.1970	−1.0759	−0.4540	0.073*
H38B	−0.2369	−0.9878	−0.5107	0.073*
H38C	−0.2537	−0.9695	−0.4514	0.073*

C39	−0.17293 (18)	−1.2719 (2)	−0.10772 (13)	0.0412 (6)
H39A	−0.1493	−1.3497	−0.1056	0.062*
H39B	−0.2343	−1.2775	−0.1232	0.062*
H39C	−0.1487	−1.2372	−0.0666	0.062*
C40	−0.11052 (14)	−0.8116 (2)	−0.11892 (11)	0.0309 (5)
H40	−0.1078	−0.8816	−0.0974	0.037*
C41	−0.16966 (15)	−0.7289 (3)	−0.12329 (12)	0.0404 (6)
H41	−0.2073	−0.7425	−0.1054	0.048*
C42	−0.17342 (16)	−0.6268 (3)	−0.15379 (14)	0.0469 (7)
H42	−0.2134	−0.5687	−0.1571	0.056*
C43	−0.11816 (16)	−0.6101 (2)	−0.17945 (14)	0.0433 (7)
H43	−0.1197	−0.5405	−0.2010	0.052*
C44	−0.06048 (15)	−0.6962 (2)	−0.17334 (12)	0.0321 (5)
H44	−0.0219	−0.6838	−0.1906	0.039*
C45	0.07098 (14)	−0.9557 (2)	−0.05497 (11)	0.0296 (5)
C46	0.10886 (15)	−1.0393 (2)	−0.14267 (11)	0.0292 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01879 (7)	0.02368 (9)	0.01814 (8)	0.00362 (6)	0.00806 (6)	0.00113 (6)
Cl1	0.0248 (2)	0.0340 (3)	0.0337 (3)	0.0095 (2)	0.0123 (2)	0.0035 (2)
O1	0.0583 (13)	0.0827 (17)	0.0225 (9)	0.0134 (12)	0.0137 (9)	−0.0024 (10)
O2	0.0385 (10)	0.0446 (12)	0.0550 (12)	−0.0135 (9)	0.0207 (9)	−0.0104 (9)
N1	0.0183 (7)	0.0199 (8)	0.0196 (8)	0.0009 (6)	0.0092 (6)	0.0001 (6)
N2	0.0213 (8)	0.0224 (9)	0.0207 (8)	0.0077 (7)	0.0109 (7)	0.0078 (7)
C1	0.0239 (10)	0.0236 (11)	0.0257 (10)	0.0037 (8)	0.0121 (8)	0.0001 (8)
C2	0.0269 (10)	0.0237 (11)	0.0281 (11)	0.0007 (8)	0.0154 (9)	−0.0044 (9)
C3	0.0266 (10)	0.0222 (10)	0.0197 (9)	−0.0047 (8)	0.0097 (8)	−0.0024 (8)
C4	0.0235 (10)	0.0213 (10)	0.0202 (9)	0.0002 (8)	0.0076 (8)	−0.0005 (8)
C5	0.0210 (9)	0.0168 (9)	0.0206 (9)	−0.0011 (7)	0.0090 (8)	0.0009 (7)
C6	0.0193 (9)	0.0187 (10)	0.0218 (9)	−0.0004 (7)	0.0103 (8)	0.0015 (7)
C7	0.0234 (10)	0.0250 (11)	0.0240 (10)	0.0038 (8)	0.0104 (8)	0.0052 (8)

C8	0.0250 (10)	0.0248 (11)	0.0322 (11)	0.0074 (8)	0.0154 (9)	0.0076 (9)
C9	0.0247 (10)	0.0211 (10)	0.0325 (11)	0.0024 (8)	0.0176 (9)	0.0023 (8)
C10	0.0233 (10)	0.0228 (10)	0.0225 (10)	0.0018 (8)	0.0117 (8)	0.0018 (8)
C11	0.0179 (9)	0.0223 (10)	0.0210 (9)	−0.0010 (7)	0.0088 (8)	0.0017 (8)
C12	0.0361 (12)	0.0311 (12)	0.0198 (10)	−0.0036 (10)	0.0118 (9)	−0.0037 (9)
C13	0.087 (2)	0.0402 (16)	0.0262 (13)	−0.0023 (16)	0.0180 (14)	−0.0106 (12)
C14	0.0559 (18)	0.103 (3)	0.0276 (13)	−0.0290 (19)	0.0188 (13)	0.0054 (16)
C15	0.0545 (17)	0.065 (2)	0.0203 (12)	0.0109 (15)	0.0066 (11)	−0.0014 (12)
C16	0.0388 (13)	0.0338 (13)	0.0386 (13)	0.0105 (11)	0.0234 (11)	−0.0005 (11)
C17	0.0273 (11)	0.0364 (13)	0.0271 (11)	0.0077 (9)	0.0154 (9)	0.0079 (9)
C18	0.0279 (11)	0.0474 (16)	0.0368 (13)	0.0057 (11)	0.0187 (10)	0.0150 (12)
C19	0.0285 (12)	0.0349 (14)	0.0473 (15)	−0.0002 (10)	0.0135 (11)	0.0141 (11)
C20	0.0340 (12)	0.0255 (12)	0.0464 (15)	0.0013 (10)	0.0167 (11)	0.0026 (10)
C21	0.0275 (11)	0.0271 (12)	0.0364 (12)	0.0051 (9)	0.0178 (10)	0.0036 (9)
C22	0.0273 (11)	0.0403 (14)	0.0273 (11)	0.0055 (10)	0.0098 (9)	−0.0022 (10)
C23	0.0243 (10)	0.0310 (12)	0.0265 (11)	0.0047 (9)	0.0096 (9)	−0.0048 (9)
Ru2	0.01969 (8)	0.02131 (8)	0.02040 (8)	−0.00284 (6)	0.01076 (6)	−0.00200 (6)
Cl2	0.0233 (2)	0.0289 (3)	0.0336 (3)	−0.0056 (2)	0.0121 (2)	−0.0011 (2)
O3	0.0468 (11)	0.0701 (14)	0.0249 (9)	−0.0095 (10)	0.0151 (8)	0.0001 (9)
O4	0.0523 (12)	0.0416 (11)	0.0758 (15)	0.0182 (9)	0.0435 (11)	0.0123 (10)
N3	0.0226 (8)	0.0210 (9)	0.0227 (8)	−0.0021 (7)	0.0127 (7)	−0.0012 (7)
N4	0.0197 (8)	0.0257 (9)	0.0299 (9)	−0.0091 (7)	0.0133 (7)	−0.0117 (8)
C24	0.0301 (11)	0.0271 (11)	0.0277 (11)	−0.0039 (9)	0.0145 (9)	−0.0003 (9)
C25	0.0393 (13)	0.0282 (12)	0.0297 (11)	−0.0034 (10)	0.0168 (10)	0.0055 (10)
C26	0.0345 (11)	0.0255 (11)	0.0217 (10)	0.0049 (9)	0.0115 (9)	0.0000 (8)
C27	0.0279 (10)	0.0231 (11)	0.0225 (10)	−0.0003 (8)	0.0078 (8)	−0.0034 (8)
C28	0.0222 (9)	0.0198 (10)	0.0234 (10)	0.0008 (8)	0.0110 (8)	−0.0027 (8)
C29	0.0225 (9)	0.0173 (10)	0.0273 (10)	−0.0004 (8)	0.0132 (8)	−0.0039 (8)
C30	0.0255 (10)	0.0258 (11)	0.0299 (11)	−0.0049 (9)	0.0127 (9)	−0.0073 (9)
C31	0.0288 (11)	0.0252 (11)	0.0398 (13)	−0.0090 (9)	0.0182 (10)	−0.0081 (10)
C32	0.0326 (11)	0.0226 (11)	0.0395 (13)	−0.0029 (9)	0.0246 (10)	−0.0022 (9)
C33	0.0296 (11)	0.0242 (11)	0.0270 (10)	−0.0036 (9)	0.0179 (9)	−0.0027 (8)

C34	0.0223 (9)	0.0200 (10)	0.0251 (10)	−0.0004 (8)	0.0135 (8)	−0.0060 (8)
C35	0.0488 (15)	0.0360 (14)	0.0200 (10)	0.0050 (11)	0.0112 (10)	−0.0007 (10)
C36	0.074 (2)	0.0448 (17)	0.0266 (13)	0.0036 (15)	0.0162 (13)	0.0072 (12)
C37	0.069 (2)	0.091 (3)	0.0323 (15)	0.018 (2)	0.0244 (15)	−0.0082 (16)
C38	0.0597 (18)	0.0458 (16)	0.0242 (12)	−0.0009 (14)	0.0025 (12)	−0.0022 (11)
C39	0.0497 (15)	0.0364 (14)	0.0495 (16)	−0.0131 (12)	0.0328 (13)	0.0000 (12)
C40	0.0266 (11)	0.0402 (14)	0.0286 (11)	−0.0066 (10)	0.0145 (9)	−0.0122 (10)
C41	0.0282 (12)	0.0580 (18)	0.0393 (14)	−0.0062 (12)	0.0189 (11)	−0.0239 (13)
C42	0.0279 (12)	0.0486 (17)	0.0585 (18)	0.0034 (12)	0.0137 (12)	−0.0236 (14)
C43	0.0325 (13)	0.0318 (14)	0.0596 (18)	0.0040 (11)	0.0146 (12)	−0.0063 (12)
C44	0.0273 (11)	0.0266 (12)	0.0432 (14)	−0.0035 (9)	0.0162 (10)	−0.0026 (10)
C45	0.0230 (10)	0.0357 (13)	0.0301 (12)	−0.0059 (9)	0.0116 (9)	0.0002 (10)
C46	0.0295 (11)	0.0269 (12)	0.0341 (12)	−0.0029 (9)	0.0167 (10)	0.0022 (9)

Geometric parameters (Å, °)

Ru1—C23	1.870 (2)	Ru2—C46	1.862 (2)
Ru1—C22	1.878 (2)	Ru2—C45	1.880 (2)
Ru1—C11	2.055 (2)	Ru2—C34	2.057 (2)
Ru1—N1	2.1295 (16)	Ru2—N3	2.1281 (17)
Ru1—N2	2.1758 (18)	Ru2—N4	2.1742 (18)
Ru1—Cl1	2.4737 (6)	Ru2—Cl2	2.4747 (6)
O1—C22	1.125 (3)	O3—C45	1.127 (3)
O2—C23	1.126 (3)	O4—C46	1.130 (3)
N1—C1	1.351 (3)	N3—C24	1.348 (3)
N1—C5	1.355 (2)	N3—C28	1.356 (3)
N2—C21	1.335 (3)	N4—C44	1.338 (3)
N2—C17	1.342 (3)	N4—C40	1.347 (3)
C1—C2	1.384 (3)	C24—C25	1.376 (3)
C1—H1	0.9500	C24—H24	0.9500
C2—C3	1.397 (3)	C25—C26	1.397 (3)
C2—H2	0.9500	C25—H25	0.9500
C3—C4	1.384 (3)	C26—C27	1.385 (3)

C3—C12	1.530 (3)	C26—C35	1.535 (3)
C4—C5	1.397 (3)	C27—C28	1.396 (3)
C4—H4	0.9500	C27—H27	0.9500
C5—C6	1.468 (3)	C28—C29	1.469 (3)
C6—C7	1.395 (3)	C29—C30	1.397 (3)
C6—C11	1.416 (3)	C29—C34	1.415 (3)
C7—C8	1.383 (3)	C30—C31	1.384 (3)
C7—H7	0.9500	C30—H30	0.9500
C8—C9	1.391 (3)	C31—C32	1.394 (3)
C8—H8	0.9500	C31—H31	0.9500
C9—C10	1.395 (3)	C32—C33	1.396 (3)
C9—C16	1.509 (3)	C32—C39	1.511 (3)
C10—C11	1.397 (3)	C33—C34	1.393 (3)
C10—H10	0.9500	C33—H33	0.9500
C12—C14	1.527 (4)	C35—C38	1.525 (4)
C12—C13	1.529 (4)	C35—C37	1.532 (4)
C12—C15	1.530 (4)	C35—C36	1.537 (4)
C13—H13A	0.9800	C36—H36A	0.9800
C13—H13B	0.9800	C36—H36B	0.9800
C13—H13C	0.9800	C36—H36C	0.9800
C14—H14A	0.9800	C37—H37A	0.9800
C14—H14B	0.9800	C37—H37B	0.9800
C14—H14C	0.9800	C37—H37C	0.9800
C15—H15A	0.9800	C38—H38A	0.9800
C15—H15B	0.9800	C38—H38B	0.9800
C15—H15C	0.9800	C38—H38C	0.9800
C16—H16A	0.9800	C39—H39A	0.9800
C16—H16B	0.9800	C39—H39B	0.9800
C16—H16C	0.9800	C39—H39C	0.9800
C17—C18	1.380 (3)	C40—C41	1.382 (4)
C17—H17	0.9500	C40—H40	0.9500
C18—C19	1.377 (4)	C41—C42	1.374 (4)

C18—H18	0.9500	C41—H41	0.9500
C19—C20	1.382 (4)	C42—C43	1.378 (4)
C19—H19	0.9500	C42—H42	0.9500
C20—C21	1.380 (3)	C43—C44	1.381 (3)
C20—H20	0.9500	C43—H43	0.9500
C21—H21	0.9500	C44—H44	0.9500
C23—Ru1—C22	91.10 (11)	C46—Ru2—C45	90.88 (10)
C23—Ru1—C11	91.34 (9)	C46—Ru2—C34	92.12 (9)
C22—Ru1—C11	94.16 (9)	C45—Ru2—C34	94.20 (9)
C23—Ru1—N1	90.21 (8)	C46—Ru2—N3	88.56 (9)
C22—Ru1—N1	173.22 (8)	C45—Ru2—N3	173.32 (8)
C11—Ru1—N1	79.15 (7)	C34—Ru2—N3	79.17 (7)
C23—Ru1—N2	176.02 (8)	C46—Ru2—N4	174.85 (9)
C22—Ru1—N2	92.83 (9)	C45—Ru2—N4	94.05 (9)
C11—Ru1—N2	89.04 (7)	C34—Ru2—N4	89.01 (7)
N1—Ru1—N2	85.97 (6)	N3—Ru2—N4	86.72 (7)
C23—Ru1—Cl1	90.90 (7)	C46—Ru2—Cl2	90.54 (7)
C22—Ru1—Cl1	92.73 (7)	C45—Ru2—Cl2	92.88 (7)
C11—Ru1—Cl1	172.71 (6)	C34—Ru2—Cl2	172.39 (6)
N1—Ru1—Cl1	93.90 (5)	N3—Ru2—Cl2	93.77 (5)
N2—Ru1—Cl1	88.25 (5)	N4—Ru2—Cl2	87.73 (5)
C1—N1—C5	118.54 (17)	C24—N3—C28	118.71 (18)
C1—N1—Ru1	126.08 (14)	C24—N3—Ru2	125.69 (14)
C5—N1—Ru1	115.37 (13)	C28—N3—Ru2	115.56 (14)
C21—N2—C17	118.2 (2)	C44—N4—C40	117.9 (2)
C21—N2—Ru1	120.21 (14)	C44—N4—Ru2	120.30 (15)
C17—N2—Ru1	121.55 (16)	C40—N4—Ru2	121.78 (17)
N1—C1—C2	122.48 (19)	N3—C24—C25	122.6 (2)
N1—C1—H1	118.8	N3—C24—H24	118.7
C2—C1—H1	118.8	C25—C24—H24	118.7
C1—C2—C3	119.9 (2)	C24—C25—C26	120.2 (2)
C1—C2—H2	120.0	C24—C25—H25	119.9

C3—C2—H2	120.0	C26—C25—H25	119.9
C4—C3—C2	117.10 (19)	C27—C26—C25	116.7 (2)
C4—C3—C12	122.7 (2)	C27—C26—C35	123.5 (2)
C2—C3—C12	120.16 (19)	C25—C26—C35	119.8 (2)
C3—C4—C5	121.04 (19)	C26—C27—C28	121.4 (2)
C3—C4—H4	119.5	C26—C27—H27	119.3
C5—C4—H4	119.5	C28—C27—H27	119.3
N1—C5—C4	120.92 (19)	N3—C28—C27	120.5 (2)
N1—C5—C6	114.46 (17)	N3—C28—C29	114.19 (18)
C4—C5—C6	124.58 (18)	C27—C28—C29	125.34 (19)
C7—C6—C11	120.28 (19)	C30—C29—C34	120.1 (2)
C7—C6—C5	122.92 (19)	C30—C29—C28	122.91 (19)
C11—C6—C5	116.77 (18)	C34—C29—C28	117.02 (18)
C8—C7—C6	120.5 (2)	C31—C30—C29	120.5 (2)
C8—C7—H7	119.8	C31—C30—H30	119.8
C6—C7—H7	119.8	C29—C30—H30	119.8
C7—C8—C9	120.5 (2)	C30—C31—C32	120.6 (2)
C7—C8—H8	119.7	C30—C31—H31	119.7
C9—C8—H8	119.7	C32—C31—H31	119.7
C8—C9—C10	118.8 (2)	C31—C32—C33	118.6 (2)
C8—C9—C16	120.1 (2)	C31—C32—C39	120.8 (2)
C10—C9—C16	121.0 (2)	C33—C32—C39	120.6 (2)
C9—C10—C11	122.2 (2)	C34—C33—C32	122.3 (2)
C9—C10—H10	118.9	C34—C33—H33	118.8
C11—C10—H10	118.9	C32—C33—H33	118.8
C10—C11—C6	117.61 (18)	C33—C34—C29	117.90 (19)
C10—C11—Ru1	128.20 (15)	C33—C34—Ru2	128.05 (16)
C6—C11—Ru1	114.19 (15)	C29—C34—Ru2	114.02 (15)
C14—C12—C13	110.3 (3)	C38—C35—C37	108.8 (2)
C14—C12—C3	108.40 (19)	C38—C35—C26	112.3 (2)
C13—C12—C3	109.5 (2)	C37—C35—C26	108.4 (2)
C14—C12—C15	108.3 (2)	C38—C35—C36	108.0 (2)

C13—C12—C15	108.1 (2)	C37—C35—C36	110.5 (3)
C3—C12—C15	112.2 (2)	C26—C35—C36	108.8 (2)
C12—C13—H13A	109.5	C35—C36—H36A	109.5
C12—C13—H13B	109.5	C35—C36—H36B	109.5
H13A—C13—H13B	109.5	H36A—C36—H36B	109.5
C12—C13—H13C	109.5	C35—C36—H36C	109.5
H13A—C13—H13C	109.5	H36A—C36—H36C	109.5
H13B—C13—H13C	109.5	H36B—C36—H36C	109.5
C12—C14—H14A	109.5	C35—C37—H37A	109.5
C12—C14—H14B	109.5	C35—C37—H37B	109.5
H14A—C14—H14B	109.5	H37A—C37—H37B	109.5
C12—C14—H14C	109.5	C35—C37—H37C	109.5
H14A—C14—H14C	109.5	H37A—C37—H37C	109.5
H14B—C14—H14C	109.5	H37B—C37—H37C	109.5
C12—C15—H15A	109.5	C35—C38—H38A	109.5
C12—C15—H15B	109.5	C35—C38—H38B	109.5
H15A—C15—H15B	109.5	H38A—C38—H38B	109.5
C12—C15—H15C	109.5	C35—C38—H38C	109.5
H15A—C15—H15C	109.5	H38A—C38—H38C	109.5
H15B—C15—H15C	109.5	H38B—C38—H38C	109.5
C9—C16—H16A	109.5	C32—C39—H39A	109.5
C9—C16—H16B	109.5	C32—C39—H39B	109.5
H16A—C16—H16B	109.5	H39A—C39—H39B	109.5
C9—C16—H16C	109.5	C32—C39—H39C	109.5
H16A—C16—H16C	109.5	H39A—C39—H39C	109.5
H16B—C16—H16C	109.5	H39B—C39—H39C	109.5
N2—C17—C18	122.3 (2)	N4—C40—C41	122.3 (3)
N2—C17—H17	118.8	N4—C40—H40	118.9
C18—C17—H17	118.8	C41—C40—H40	118.9
C19—C18—C17	119.2 (2)	C42—C41—C40	119.2 (2)
C19—C18—H18	120.4	C42—C41—H41	120.4
C17—C18—H18	120.4	C40—C41—H41	120.4

C18—C19—C20	118.7 (2)	C41—C42—C43	118.9 (3)
C18—C19—H19	120.7	C41—C42—H42	120.5
C20—C19—H19	120.7	C43—C42—H42	120.5
C21—C20—C19	119.1 (2)	C42—C43—C44	119.0 (3)
C21—C20—H20	120.5	C42—C43—H43	120.5
C19—C20—H20	120.5	C44—C43—H43	120.5
N2—C21—C20	122.5 (2)	N4—C44—C43	122.7 (2)
N2—C21—H21	118.7	N4—C44—H44	118.6
C20—C21—H21	118.7	C43—C44—H44	118.6
O1—C22—Ru1	177.1 (2)	O3—C45—Ru2	176.5 (2)
O2—C23—Ru1	177.4 (2)	O4—C46—Ru2	175.4 (2)
C23—Ru1—N1—C1	85.59 (18)	C46—Ru2—N3—C24	−84.31 (19)
C11—Ru1—N1—C1	176.91 (18)	C34—Ru2—N3—C24	−176.74 (19)
N2—Ru1—N1—C1	−93.29 (17)	N4—Ru2—N3—C24	93.64 (18)
Cl1—Ru1—N1—C1	−5.33 (17)	Cl2—Ru2—N3—C24	6.14 (18)
C23—Ru1—N1—C5	−93.20 (15)	C46—Ru2—N3—C28	93.39 (16)
C11—Ru1—N1—C5	−1.88 (14)	C34—Ru2—N3—C28	0.96 (15)
N2—Ru1—N1—C5	87.92 (14)	N4—Ru2—N3—C28	−88.66 (15)
Cl1—Ru1—N1—C5	175.88 (13)	Cl2—Ru2—N3—C28	−176.16 (14)
C22—Ru1—N2—C21	−136.21 (17)	C45—Ru2—N4—C44	132.99 (18)
C11—Ru1—N2—C21	129.67 (16)	C34—Ru2—N4—C44	−132.87 (17)
N1—Ru1—N2—C21	50.48 (16)	N3—Ru2—N4—C44	−53.66 (17)
Cl1—Ru1—N2—C21	−43.56 (15)	Cl2—Ru2—N4—C44	40.25 (16)
C22—Ru1—N2—C17	44.31 (17)	C45—Ru2—N4—C40	−48.08 (17)
C11—Ru1—N2—C17	−49.81 (16)	C34—Ru2—N4—C40	46.07 (17)
N1—Ru1—N2—C17	−129.00 (16)	N3—Ru2—N4—C40	125.28 (17)
Cl1—Ru1—N2—C17	136.96 (16)	Cl2—Ru2—N4—C40	−140.81 (16)
C5—N1—C1—C2	0.9 (3)	C28—N3—C24—C25	0.3 (3)
Ru1—N1—C1—C2	−177.85 (16)	Ru2—N3—C24—C25	177.96 (18)
N1—C1—C2—C3	−0.5 (3)	N3—C24—C25—C26	0.1 (4)
C1—C2—C3—C4	−0.8 (3)	C24—C25—C26—C27	0.1 (4)
C1—C2—C3—C12	177.1 (2)	C24—C25—C26—C35	−178.9 (2)

C2—C3—C4—C5	1.7 (3)	C25—C26—C27—C28	−0.7 (3)
C12—C3—C4—C5	−176.2 (2)	C35—C26—C27—C28	178.2 (2)
C1—N1—C5—C4	0.0 (3)	C24—N3—C28—C27	−1.0 (3)
Ru1—N1—C5—C4	178.87 (15)	Ru2—N3—C28—C27	−178.83 (16)
C1—N1—C5—C6	−177.71 (18)	C24—N3—C28—C29	177.76 (18)
Ru1—N1—C5—C6	1.2 (2)	Ru2—N3—C28—C29	−0.1 (2)
C3—C4—C5—N1	−1.3 (3)	C26—C27—C28—N3	1.2 (3)
C3—C4—C5—C6	176.14 (19)	C26—C27—C28—C29	−177.4 (2)
N1—C5—C6—C7	178.72 (19)	N3—C28—C29—C30	179.44 (19)
C4—C5—C6—C7	1.1 (3)	C27—C28—C29—C30	−1.9 (3)
N1—C5—C6—C11	0.7 (3)	N3—C28—C29—C34	−1.3 (3)
C4—C5—C6—C11	−176.86 (19)	C27—C28—C29—C34	177.3 (2)
C11—C6—C7—C8	1.7 (3)	C34—C29—C30—C31	0.1 (3)
C5—C6—C7—C8	−176.2 (2)	C28—C29—C30—C31	179.3 (2)
C6—C7—C8—C9	−0.5 (3)	C29—C30—C31—C32	−0.1 (3)
C7—C8—C9—C10	−1.6 (3)	C30—C31—C32—C33	0.4 (3)
C7—C8—C9—C16	176.0 (2)	C30—C31—C32—C39	−179.0 (2)
C8—C9—C10—C11	2.7 (3)	C31—C32—C33—C34	−0.5 (3)
C16—C9—C10—C11	−175.0 (2)	C39—C32—C33—C34	178.8 (2)
C9—C10—C11—C6	−1.5 (3)	C32—C33—C34—C29	0.5 (3)
C9—C10—C11—Ru1	178.12 (16)	C32—C33—C34—Ru2	178.59 (16)
C7—C6—C11—C10	−0.7 (3)	C30—C29—C34—C33	−0.2 (3)
C5—C6—C11—C10	177.35 (18)	C28—C29—C34—C33	−179.48 (19)
C7—C6—C11—Ru1	179.64 (15)	C30—C29—C34—Ru2	−178.61 (16)
C5—C6—C11—Ru1	−2.3 (2)	C28—C29—C34—Ru2	2.1 (2)
C23—Ru1—C11—C10	−87.5 (2)	C46—Ru2—C34—C33	92.1 (2)
C22—Ru1—C11—C10	3.7 (2)	C45—Ru2—C34—C33	1.0 (2)
N1—Ru1—C11—C10	−177.4 (2)	N3—Ru2—C34—C33	−179.8 (2)
N2—Ru1—C11—C10	96.49 (19)	N4—Ru2—C34—C33	−92.96 (19)
C23—Ru1—C11—C6	92.15 (16)	C46—Ru2—C34—C29	−89.75 (16)
C22—Ru1—C11—C6	−176.65 (16)	C45—Ru2—C34—C29	179.21 (16)
N1—Ru1—C11—C6	2.20 (14)	N3—Ru2—C34—C29	−1.63 (14)

N2—Ru1—C11—C6	−83.88 (15)	N4—Ru2—C34—C29	85.23 (15)
C4—C3—C12—C14	110.6 (3)	C27—C26—C35—C38	4.7 (3)
C2—C3—C12—C14	−67.2 (3)	C25—C26—C35—C38	−176.4 (2)
C4—C3—C12—C13	−129.0 (3)	C27—C26—C35—C37	−115.6 (3)
C2—C3—C12—C13	53.2 (3)	C25—C26—C35—C37	63.3 (3)
C4—C3—C12—C15	−9.0 (3)	C27—C26—C35—C36	124.2 (3)
C2—C3—C12—C15	173.2 (2)	C25—C26—C35—C36	−56.9 (3)
C21—N2—C17—C18	−0.5 (3)	C44—N4—C40—C41	1.2 (3)
Ru1—N2—C17—C18	179.01 (17)	Ru2—N4—C40—C41	−177.75 (17)
N2—C17—C18—C19	−0.4 (3)	N4—C40—C41—C42	−0.7 (4)
C17—C18—C19—C20	0.2 (4)	C40—C41—C42—C43	0.3 (4)
C18—C19—C20—C21	0.8 (4)	C41—C42—C43—C44	−0.4 (4)
C17—N2—C21—C20	1.5 (3)	C40—N4—C44—C43	−1.3 (3)
Ru1—N2—C21—C20	−177.97 (18)	Ru2—N4—C44—C43	177.64 (19)
C19—C20—C21—N2	−1.7 (4)	C42—C43—C44—N4	1.0 (4)

Computing details

Data collection: Bruker *APEX2*; cell refinement: Bruker *SAINT*; data reduction: Bruker *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: Bruker *SHELXTL*; software used to prepare material for publication: Bruker *SHELXTL*.

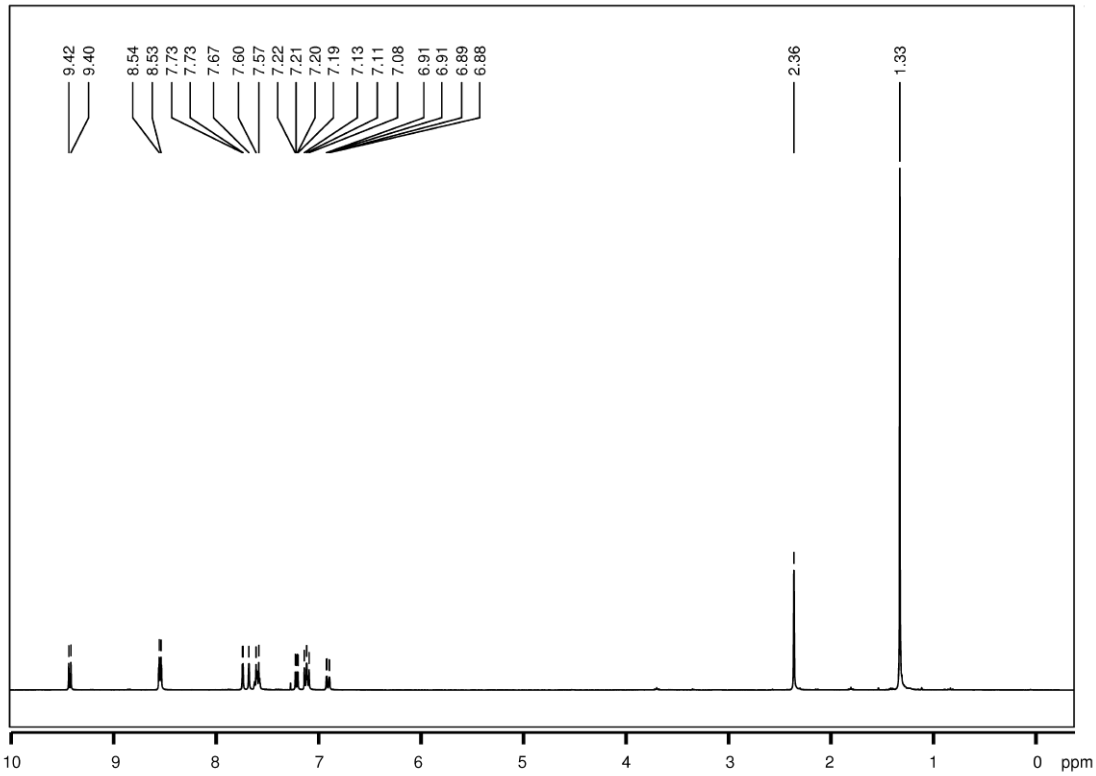

Figure S1. ^{1}H NMR spectrum of complex **7** in $CDCl_3$

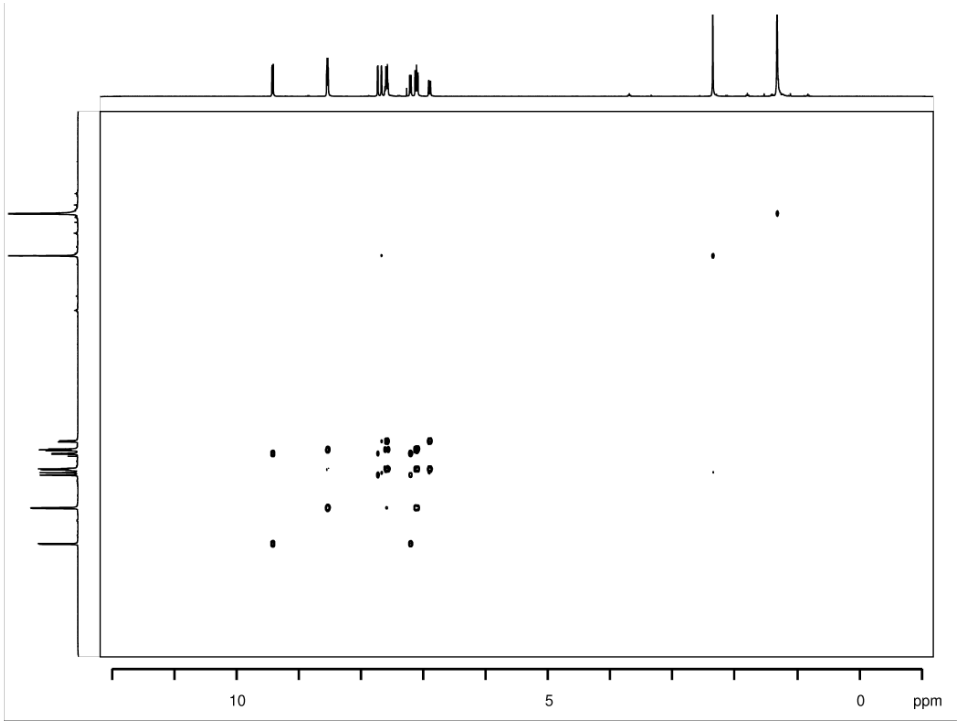

Figure S2. COSY (^{1}H) spectrum of complex **7** in $CDCl_3$

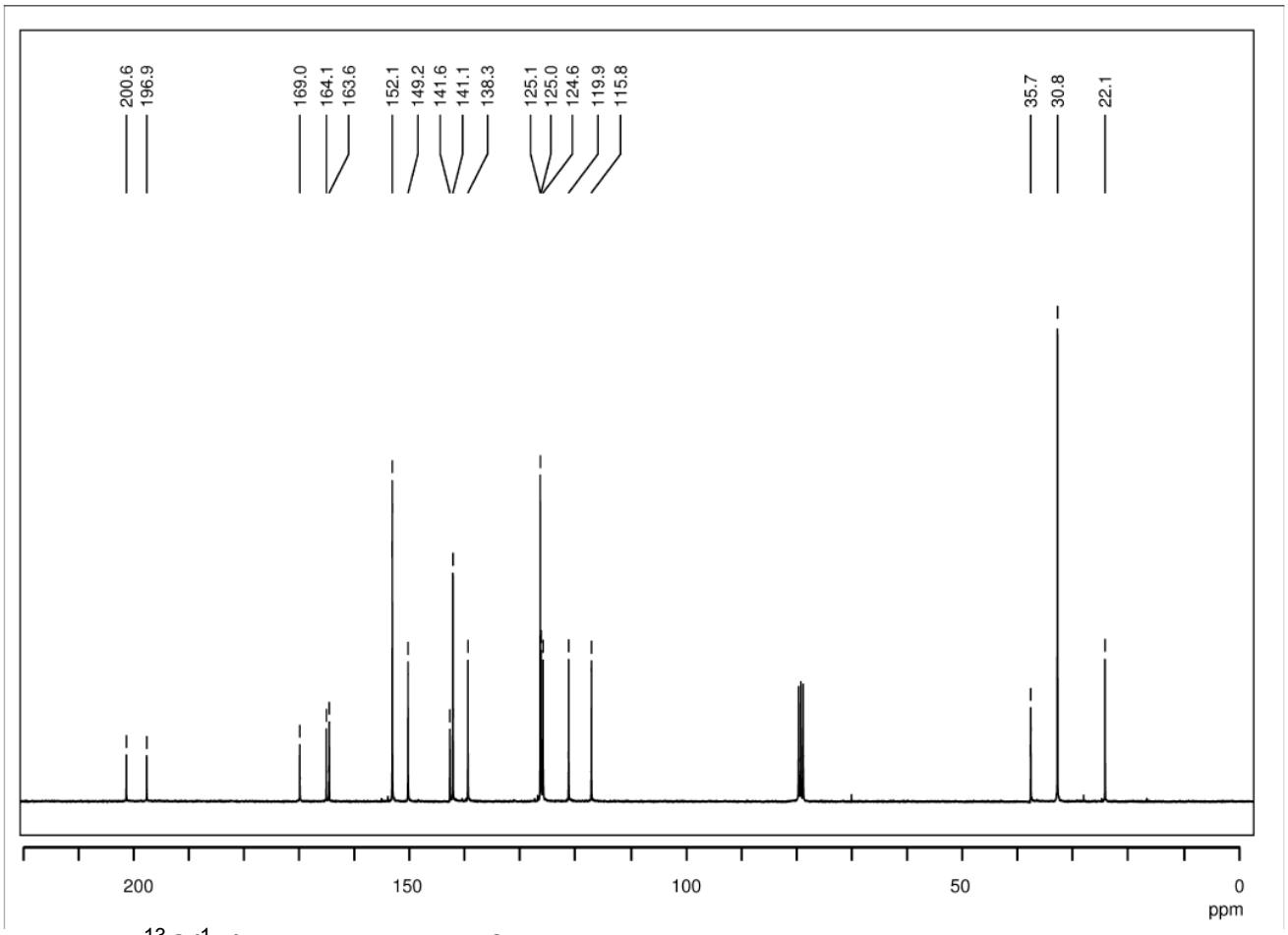

Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of complex **7**

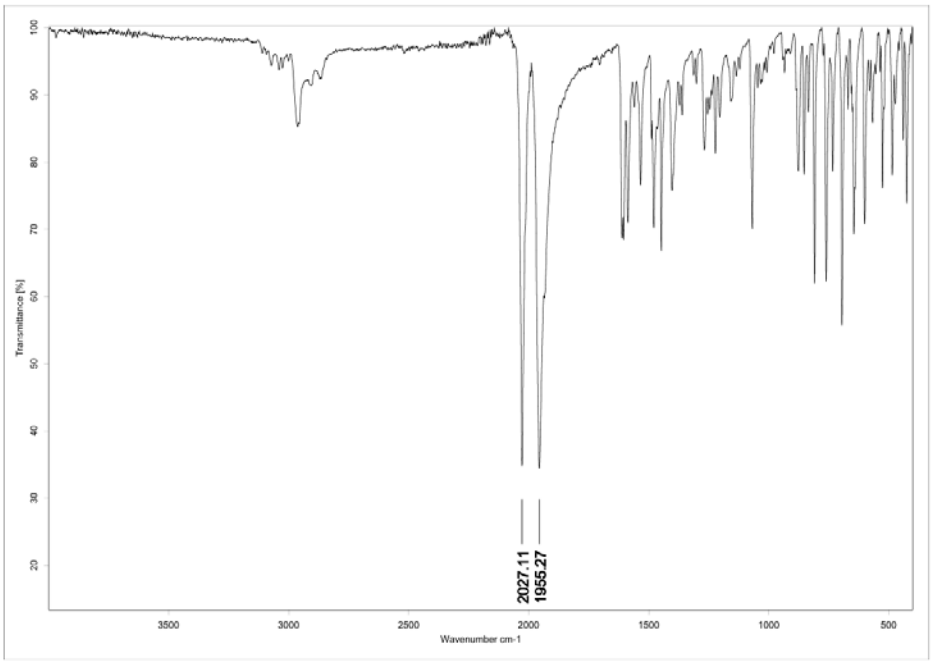

Figure S4. Solid state IR spectrum of complex **7** (ATR)

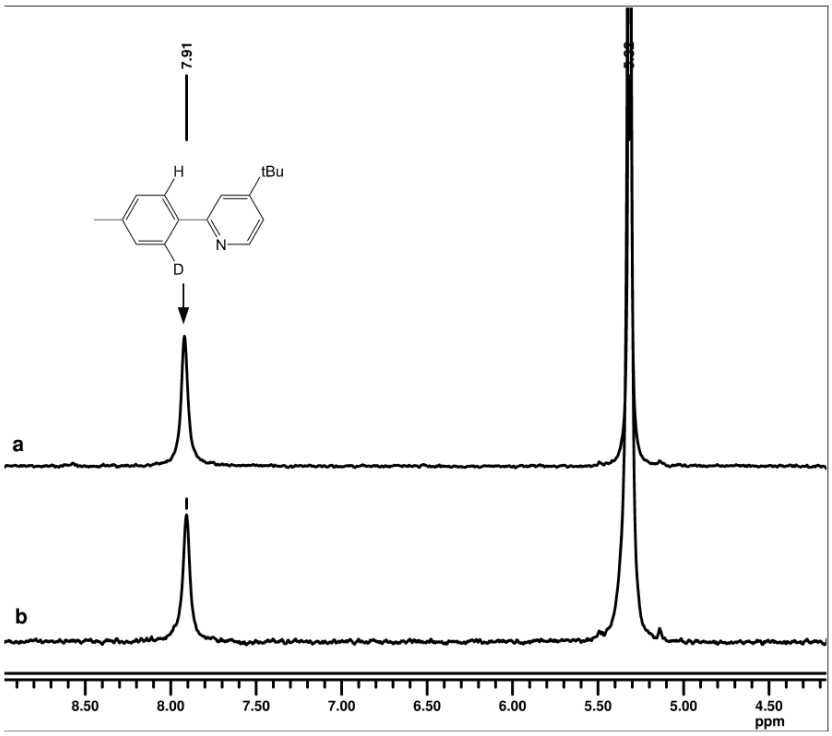

Figure S5. $^{2}H\{^{1}H\}$ NMR spectra (in CH_2Cl_2, locked on ^{19}F C_6F_6, internal reference CD_2Cl_2) of the ligand **9** (2-(*p*-tolyl)-4-tertbutylpyridine) after reaction of complex **1** in THF with a) ND_3BH_3 and b) NH_3BD_3

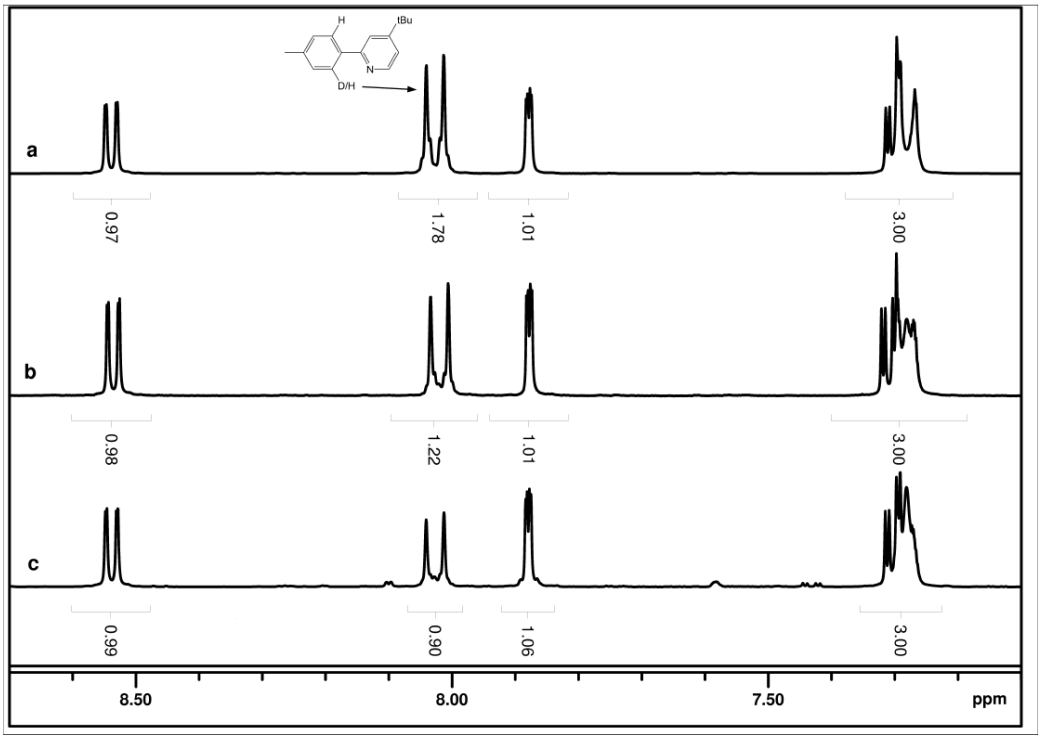

Figure S6. ^{1}H NMR spectra (in d_6-acetone) of the partially deuterated ligand **9** after reaction of complex **1** in THF with a) ND_3BH_3, b) NH_3BD_3 and c) ND_3BD_3

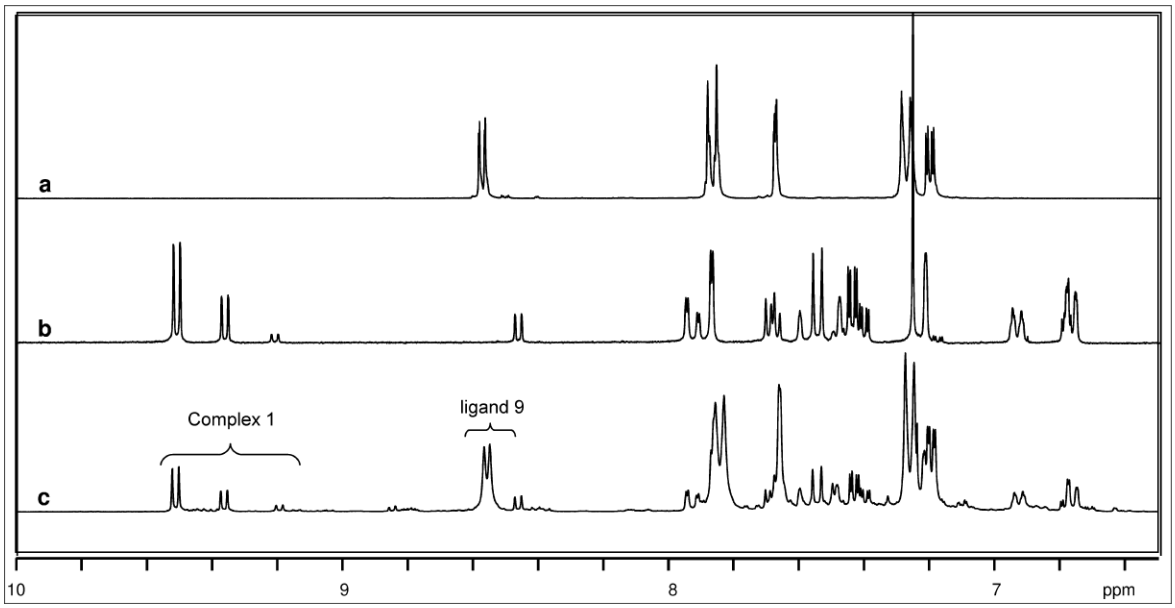

Figure S7. ^{1}H NMR spectra of a) ligand **9**, b) pure complex **1** and c) the reaction of complex **1** with $LiEt_3BH$ and ligand **9**.

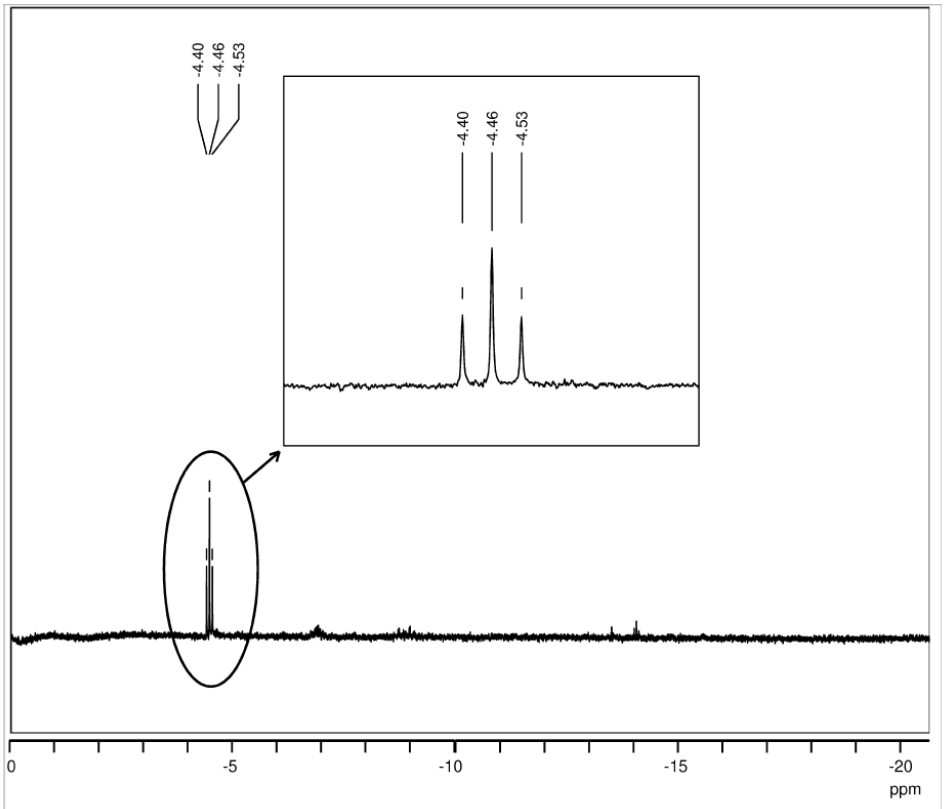

Figure S8. ^{1}H NMR spectrum in the hydrido region of $Ru(CO)_2(PPh_3)_2ClH$

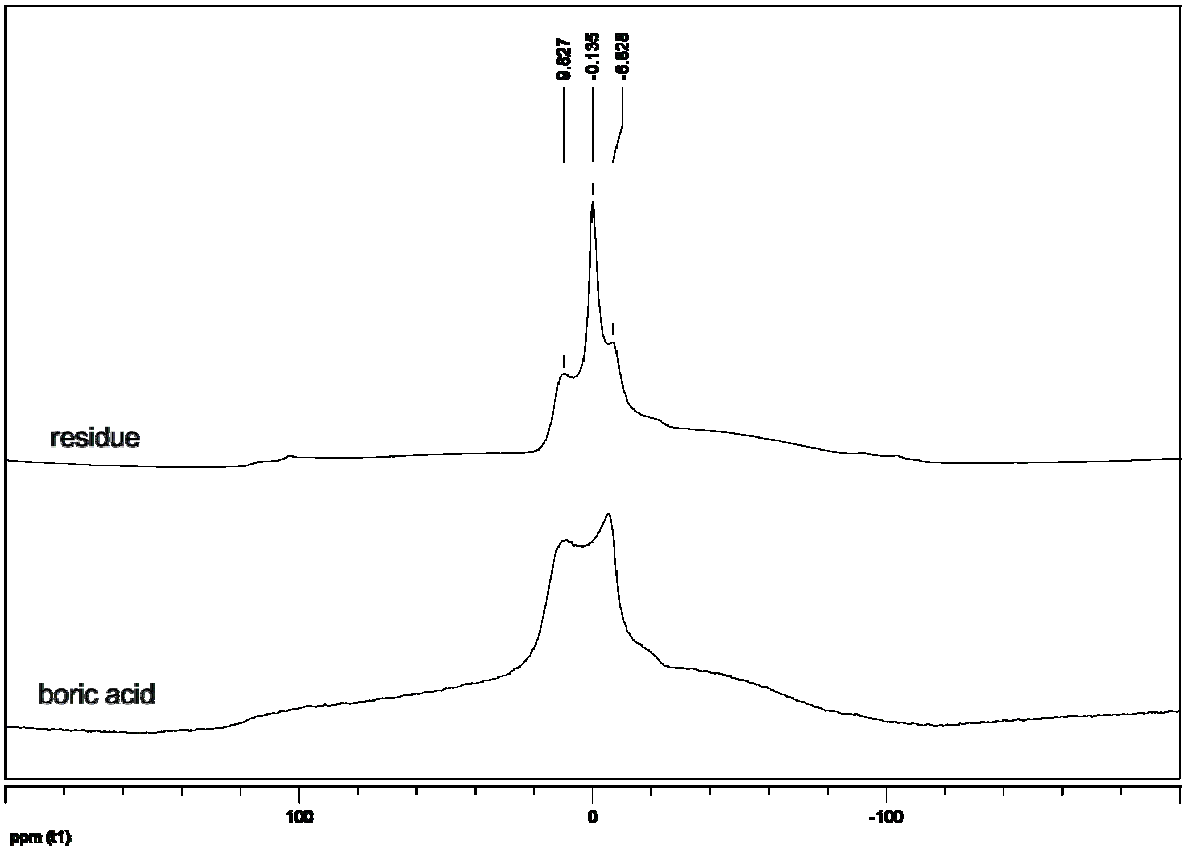

Figure S9. Magic Angle Spining ^{11}B NMR spectrum of the off-white solid residue (above) and the spectrum of boric acid $B(OH)_3$ (below).

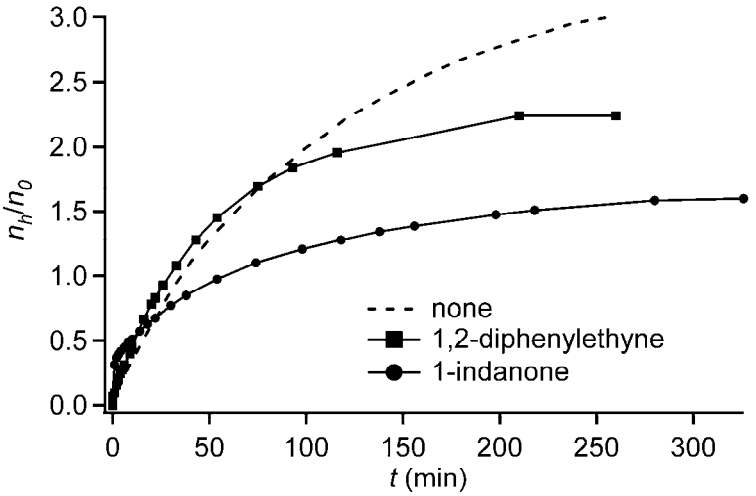

Fig. 10 Inhibition of the production of H_2 by notorious hydrogen acceptors such as 1,2-diphenylethyne (■) and 1-indanone (●).

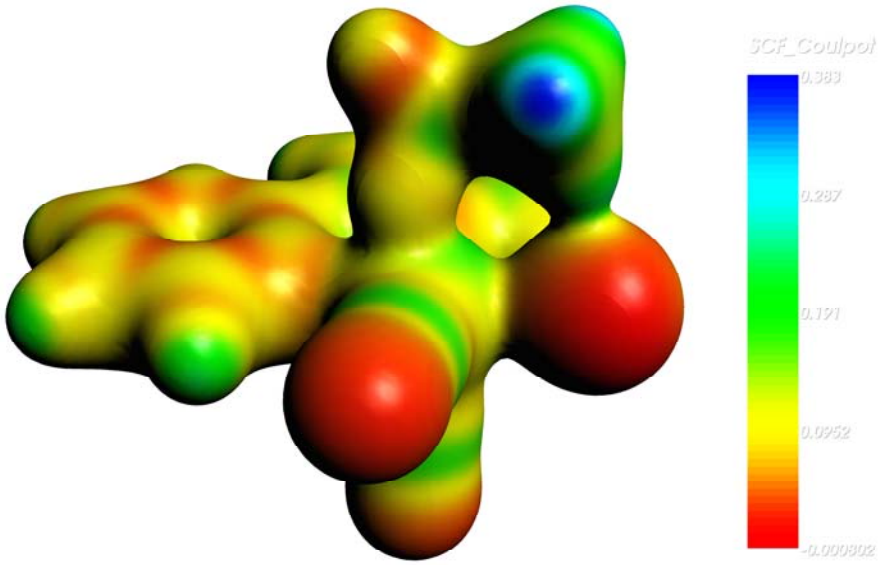

Figure S11. Coulombic map (bar graph in a.u.) drawn over the isosurface of the SCF electron density (0.030 e/bohr^3) for conformer **A1.**

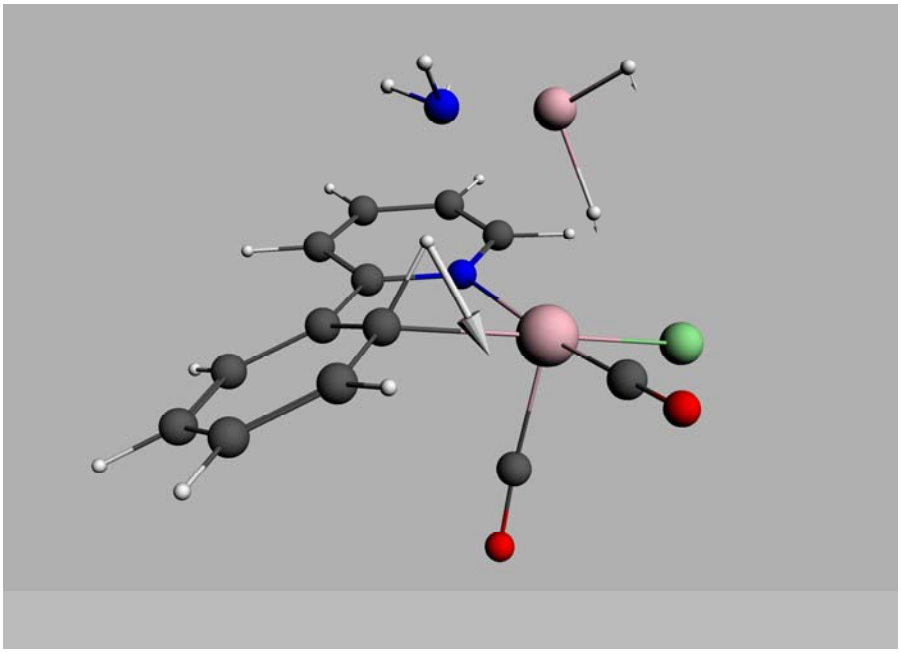

Figure S12. Displacement vectors for **TS1** in the gas phase showing the direction of the imaginary vibrational mode.

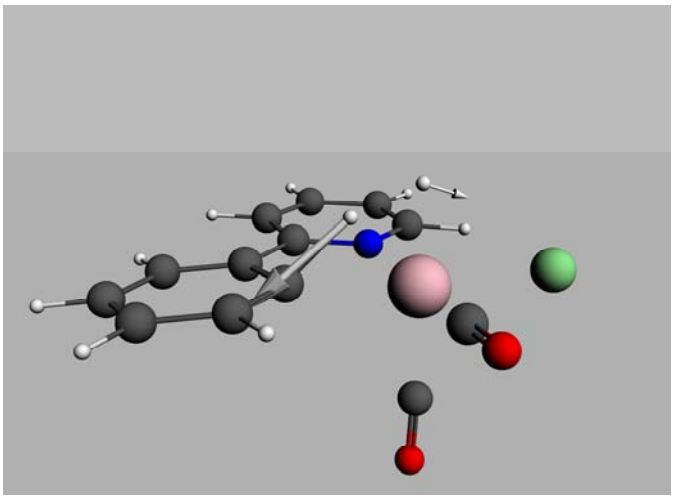

Figure S13. Displacement vectors for **TS2** in the gas phase showing the direction of the imaginary vibrational mode.

Computational data (BP86-D/TZP (ZORA)): Cartesian coordinates, energies and vibrational modes.

Gas Phase

NH_3BH3

Geometry CYCLE 4
==========

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

Atom	Cartesian (a.u./angstrom) X	Y	Z
1 N	-0.000065	-0.000604	-0.000002
2 H	0.000019	-0.000032	0.000419
3 H	0.000021	-0.000025	0.000058
4 H	0.000032	0.000213	-0.000126
5 B	0.000209	0.000338	-0.000525
6 H	-0.000101	0.000114	0.000005
7 H	-0.000081	0.000040	0.000120
8 H	-0.000034	-0.000044	0.000052

Geometry Convergence after Step 4

current energy	-1.34142056 Hartree		
abs of energy change	0.00000804	0.00100000	T
constrained gradient max	0.00060363	0.00100000	T
constrained gradient rms	0.00021376	0.00066667	T
gradient max	0.00060363		
gradient rms	0.00021376		
cart. step max	0.00804663	0.01000000	T
cart. step rms	0.00280078	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	9.475363101412809	257.8377	5945.88	24877.56
Delta V^Pauli Coulomb:	-4.244486946053502	-115.4984	-2663.46	-11143.90
Delta V^Pauli LDA-XC:	-1.329331157064725	-36.1729	-834.17	-3490.16
Delta V^Pauli GGA-Exchange:	0.059695812782594	1.6244	37.46	156.73
Delta V^Pauli GGA-Correlation:	-0.013815718520040	-0.3759	-8.67	-36.27
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	3.947425092557136	107.4149	2477.05	10363.96
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	3.947425092557136	107.4149	2477.05	10363.96
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-0.669881778438920	-18.2284	-420.36	-1758.77
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	3.277543314118216	89.1865	2056.69	8605.19
Orbital Interactions				
A:	-4.613973735726518	-125.5526	-2895.31	-12113.99
Total Orbital Interactions:	-4.614202057258072	-125.5588	-2895.46	-12114.59
Alternative Decomposition Orb.Int.				
Kinetic:	-8.240635362366771	-224.2391	-5171.08	-21635.79
Coulomb:	3.509859504204933	95.5081	2202.47	9215.13
XC:	0.116573800903766	3.1721	73.15	306.06
Total Orbital Interactions:	-4.614202057258072	-125.5588	-2895.46	-12114.59
Residu (E=Steric+OrbInt+Res):	0.000000073359140	0.0000	0.00	0.00
Dispersion Energy:	-0.004767002071385	-0.1297	-2.99	-12.52
Total Bonding Energy:	-1.341425671852101	-36.5020	-841.76	-3521.91

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

Electrostatic Energy:	-0.669881778438920	-18.2284	-420.36	-1758.77
Kinetic Energy:	1.234727739046038	33.5987	774.80	3241.78
Coulomb (Steric+OrbInt) Energy:	-0.734627368489428	-19.9902	-460.99	-1928.76
XC Energy:	-1.166877261898406	-31.7523	-732.23	-3063.64

Dispersion Energy:	-0.004767002071385	-0.1297	-2.99	-12.52
Total Bonding Energy:	-1.341425671852102	-36.5020	-841.76	-3521.91

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:	-10.155392089080674	-276.3423	-6372.61	-26662.98
Exchange GGA:	-1.418171653554853	-38.5904	-889.92	-3723.41
Correlation LDA:	-0.992813018429513	-27.0158	-623.00	-2606.63
Correlation GGA:	0.540447948412429	14.7063	339.14	1418.95
Total XC:	-12.025928812652612	-327.2422	-7546.39	-31574.07

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

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
250.669286	0.006631	0.000417
606.374899	8.561525	1.301279
607.655663	8.626302	1.313894
619.891690	64.507785	10.023191
1032.411967	104.062932	26.929430
1033.185027	104.325374	27.017560
1152.320646	463.522568	133.882033
1171.042437	14.690612	4.312118
1171.306193	15.614433	4.584318
1282.323884	264.205148	84.921387
1617.099743	57.790232	23.424445
1617.921136	57.176931	23.187624
2416.357490	85.480265	51.773213
2437.187610	386.635944	236.194216
2439.443343	386.061399	236.061513
3341.955033	0.551385	0.461885
3452.942519	34.251964	29.645099
3453.497434	34.495823	29.860957

Zero-Point Energy : 0.067670 a.u.
================== 1.841388 eV

```
NH2BH2
Geometry CYCLE 7
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 N    -0.000184 -0.000414 -0.000236
     2 H     0.000147  0.000074  0.000137
     3 H    -0.000054  0.000189  0.000086
     4 B     0.000163  0.000206 -0.000006
     5 H    -0.000089  0.000001 -0.000001
     6 H     0.000016 -0.000056  0.000018
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step   7
-------------------------------------
current energy                          -1.09202318 Hartree
abs of energy change               0.00001186     0.00100000    T
constrained gradient max           0.00041409     0.00100000    T
constrained gradient rms           0.00015524     0.00066667    T
gradient max                       0.00041409
gradient rms                       0.00015524
cart. step max                     0.00019249     0.01000000    T
cart. step rms                     0.00010776     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              8.330865559202879        226.6944         5227.70         21872.68
  Delta V^Pauli Coulomb:           -3.786877152067238       -103.0462        -2376.30         -9942.44
  Delta V^Pauli LDA-XC:            -1.104940156426055        -30.0670         -693.36         -2901.02
  Delta V^Pauli GGA-Exchange:       0.042996678775991          1.1700           26.98           112.89
  Delta V^Pauli GGA-Correlation:   -0.007728236534039         -0.2103           -4.85           -20.29
                                   --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:            3.474316692951537         94.5410         2180.17          9121.82
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  3.474316692951537         94.5410         2180.17          9121.82
  Electrostatic Interaction:       -0.582264715648477        -15.8442         -365.38         -1528.74
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                   --------------------     -----------     ----------     -----------
  Total Steric Interaction:         2.892051977303060         78.6967         1814.79          7593.08
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -3.980991805861237       -108.3283        -2498.11        -10452.09
                                   --------------------     -----------     ----------     -----------
  Total Orbital Interactions:      -3.982099875130255       -108.3585        -2498.81        -10455.00

Alternative Decomposition Orb.Int.
  Kinetic:                         -7.322187980673743       -199.2469        -4594.74        -19224.40
  Coulomb:                          3.222568404270911         87.6905         2022.19          8460.85
  XC:                               0.117519701272575          3.1979           73.74           308.55
                                   --------------------     -----------     ----------     -----------
  Total Orbital Interactions:      -3.982099875130257       -108.3585        -2498.81        -10455.00

  Residu (E=Steric+OrbInt+Res):     0.000000123990338          0.0000            0.00            0.00
  Dispersion Energy:               -0.001975807134409         -0.0538           -1.24           -5.19

Total Bonding Energy:              -1.092023580971266        -29.7155         -685.26         -2867.11


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

  Electrostatic Energy:            -0.582264715648477        -15.8442         -365.38         -1528.74
  Kinetic Energy:                   1.008677578529136         27.4475          632.95          2648.28
  Coulomb (Steric+OrbInt) Energy:  -0.564308623805989        -15.3556         -354.11         -1481.59
  XC Energy:                       -0.952152012911528        -25.9094         -597.48         -2499.87
  Dispersion Energy:               -0.001975807134409         -0.0538           -1.24           -5.19
                                   --------------------     -----------     ----------     -----------
  Total Bonding Energy:            -1.092023580971266        -29.7155         -685.26         -2867.11
```

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:	-9.758673086480334	-265.5470	-6123.66	-25621.39
Exchange GGA:	-1.330697359523562	-36.2101	-835.03	-3493.75
Correlation LDA:	-0.912973364820409	-24.8433	-572.90	-2397.01
Correlation GGA:	0.492780474387309	13.4092	309.22	1293.79
Total XC:	-11.509563336436996	-313.1912	-7222.36	-30218.35

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
590.376991	1054.400821	156.031840
710.011066	0.640427	0.113976
842.338362	0.011383	0.002403
971.208898	85.840138	20.896865
1098.654340	115.192303	31.722150
1119.385973	1.746262	0.489968
1317.917496	158.210305	52.263810
1586.633385	170.620150	67.855488
2528.118534	131.140351	83.102070
2587.737211	234.978067	152.414248
3473.369455	18.626334	16.216474
3572.492492	29.325987	26.260442

Zero-Point Energy : 0.046471 a.u.
1.264530 eV

```
THF

 Geometry CYCLE 5
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 O    -0.000047  0.000385 -0.000079
     2 C     0.000007  0.000089  0.000231
     3 C    -0.000240 -0.000413 -0.000265
     4 C     0.000575 -0.000117 -0.000043
     5 C    -0.000261  0.000020  0.000197
     6 H     0.000013 -0.000055 -0.000066
     7 H     0.000002  0.000014 -0.000057
     8 H    -0.000008  0.000090  0.000042
     9 H     0.000011 -0.000021  0.000059
    10 H    -0.000083 -0.000002  0.000037
    11 H    -0.000016  0.000024  0.000083
    12 H     0.000022  0.000038 -0.000050
    13 H     0.000025 -0.000051 -0.000089
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step   5
-------------------------------------
current energy                          -2.61277822 Hartree
abs of energy change              0.00000365     0.00100000    T
constrained gradient max          0.00057514     0.00100000    T
constrained gradient rms          0.00016224     0.00066667    T
gradient max                      0.00057514
gradient rms                      0.00016224
cart. step max                    0.00090178     0.01000000    T
cart. step rms                    0.00028594     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              22.890281443009279       622.8763        14363.87         60098.43
  Delta V^Pauli Coulomb:           -11.038243781658490      -300.3659        -6926.60        -28980.90
  Delta V^Pauli LDA-XC:             -3.101531706304075       -84.3970        -1946.24         -8143.07
  Delta V^Pauli GGA-Exchange:        0.175555220962442         4.7771          110.16           460.92
  Delta V^Pauli GGA-Correlation:    -0.048966164215446        -1.3324          -30.73          -128.56
                                  --------------------  -----------  ----------  -----------
  Total Pauli Repulsion:            8.877095011793708       241.5580         5570.46         23306.81
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  8.877095011793708       241.5580         5570.46         23306.81
  Electrostatic Interaction:       -1.784941411517720       -48.5707        -1120.07         -4686.36
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------  -----------  ----------  -----------
  Total Steric Interaction:         7.092153600275988       192.9873         4450.39         18620.45
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -9.692871193071523      -263.7564        -6082.37        -25448.63
                                  --------------------  -----------  ----------  -----------
  Total Orbital Interactions:      -9.694441132285752      -263.7992        -6083.35        -25452.75

Alternative Decomposition Orb.Int.
  Kinetic:                        -20.473966738628711      -557.1250       -12847.61        -53754.39
  Coulomb:                         10.164291456065923       276.5844         6378.19         26686.34
  XC:                               0.615234150277038        16.7414          386.07          1615.30
                                  --------------------  -----------  ----------  -----------
  Total Orbital Interactions:      -9.694441132285750      -263.7992        -6083.35        -25452.75

  Residu (E=Steric+OrbInt+Res):     0.000011387989756         0.0003            0.01            0.03
  Dispersion Energy:               -0.010502093247352        -0.2858           -6.59           -27.57

Total Bonding Energy:              -2.612778237267360       -71.0973        -1639.54         -6859.85


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

Electrostatic Energy:	-1.784941411517720	-48.5707	-1120.07	-4686.36
Kinetic Energy:	2.416314704380568	65.7513	1516.26	6344.03
Coulomb (Steric+OrbInt) Energy:	-0.873940937602811	-23.7811	-548.41	-2294.53
XC Energy:	-2.359708499280041	-64.2109	-1480.74	-6195.41
Dispersion Energy:	-0.010502093247352	-0.2858	-6.59	-27.57
Total Bonding Energy:	-2.612778237267356	-71.0973	-1639.54	-6859.85

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:	-26.366666276461654	-717.4735	-16545.33	-69225.67
Exchange GGA:	-3.477241068681778	-94.6205	-2182.00	-9129.50
Correlation LDA:	-2.361509048595487	-64.2599	-1481.87	-6200.14
Correlation GGA:	1.254069282264207	34.1250	786.94	3292.56
Total XC:	-30.951347111474707	-842.2290	-19422.27	-81262.75

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
68.419279	3.223696	0.055285
281.425128	95.667244	6.748453
609.411526	18.588708	2.839474
629.997955	10.982929	1.734345
770.490969	31.444152	6.072751
835.578726	23.751746	4.974632
871.935522	36.258241	7.924451
898.192506	5.670540	1.276650
902.284602	104.749607	23.690489
920.490305	69.127242	15.949480
1006.384249	17.733985	4.473508
1039.690042	270.823952	70.577948
1105.498778	5.115224	1.417428
1163.871521	16.438091	4.795507
1178.785432	10.361255	3.061436
1210.325821	13.876053	4.209653
1220.245544	14.311725	4.377410
1259.463559	3.272073	1.032967
1266.616758	0.341808	0.108519
1303.722575	4.483227	1.465055
1337.464945	21.554361	7.225961
1430.245395	2.651739	0.950647
1445.166963	14.291761	5.177044
1449.751965	0.104408	0.037941
1464.104832	3.004081	1.102458
2860.795612	78.360093	56.190105
2867.031333	131.854608	94.755804
2958.981900	33.604222	24.923798
2969.593278	48.247891	35.913140
2999.386912	32.956094	24.776862
3007.967128	2.397602	1.807708
3011.684710	20.768012	15.677706
3026.971486	66.060515	50.121996

Zero-Point Energy : 0.112478 a.u.
========== 3.060672 eV

```
H2

 Geometry CYCLE 2
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 H     0.000000  0.000000  0.000012
     2 H     0.000000  0.000000 -0.000012
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step   2
-------------------------------------
current energy                          -0.24701946 Hartree
abs of energy change               0.00000001     0.00100000    T
constrained gradient max           0.00001224     0.00100000    T
constrained gradient rms           0.00000707     0.00066667    T
gradient max                       0.00001224
gradient rms                       0.00000707
cart. step max                     0.00000487     0.01000000    T
cart. step rms                     0.00000281     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              0.586657888097204         15.9638          368.13          1540.27
  Delta V^Pauli Coulomb:           -0.124043204450532         -3.3754          -77.84          -325.68
  Delta V^Pauli LDA-XC:            -0.093608449913325         -2.5472          -58.74          -245.77
  Delta V^Pauli GGA-Exchange:      -0.002585610259500         -0.0704           -1.62            -6.79
  Delta V^Pauli GGA-Correlation:    0.001753742413758          0.0477            1.10             4.60
                                   --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:            0.368174365887605         10.0185          231.03          966.64
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  0.368174365887605         10.0185          231.03          966.64
  Electrostatic Interaction:        0.009131239247804          0.2485            5.73           23.97
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                   --------------------     -----------     ----------     -----------
  Total Steric Interaction:         0.377305605135409         10.2670          236.76          990.62
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  SIGMA.g:                         -0.478572041547944        -13.0226         -300.31        -1256.49
  SIGMA.u:                         -0.145625006965815         -3.9627          -91.38          -382.34
  PI.g:                             0.000000000000000          0.0000            0.00            0.00
  PI.u:                             0.000000000000000          0.0000            0.00            0.00
                                   --------------------     -----------     ----------     -----------
  Total Orbital Interactions:      -0.624323907551419        -16.9887         -391.77        -1639.16

Alternative Decomposition Orb.Int.
  Kinetic:                         -0.348648410664324         -9.4872         -218.78          -915.38
  Coulomb:                         -0.187379696954795         -5.0989         -117.58          -491.97
  XC:                              -0.088295799932301         -2.4027          -55.41          -231.82
                                   --------------------     -----------     ----------     -----------
  Total Orbital Interactions:      -0.624323907551419        -16.9887         -391.77        -1639.16

  Residu (E=Steric+OrbInt+Res):     0.000000007331080          0.0000            0.00            0.00
  Dispersion Energy:               -0.000001163948600          0.0000            0.00            0.00

Total Bonding Energy:              -0.247019459033531         -6.7217         -155.01         -648.55


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

  Electrostatic Energy:             0.009131239247804          0.2485            5.73           23.97
  Kinetic Energy:                   0.238009477432881          6.4766          149.35          624.89
  Coulomb (Steric+OrbInt) Energy:  -0.311422894074247         -8.4742         -195.42         -817.64
  XC Energy:                       -0.182736117691369         -4.9725         -114.67         -479.77
  Dispersion Energy:               -0.000001163948600          0.0000            0.00            0.00
                                   --------------------     -----------     ----------     -----------
  Total Bonding Energy:            -0.247019459033531         -6.7217         -155.01         -648.55
```

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:	-0.396722097407383	-10.7954	-248.95	-1041.59
Exchange GGA:	-0.087472208603464	-2.3802	-54.89	-229.66
Correlation LDA:	-0.079840340640093	-2.1726	-50.10	-209.62
Correlation GGA:	0.047665891717013	1.2971	29.91	125.15
Total XC:	-0.516368754933928	-14.0511	-324.03	-1355.73

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
4300.547628	0.000000	0.000000

Zero-Point Energy : 0.009797 a.u.
0.266600 eV

S1

Geometry CYCLE 31
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	-0.000068	-0.000033	0.000001
2	H	-0.000031	-0.000070	-0.000018
3	C	0.000017	-0.000008	0.000009
4	C	0.000006	0.000027	-0.000024
5	Cl	-0.000138	-0.000060	-0.000180
6	N	0.000133	-0.000058	-0.000081
7	O	0.000069	-0.000080	-0.000135
8	C	-0.000054	-0.000045	-0.000039
9	O	-0.000084	-0.000068	-0.000088
10	H	-0.000041	-0.000051	0.000036
11	C	-0.000007	0.000065	0.000229
12	C	0.000005	-0.000001	-0.000008
13	C	0.000196	0.000144	0.000140
14	Ru	0.000362	-0.000253	0.000004
15	H	-0.000060	-0.000104	0.000029
16	Ru	0.000454	0.000171	0.000049
17	C	-0.000029	-0.000034	0.000007
18	C	-0.000342	0.000011	0.000202
19	C	0.000017	0.000040	-0.000025
20	C	-0.000054	-0.000060	0.000046
21	H	-0.000022	0.000018	0.000047
22	H	0.000087	0.000061	0.000012
23	C	0.000021	0.000024	-0.000013
24	O	-0.000128	0.000088	0.000030
25	N	0.000175	0.000120	-0.000002
26	H	-0.000017	-0.000037	0.000032
27	C	0.000086	0.000051	0.000004
28	C	-0.000007	-0.000032	-0.000072
29	H	0.000012	-0.000005	0.000009
30	C	-0.000064	-0.000149	0.000105
31	C	-0.000031	-0.000018	0.000008
32	C	-0.000073	0.000021	-0.000055
33	C	0.000015	0.000032	0.000003
34	H	-0.000025	-0.000033	0.000022
35	C	-0.000162	-0.000066	-0.000070
36	C	-0.000083	-0.000102	-0.000010
37	H	0.000020	-0.000024	-0.000003
38	C	-0.000073	-0.000081	-0.000013
39	C	0.000065	0.000022	0.000033
40	C	0.000011	0.000010	0.000024
41	H	-0.000031	0.000028	-0.000039
42	H	-0.000033	-0.000045	-0.000004
43	C	-0.000011	0.000048	-0.000015
44	H	0.000051	0.000037	-0.000032
45	C	-0.000051	-0.000008	-0.000006
46	H	-0.000014	0.000014	-0.000005
47	H	-0.000034	-0.000001	-0.000001
48	H	0.000033	0.000018	-0.000026
49	H	-0.000026	-0.000033	-0.000013
50	Cl	-0.000095	0.000162	-0.000109
51	C	-0.000124	0.000278	-0.000045
52	O	0.000176	0.000074	0.000047

Geometry Convergence after Step 31

---

current energy -13.12371103 Hartree

abs of energy change	0.00001438	0.00100000	T
constrained gradient max	0.00045415	0.00100000	T
constrained gradient rms	0.00009281	0.00066667	T
gradient max	0.00045415		
gradient rms	0.00009281		
cart. step max	0.00814301	0.01000000	T
cart. step rms	0.00229654	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	153.952132502709020	4189.2507	96606.43	404201.27

```
  Delta V^Pauli Coulomb:          -80.347159564187194      -2186.3575       -50418.61       -210951.44
  Delta V^Pauli LDA-XC:           -18.978088241945624       -516.4201       -11908.93        -49826.96
  Delta V^Pauli GGA-Exchange:       1.111431930123906         30.2436          697.43          2918.06
  Delta V^Pauli GGA-Correlation:   -0.313327236086980         -8.5261         -196.62          -822.64
                                  --------------------     -----------     ----------      -----------
  Total Pauli Repulsion:           55.424989390613121       1508.1907        34779.71        145518.29
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 55.424989390613121       1508.1907        34779.71        145518.29
  Electrostatic Interaction:      -11.830276015325479       -321.9182        -7423.61        -31060.39
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------     -----------     ----------      -----------
  Total Steric Interaction:        43.594713375287640       1186.2725        27356.10        114457.90
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                              -56.603504382532336      -1540.2597       -35519.24       -148612.48
                                  --------------------     -----------     ----------      -----------
  Total Orbital Interactions:     -56.610529736491607      -1540.4509       -35523.65       -148630.92

Alternative Decomposition Orb.Int.
  Kinetic:                       -141.565142472235721      -3852.1835       -88833.48       -371679.23
  Coulomb:                         78.217373469240698       2128.4030        49082.15        205359.68
  XC:                               6.737239266503427        183.3296         4227.68         17688.62
                                  --------------------     -----------     ----------      -----------
  Total Orbital Interactions:     -56.610529736491593      -1540.4509       -35523.65       -148630.92

  Residu (E=Steric+OrbInt+Res):    -0.000018446508690         -0.0005          -0.01           -0.05
  Dispersion Energy:               -0.107876461011881         -2.9355         -67.69          -283.23

Total Bonding Energy:              -13.123711268724540       -357.1144        -8235.25        -34456.30


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

  Electrostatic Energy:           -11.830276015325479       -321.9182        -7423.61        -31060.39
  Kinetic Energy:                  12.386990030473299        337.0671         7772.95         32522.04
  Coulomb (Steric+OrbInt) Energy:  -2.129804541455186        -57.9549        -1336.47         -5591.80
  XC Energy:                      -11.442744281405272       -311.3729        -7180.43        -30042.92
  Dispersion Energy:               -0.107876461011881         -2.9355         -67.69          -283.23
                                  --------------------     -----------     ----------      -----------
  Total Bonding Energy:           -13.123711268724520       -357.1144        -8235.25        -34456.30


 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:                   -459.234343486345836     -12496.4023      -288173.93      -1205719.60
  Exchange GGA:                    -38.707740255224188      -1053.2912       -24289.48       -101627.16
  Correlation LDA:                 -24.378269980365868       -663.3665       -15297.60        -64005.14
  Correlation GGA:                  11.324532059261134        308.1562         7106.25         29732.55
                                  --------------------     -----------     ----------      -----------
  Total XC:                       -510.995821662674700     -13904.9038      -320654.75      -1341619.34

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2                km/mole
             ----------          ----------           ----------
              16.407522          122.426407             0.503496
              27.640788          239.282897             1.657831
              32.629782          105.467618             0.862604
              34.376802           13.502056             0.116344
              42.527907            0.970340             0.010344
              66.184792            5.925825             0.098307
              67.881432            4.167426             0.070908
              69.190312            1.966606             0.034107
              76.260582            0.083871             0.001603
              84.106624          121.686461             2.565373
              87.505705            0.477713             0.010478
              90.461567            3.019843             0.068474
              90.777980            1.426425             0.032457
              95.867225            0.184745             0.004439
             106.380128            5.334753             0.142250
```

107.327134	34.490071	0.927858
117.814900	2.745834	0.081087
128.061312	0.026047	0.000836
139.177032	0.010590	0.000369
152.806689	41.658050	1.595583
186.366421	38.702382	1.807938
198.686069	0.006173	0.000307
200.894378	10.406037	0.524000
203.941158	0.035306	0.001805
216.081160	224.564695	12.162881
219.615479	3.385921	0.186388
254.137172	42.625080	2.715260
254.968722	1.238357	0.079143
261.395074	0.942605	0.061760
263.834325	56.105112	3.710324
269.341821	0.017492	0.001181
284.380546	744.191154	53.047199
290.541272	5.944062	0.432882
292.248047	73.836282	5.408782
371.337824	8.839940	0.822804
372.018280	24.360502	2.271583
413.370890	65.781893	6.815917
414.301720	18.834723	1.955933
423.950451	12.976465	1.378953
425.107333	0.008438	0.000899
465.281802	0.172425	0.020109
466.030212	21.824777	2.549423
468.469252	0.041778	0.004906
468.957408	14.345462	1.686266
486.907761	1.311448	0.160057
487.288662	19.640757	2.398958
507.964490	0.345321	0.043968
510.388036	66.519261	8.509930
519.797473	128.116765	16.692378
520.129257	17.469688	2.277585
542.408452	7.851903	1.067528
543.006654	52.648290	7.165846
554.776924	3.573570	0.496934
555.388015	0.080829	0.011252
592.703991	49.606325	7.369754
593.526305	176.435302	26.248442
624.129246	22.948505	3.590104
624.810702	52.104796	8.160264
635.707208	233.553693	37.215336
636.542768	15.176010	2.421382
643.313539	28.730609	4.632822
643.643949	23.408040	3.776494
659.524315	1.727507	0.285581
659.907868	14.844217	2.455380
712.304460	22.902611	4.089109
713.148855	27.376164	4.893627
721.606078	0.055141	0.009974
721.919098	224.315542	40.590646
737.693391	286.438032	52.964472
738.051020	459.180923	84.947048
754.564876	2.852259	0.539465
755.301810	3.416214	0.646761
780.435433	5.188794	1.015036
780.731441	20.756200	4.061885
843.173605	3.738542	0.790128
843.708445	3.117751	0.659344
860.466680	7.132538	1.538354
860.956359	4.406271	0.950890
921.099001	0.415603	0.095954
921.655250	0.516019	0.119210
960.386771	5.407271	1.301674
960.625340	0.970081	0.233583
962.624474	4.225411	1.019539
962.718834	1.833422	0.442425
974.865531	1.689495	0.412838
975.329480	0.896734	0.219227
998.532290	6.221002	1.557043
998.611207	30.380036	7.604362
1004.740355	157.569607	39.682988
1005.179430	70.864066	17.854502
1015.266556	0.062701	0.015956
1015.503228	27.981538	7.122475
1045.204084	4.226615	1.107317
1045.506138	4.652195	1.219165
1048.376777	58.043351	15.252743
1049.155560	49.148424	12.924911
1093.878480	6.916022	1.896285
1094.515879	7.286476	1.999023
1106.316182	2.971740	0.824078
1106.811638	3.717122	1.031237

1133.999792	7.161952	2.035741
1134.114603	15.606982	4.436638
1150.191839	43.610631	12.573052
1150.291946	4.655622	1.342344
1240.131000	13.305606	4.135998
1240.913860	19.357581	6.021030
1268.904619	89.865861	28.582604
1269.376871	3.592448	1.143034
1283.434252	12.390445	3.986012
1283.911407	10.274056	3.306397
1302.953349	40.347270	13.177138
1304.370996	34.532709	11.290414
1314.496246	35.771572	11.786245
1315.009595	32.717968	10.784334
1408.797107	35.072530	12.384932
1409.100749	103.806739	36.664491
1423.657323	11.509760	4.107237
1423.910325	14.839959	5.296554
1441.549735	3.896525	1.407943
1442.129006	14.743891	5.329596
1468.867467	18.157696	6.685308
1469.579770	283.674148	104.493913
1538.437814	18.573892	7.162439
1538.847146	31.728182	12.238234
1551.720135	88.054724	34.248703
1552.322795	78.107671	30.391616
1570.575561	125.914970	49.569469
1571.372162	102.966171	40.555680
1594.113370	124.087632	49.582198
1594.665125	167.088583	66.787370
1941.636128	85.858613	41.785902
1943.411662	2347.436678	1143.501558
2003.408481	2509.712728	1260.293195
2007.336012	13.357281	6.720726
3077.167214	2.482910	1.915094
3077.958719	1.869286	1.442170
3088.083295	8.886580	6.878627
3088.594978	8.944362	6.924500
3096.274878	17.119545	13.286476
3096.646663	16.765519	13.013278
3098.600985	8.509888	6.609484
3098.763552	9.919582	7.704774
3106.007018	15.950647	12.418204
3106.738301	23.316822	18.157334
3110.402318	73.699512	57.459157
3110.505632	12.943652	10.091736
3128.732167	2.329308	1.826726
3129.109642	2.479769	1.944957
3133.682208	10.459928	8.216024
3134.084277	8.249392	6.480532

Zero-Point Energy : **0.348378 a.u.**
========== **9.479854 eV**

A1

Geometry CYCLE 20
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	O	0.000027	0.000008	-0.000065
2	O	0.000121	-0.000073	0.000012
3	C	-0.000058	0.000097	0.000193
4	C	-0.000334	-0.000107	-0.000023
5	H	0.000023	0.000088	-0.000003
6	Ru	-0.000145	-0.000669	-0.000057
7	C	0.000217	0.000007	-0.000017
8	H	0.000010	0.000018	0.000003
9	N	-0.000446	-0.000002	0.000198
10	H	0.000000	-0.000002	0.000023
11	C	-0.000106	-0.000016	0.000059
12	C	-0.000052	0.000542	0.000078
13	C	0.000087	-0.000151	0.000089
14	C	0.000093	-0.000088	-0.000058
15	C	0.000029	0.000011	-0.000095
16	C	0.000017	0.000011	0.000026
17	C	-0.000028	0.000060	-0.000011
18	C	0.000032	-0.000013	-0.000038
19	H	-0.000006	-0.000050	-0.000038
20	H	0.000040	0.000012	-0.000015
21	C	0.000040	-0.000081	0.000016
22	H	0.000014	0.000043	-0.000012
23	C	0.000008	0.000049	0.000014
24	H	0.000018	0.000056	-0.000008
25	H	0.000007	-0.000018	-0.000029
26	Cl	-0.000180	0.000177	-0.000055
27	N	-0.000038	-0.000214	0.000279
28	H	0.000289	-0.000226	-0.000254
29	H	-0.000047	0.000178	-0.000168
30	H	-0.000007	-0.000116	0.000011
31	B	-0.000026	0.000173	0.000065
32	H	-0.000059	0.000015	-0.000101
33	H	0.000479	0.000126	-0.000040
34	H	-0.000021	0.000153	0.000021

Geometry Convergence after Step 20

current energy	-7.91684126 Hartree		
abs of energy change	0.00001542	0.00100000	T
constrained gradient max	0.00066907	0.00100000	T
constrained gradient rms	0.00014583	0.00066667	T
gradient max	0.00066907		
gradient rms	0.00014583		
cart. step max	0.00916826	0.01000000	T
cart. step rms	0.00255898	0.00666667	T

Number of elements of the density matrix on this node (used, total): 37258 148240

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	87.082607436524015	2369.6383	54645.17	228635.35
Delta V^Pauli Coulomb:	-44.722204339322715	-1216.9531	-28063.61	-117418.13
Delta V^Pauli LDA-XC:	-10.924865562227266	-297.2807	-6855.46	-28683.23
Delta V^Pauli GGA-Exchange:	0.616210475069398	16.7679	386.68	1617.86
Delta V^Pauli GGA-Correlation:	-0.170541876599161	-4.6407	-107.02	-447.76
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	31.881206133444266	867.5318	20005.76	83704.09
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	31.881206133444266	867.5318	20005.76	83704.09
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-6.642512807162000	-180.7520	-4168.24	-17439.91

```
  Total Steric Interaction:         25.238693326282267        686.7798         15837.52         66264.18
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -33.092389030855855       -900.4897        -20765.79        -86884.06
                                   --------------------     -----------      ----------       -----------
  Total Orbital Interactions:      -33.095200744598152       -900.5662        -20767.55        -86891.44

Alternative Decomposition Orb.Int.
  Kinetic:                         -79.636659051085687      -2167.0238        -49972.76       -209086.02
  Coulomb:                          42.957958291003600       1168.9455         26956.53        112786.10
  XC:                                3.583500015483937         97.5120          2248.68          9408.48
                                   --------------------     -----------      ----------       -----------
  Total Orbital Interactions:      -33.095200744598152       -900.5662        -20767.55        -86891.44

  Residu (E=Steric+OrbInt+Res):     -0.000010618053354         -0.0003           -0.01            -0.03
  Dispersion Energy:                -0.060323228342564         -1.6415          -37.85           -158.38

Total Bonding Energy:               -7.916841264711804       -215.4282         -4967.89        -20785.66


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

  Electrostatic Energy:             -6.642512807162000       -180.7520         -4168.24        -17439.91
  Kinetic Energy:                    7.445948385438328        202.6146          4672.40         19549.33
  Coulomb (Steric+OrbInt) Energy:   -1.764256666372468        -48.0079         -1107.09         -4632.06
  XC Energy:                        -6.895696948273093       -187.6415         -4327.12        -18104.65
  Dispersion Energy:                -0.060323228342564         -1.6415          -37.85           -158.38
                                   --------------------     -----------      ----------       -----------
  Total Bonding Energy:             -7.916841264711797       -215.4282         -4967.89        -20785.66


 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:                   -239.772684219817620      -6524.5467       -150459.65       -629523.09
  Exchange GGA:                    -20.772099868263194       -565.2376        -13034.69        -54537.14
  Correlation LDA:                 -13.181956846791044       -358.6993         -8271.80        -34609.22
  Correlation GGA:                   6.202755285868969        168.7856          3892.29         16285.33
                                   --------------------     -----------      ----------       -----------
  Total XC:                       -267.523985649002839      -7279.6980       -167873.85       -702384.12

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2           km/mole
             ----------          ----------          ----------
              33.844797          811.446896            6.883829
              39.640532           51.099372            0.507730
              57.510083          105.233557            1.516968
              69.739823           42.256800            0.738679
              86.006977           42.024931            0.905980
              88.578074           13.825428            0.306961
              93.399033           15.178336            0.355340
             113.309823           64.995692            1.845994
             118.358020           20.807604            0.617302
             143.854597          104.295881            3.760702
             147.640671          122.593731            4.536828
             196.413312           27.144032            1.336360
             203.031282           33.732829            1.716698
             211.064751          163.624482            8.656495
             224.061954          119.717223            6.723615
             256.724961          146.384580            9.419796
             266.318321          208.373282           13.909808
             272.304937          218.340052           14.902770
             292.975023           96.431454            7.081535
             315.886678          253.569608           20.077359
             371.996662           26.146768            2.438008
             412.361209           35.971599            3.718053
             422.607654            0.830312            0.087954
             464.649967            8.822109            1.027487
             468.677587           10.168905            1.194611
             472.785115           50.874710            6.028980
             502.219290           32.003114            4.028689
             514.201830           80.826085           10.417493
             538.747015           60.865652            8.219307
             553.245349            0.639733            0.088715
```

571.563314	98.664897	14.135302
591.012480	92.106628	13.644751
624.487642	29.388253	4.600189
634.205312	196.437735	31.227187
642.887498	19.696563	3.173975
659.243370	12.404983	2.049840
683.234392	35.671812	6.109040
711.762940	53.259960	9.501984
721.337863	97.581773	17.643531
738.478827	191.982480	35.536751
740.582428	217.580603	40.389795
755.332775	3.508219	0.664207
770.409056	123.763484	23.899674
781.619951	3.938793	0.771679
842.422961	1.558499	0.329090
860.313228	0.312214	0.067327
920.079640	0.096243	0.022196
960.259639	0.401218	0.096571
963.029790	2.459868	0.593786
968.387400	58.372579	14.168898
976.580152	1.772428	0.433865
997.367636	23.678801	5.919609
1007.019361	91.683345	23.142290
1014.222327	26.121924	6.640739
1042.637872	1.907353	0.498474
1048.142628	69.581718	18.280733
1056.532236	205.253483	54.356484
1086.471437	310.111908	84.452950
1094.616719	4.090084	1.122206
1105.896866	5.842483	1.619534
1133.178127	12.158210	3.453392
1149.199782	19.006710	5.474955
1160.831348	95.403770	27.759570
1222.470045	70.714985	21.668445
1238.373635	19.641605	6.096867
1268.260027	62.770317	19.954493
1281.932481	6.739047	2.165418
1304.531776	40.159172	13.131595
1315.302251	34.152226	11.259592
1365.102057	316.935562	108.446156
1407.705828	64.229479	22.663364
1423.632193	16.628725	5.933826
1440.514832	12.035982	4.345876
1469.210388	212.943226	78.419829
1537.262571	32.486639	12.517884
1550.866569	66.212525	25.739058
1571.869613	110.906234	43.696892
1586.459087	18.522664	7.365638
1593.630503	143.813882	57.446889
1604.941690	45.934806	18.479032
1950.321360	1264.335262	618.082572
2008.560842	1087.673128	547.597505
2156.660449	1320.936006	714.071372
2472.174494	169.161490	104.823509
2544.296281	91.247509	58.192467
2756.192885	1119.962663	773.733181
3077.652737	1.324046	1.021411
3086.989996	7.690403	5.950623
3091.644176	40.203540	31.155295
3095.222756	2.940196	2.281110
3096.577882	17.291853	13.421517
3109.576579	36.838989	28.713559
3121.023480	9.944369	7.779512
3132.808923	5.921280	4.649728
3385.897578	46.517550	39.479235
3462.207644	28.502753	24.735346

Zero-Point Energy : **0.243070 a.u.**
========== **6.614270 eV**

A2

Geometry CYCLE 57
==========

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

Atom	Cartesian (a.u./angstrom) X	Y	Z
1 O	-0.000072	-0.000059	-0.000011
2 O	0.000250	0.000292	0.000046
3 C	-0.000094	-0.000031	0.000065
4 C	0.000107	0.000209	0.000063
5 H	-0.000021	-0.000028	-0.000008
6 Ru	-0.000226	-0.000390	-0.000034
7 C	0.000060	0.000049	0.000010
8 H	0.000023	-0.000075	-0.000016
9 N	0.000017	-0.000104	-0.000074
10 H	-0.000066	-0.000005	0.000068
11 C	-0.000064	-0.000064	0.000103
12 C	0.000066	-0.000001	0.000008
13 C	0.000016	-0.000068	-0.000018
14 C	-0.000037	0.000016	0.000013
15 C	0.000145	0.000100	-0.000171
16 C	0.000019	0.000014	0.000128
17 C	0.000001	-0.000112	0.000044
18 C	-0.000024	-0.000004	-0.000049
19 H	0.000002	-0.000026	0.000002
20 H	-0.000060	0.000022	0.000127
21 C	0.000027	-0.000028	-0.000015
22 H	0.000002	0.000023	-0.000089
23 C	-0.000024	0.000030	-0.000018
24 H	0.000037	0.000030	-0.000067
25 H	0.000008	0.000012	-0.000007
26 Cl	-0.000007	-0.000053	-0.000019
27 N	0.000153	0.000100	-0.000067
28 H	-0.000043	-0.000031	-0.000012
29 H	-0.000069	-0.000020	-0.000008
30 H	-0.000150	0.000012	0.000071
31 B	0.000010	-0.000002	-0.000006
32 H	0.000035	-0.000058	-0.000015
33 H	0.000007	0.000297	-0.000002
34 H	-0.000028	-0.000046	-0.000044

Geometry Convergence after Step 57
---
current energy -7.90333702 Hartree

abs of energy change	0.00008388	0.00100000	T
constrained gradient max	0.00038980	0.00100000	T
constrained gradient rms	0.00008945	0.00066667	T
gradient max	0.00038980		
gradient rms	0.00008945		
cart. step max	0.00547879	0.01000000	T
cart. step rms	0.00150080	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	86.791910696782011	2361.7281	54462.75	227872.13
Delta V^Pauli Coulomb:	-44.515522643333682	-1211.3290	-27933.92	-116875.49
Delta V^Pauli LDA-XC:	-10.904069785152897	-296.7148	-6842.41	-28628.63
Delta V^Pauli GGA-Exchange:	0.618357620303602	16.8264	388.03	1623.50
Delta V^Pauli GGA-Correlation:	-0.171938121427853	-4.6787	-107.89	-451.42
Total Pauli Repulsion:	31.818737767171179	865.8319	19966.56	83540.08
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	31.818737767171179	865.8319	19966.56	83540.08
Electrostatic Interaction:	-6.637170583062695	-180.6066	-4164.89	-17425.89
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	25.181567184108484	685.2253	15801.67	66114.20
(Total Steric Interaction =				

Delta E^0 in the BB paper)

Orbital Interactions				
A:	-33.016794176584618	-898.4327	-20718.35	-86685.58
Total Orbital Interactions:	-33.020811212916335	-898.5420	-20720.87	-86696.13
Alternative Decomposition Orb.Int.				
Kinetic:	-79.346510883306308	-2159.1284	-49790.69	-208324.23
Coulomb:	42.758703520347751	1163.5235	26831.49	112262.96
XC:	3.566996150042213	97.0629	2238.32	9365.15
Total Orbital Interactions:	-33.020811212916342	-898.5420	-20720.87	-86696.13
Residu (E=Steric+OrbInt+Res):	0.000000727305502	0.0000	0.00	0.00
Dispersion Energy:	-0.064094113258016	-1.7441	-40.22	-168.28
Total Bonding Energy:	-7.903337414760365	-215.0608	-4959.42	-20750.21

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

Electrostatic Energy:	-6.637170583062695	-180.6066	-4164.89	-17425.89
Kinetic Energy:	7.445399813475703	202.5996	4672.06	19547.89
Coulomb (Steric+OrbInt) Energy:	-1.756818395680426	-47.8055	-1102.42	-4612.53
XC Energy:	-6.890654136234935	-187.5042	-4323.95	-18091.41
Dispersion Energy:	-0.064094113258016	-1.7441	-40.22	-168.28
Total Bonding Energy:	-7.903337414760370	-215.0608	-4959.42	-20750.21

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:	-239.772132870408399	-6524.5317	-150459.30	-629521.65
Exchange GGA:	-20.771821723475956	-565.2300	-13034.52	-54536.41
Correlation LDA:	-13.181900252580110	-358.6978	-8271.77	-34609.07
Correlation GGA:	6.202731404170991	168.7849	3892.27	16285.27
Total XC:	-267.523123442293468	-7279.6746	-167873.31	-702381.86

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
32.469745	368.336807	2.997796
46.697926	307.503896	3.599368
58.924900	130.750610	1.931171
72.629173	46.315557	0.843172
85.663649	36.199293	0.777275
86.607504	138.601088	3.008848
90.648034	24.825598	0.564074
107.129997	83.564185	2.243930
118.401987	72.379010	2.148076
122.141102	27.744639	0.849413
134.050273	117.388004	3.944296
152.071306	67.048262	2.555718
187.788022	6.130200	0.288550
197.717842	15.247373	0.755647
218.030027	44.186173	2.414798
229.832988	129.300836	7.448894
234.769771	303.389148	17.853373
277.393621	156.752560	10.899064
284.594721	167.882612	11.975968
303.518597	361.292632	27.486692
370.793735	29.657757	2.756441
415.483861	37.966365	3.953951
425.450758	6.471054	0.690085
466.500953	8.235094	0.962940
473.668704	33.421093	3.968016
481.007872	14.420095	1.738595
493.776191	19.358811	2.396000
518.743942	49.781866	6.472950
540.851443	20.193708	2.737614
555.545760	8.533902	1.188353
566.806032	191.127716	27.154149
587.649529	135.889754	20.016271

624.091698	26.491895	4.144189
634.161567	102.285376	16.258914
638.977632	17.716944	2.837609
656.012364	4.065868	0.668565
675.699577	66.701390	11.297090
705.334766	76.587120	13.540325
718.763373	55.015796	9.911774
726.457211	81.473328	14.835547
735.956982	81.758026	15.082068
743.014523	350.017737	65.187665
753.311319	6.206637	1.171950
786.835365	6.161258	1.215154
848.824751	2.630054	0.559578
864.383244	0.108646	0.023540
921.770239	0.459934	0.106267
942.275017	89.126444	21.050496
959.557899	0.250919	0.060351
967.566498	0.145567	0.035304
992.311214	0.738558	0.183701
993.463125	23.726587	5.908335
1005.723249	88.743482	22.371393
1008.429307	4.785360	1.209590
1037.566920	2.204060	0.573215
1043.293639	69.501068	18.175071
1047.619709	139.601639	36.658294
1090.357270	4.350822	1.189100
1102.214351	14.341378	3.962187
1106.489689	341.371198	94.678707
1132.200000	11.681165	3.315029
1147.827456	14.138193	4.067697
1155.446852	39.696946	11.497016
1233.160898	22.719127	7.022463
1262.857191	65.276028	20.662651
1278.724851	3.818988	1.224062
1296.689744	21.397794	6.954776
1305.550655	27.485597	8.994499
1320.617705	36.007931	11.919371
1331.972517	139.412366	46.545171
1401.926850	77.638872	27.282404
1420.228250	14.687501	5.228584
1432.808160	8.680351	3.117478
1462.376144	185.982854	68.172634
1530.586680	24.233344	9.297140
1548.746208	59.769043	23.202492
1566.248039	84.032339	32.990209
1587.449612	136.366242	54.260638
1589.732852	4.564095	1.818683
1601.577184	111.408625	44.724424
1956.075103	1146.944091	562.348892
2014.210117	1224.416702	618.175926
2186.547023	959.649478	525.956132
2464.216928	156.633092	96.747673
2544.515893	80.108633	51.093136
3056.443751	81.143556	62.165369
3078.726354	1.689300	1.303635
3085.331056	8.445982	6.531757
3093.607164	6.788149	5.263742
3096.995002	11.577425	8.987327
3109.697167	31.190036	24.311516
3122.248511	4.944504	3.869619
3129.681238	7.178876	5.631637
3258.757891	108.392790	88.538174
3389.353422	56.943189	48.376752
3450.175645	44.635672	38.601249

Zero-Point Energy : **0.243561 a.u.**
========== **6.627645 eV**

```
P1
 Geometry CYCLE 3
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ---------------------------------------
     1 O     0.000065  0.000008  0.000014
     2 O     0.000040  0.000069  0.000103
     3 C    -0.000066  0.000205 -0.000203
     4 C    -0.000185 -0.000177 -0.000202
     5 H     0.000068  0.000024  0.000005
     6 Ru   -0.000257 -0.000180  0.000314
     7 C     0.000050  0.000003  0.000022
     8 H    -0.000040  0.000000  0.000001
     9 N     0.000158 -0.000100 -0.000150
    10 H     0.000028  0.000026  0.000036
    11 C    -0.000075 -0.000013  0.000063
    12 C     0.000025 -0.000087  0.000010
    13 C     0.000047  0.000031  0.000225
    14 C     0.000019  0.000069 -0.000061
    15 C     0.000010  0.000028 -0.000026
    16 C    -0.000026 -0.000050 -0.000273
    17 C     0.000025 -0.000020  0.000043
    18 C     0.000014  0.000017 -0.000076
    19 H    -0.000028 -0.000008 -0.000041
    20 H     0.000003  0.000001  0.000011
    21 C     0.000066 -0.000037 -0.000009
    22 H    -0.000038  0.000035  0.000013
    23 C    -0.000072  0.000094  0.000093
    24 H    -0.000007 -0.000033 -0.000015
    25 H    -0.000005  0.000005  0.000047
    26 Cl    0.000041  0.000046 -0.000030
    27 N    -0.000304 -0.000245 -0.000153
    28 H     0.000036  0.000094  0.000058
    29 H     0.000090  0.000068  0.000000
    30 H     0.000071  0.000027  0.000034
    31 B     0.000304  0.000221  0.000166
    32 H    -0.000021 -0.000014  0.000012
    33 H    -0.000019 -0.000112 -0.000007
    34 H    -0.000019  0.000003 -0.000026
 ---------------------------------------

-------------------------------------
Geometry Convergence after Step   3
-------------------------------------
current energy                          -7.86812073 Hartree
abs of energy change              0.00008740     0.00100000    T
constrained gradient max          0.00031438     0.00100000    T
constrained gradient rms          0.00010318     0.00066667    T
gradient max                      0.00031438
gradient rms                      0.00010318
cart. step max                    0.00536546     0.01000000    T
cart. step rms                    0.00144127     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              85.955765073100878       2338.9754        53938.06        225676.83
  Delta V^Pauli Coulomb:           -43.875630889014872      -1193.9167       -27532.38       -115195.45
  Delta V^Pauli LDA-XC:            -10.789911345903951       -293.6084        -6770.77        -28328.91
  Delta V^Pauli GGA-Exchange:        0.609560908207353         16.5870          382.51          1600.40
  Delta V^Pauli GGA-Correlation:    -0.167688644458917         -4.5630         -105.23          -440.27
                                  --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:            31.732095101930490        863.4742        19912.19         83312.60
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  31.732095101930490        863.4742        19912.19         83312.60
  Electrostatic Interaction:        -6.580110908915994       -179.0539        -4129.08        -17276.08
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------     -----------     ----------     -----------
  Total Steric Interaction:         25.151984193014496        684.4203        15783.11         66036.53
 (Total Steric Interaction =
  Delta E^0 in the BB paper)
```

```
Orbital Interactions
  A:                              -32.951251277814521       -896.6492        -20677.22        -86513.50
                                  -------------------      -----------      ----------      -----------
  Total Orbital Interactions:     -32.955408755099342       -896.7623        -20679.83        -86524.41

Alternative Decomposition Orb.Int.
  Kinetic:                         -78.566491391817166      -2137.9030        -49301.22       -206276.29
  Coulomb:                          42.121656869917103       1146.1886         26431.74        110590.39
  XC:                                3.489425766800718         94.9521          2189.65          9161.49
                                  -------------------      -----------      ----------      -----------
  Total Orbital Interactions:     -32.955408755099342       -896.7623        -20679.83        -86524.41

  Residu (E=Steric+OrbInt+Res):     0.000001018106926          0.0000             0.00             0.00
  Dispersion Energy:               -0.064697191164353         -1.7605           -40.60           -169.86

Total Bonding Energy:               -7.868120735142273       -214.1025         -4937.32        -20657.75


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

  Electrostatic Energy:             -6.580110908915994       -179.0539         -4129.08        -17276.08
  Kinetic Energy:                    7.389273681283711        201.0724          4636.84         19400.54
  Coulomb (Steric+OrbInt) Energy:   -1.753973000990840        -47.7280         -1100.63         -4605.06
  XC Energy:                        -6.858613315354797       -186.6324         -4303.85        -18007.29
  Dispersion Energy:                -0.064697191164353         -1.7605           -40.60           -169.86
                                  -------------------      -----------      ----------      -----------
  Total Bonding Energy:             -7.868120735142272       -214.1025         -4937.32        -20657.75


 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:                   -239.772825589670475      -6524.5506       -150459.74       -629523.46
  Exchange GGA:                    -20.772118473042227       -565.2381        -13034.70        -54537.19
  Correlation LDA:                 -13.181977032669195       -358.6998         -8271.82        -34609.28
  Correlation GGA:                   6.202755231355050        168.7856          3892.29         16285.33
                                  -------------------      -----------      ----------      -----------
  Total XC:                       -267.524165864026827      -7279.7029       -167873.97       -702384.60

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2           km/mole
             ----------          ----------          ----------
              36.340909           22.171139            0.201958
              48.183344          174.724021            2.110219
              53.130439          231.575483            3.083998
              61.864266           50.144627            0.777575
              63.731379           80.899152            1.292336
              79.339052           46.202456            0.918819
              86.629499          281.405917            6.110505
              93.886509           34.091647            0.802286
              97.493795           65.646149            1.604221
             104.181729           70.857947            1.850368
             114.907631           38.475088            1.108170
             135.772898          142.043222            4.834056
             148.631958           29.671549            1.105428
             151.292745          484.686665           18.380497
             195.615898          113.156167            5.548307
             208.459740           51.452955            2.688503
             244.163085           49.566062            3.033489
             285.991609           26.795562            1.920853
             319.345164          245.219826           19.628811
             330.022788           80.144170            6.629701
             353.653422           93.596532            8.296897
             360.457105            4.612630            0.416754
             411.370392          348.576794           35.942607
             421.756639           43.069875            4.553167
             427.927073          326.723423           35.045165
             441.115960         1224.930562          135.438555
             454.149134           45.330723            5.160232
             467.141319         1748.888027          204.780386
             501.485903          147.657614           18.560627
             506.140057           39.258979            4.980670
             540.842968           22.723057            3.080463
             567.794637           77.351164           11.008704
             574.202786          218.064768           31.385487
             604.514374           26.221598            3.973231
```

618.944749	3.055498	0.474037
647.914177	3.276128	0.532055
676.093338	9.516267	1.612692
701.239843	22.402914	3.937759
730.482041	315.207453	57.714388
744.517156	83.695141	15.618993
745.804810	113.784464	21.270917
770.723887	31.398640	6.065795
779.517282	152.230420	29.744404
835.875054	61.416960	12.867902
853.522901	499.286510	106.817665
870.588391	1.256713	0.274238
884.028572	682.111600	151.147096
918.969788	570.386040	131.385728
942.794369	3.730086	0.881483
946.630795	1.652063	0.391999
963.020814	117.936362	28.468296
972.652222	10.830017	2.640370
975.924379	1.307662	0.319882
998.604157	39.159981	9.801982
1008.043144	1.422513	0.359429
1013.498273	31.057459	7.889818
1020.803752	10.777910	2.757750
1038.019949	16.902126	4.397695
1059.891517	5.297456	1.407365
1070.584892	29.251870	7.849695
1085.656215	4.765085	1.296705
1098.454587	42.818829	11.789488
1130.175804	8.443196	2.391834
1138.800628	2.076172	0.592638
1150.959742	1.615626	0.466100
1248.959346	138.119145	43.239459
1250.591421	50.023041	15.680634
1269.989015	7.646769	2.434199
1291.148034	6.509852	2.106809
1304.655624	12.333455	4.033283
1336.578488	25.991856	8.707828
1411.157107	10.428817	3.688829
1427.077675	16.412424	5.870815
1448.658065	85.324996	30.982770
1477.443015	4.245869	1.572372
1535.114064	6.578191	2.531193
1553.005450	4.501686	1.752372
1569.483008	105.551130	41.523846
1576.004317	22.282553	8.802386
1588.874070	22.725270	9.050584
1796.694552	190.778360	85.917461
1958.842356	1537.955936	755.129521
2003.540765	1467.563644	737.009690
2464.793015	126.804881	78.341972
2528.294608	161.390194	102.278156
3092.572521	0.030927	0.023973
3097.780357	46.819291	36.354111
3098.147446	11.349849	8.813943
3101.665083	9.665970	7.514817
3104.148126	7.502458	5.837462
3111.106298	1.242227	0.968710
3117.365178	6.571838	5.135143
3121.188268	11.066188	8.657571
3124.067457	6.242264	4.888106
3469.884201	19.660598	17.099751
3574.258749	10.653402	9.544482

Zero-Point Energy : **0.239065 a.u.**
========== **6.505287 eV**

```
P2

 Geometry CYCLE 20
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 O     0.000001  0.000003 -0.000059
     2 O     0.000034 -0.000098  0.000008
     3 C    -0.000150  0.000135  0.000255
     4 C     0.000461  0.000323  0.000229
     5 H     0.000001 -0.000078  0.000137
     6 Ru   -0.000539  0.000481  0.000050
     7 C    -0.000225  0.000458 -0.000032
     8 H    -0.000044  0.000001  0.000000
     9 N     0.000644 -0.000698 -0.000252
    10 H    -0.000026 -0.000043  0.000070
    11 C     0.000150 -0.000043 -0.000216
    12 C    -0.000130 -0.000080 -0.000338
    13 C     0.000133 -0.000172  0.000207
    14 C    -0.000041  0.000083  0.000103
    15 C     0.000019 -0.000053  0.000135
    16 C     0.000166  0.000351  0.000147
    17 C    -0.000061 -0.000048  0.000001
    18 C     0.000057  0.000013 -0.000205
    19 H     0.000009  0.000007 -0.000123
    20 H     0.000027  0.000053  0.000020
    21 C    -0.000111 -0.000298 -0.000174
    22 H    -0.000029  0.000010 -0.000034
    23 C    -0.000085  0.000104  0.000233
    24 H     0.000016  0.000008 -0.000152
    25 H    -0.000017  0.000014  0.000113
    26 Cl    0.000002 -0.000064  0.000053
    27 H     0.000052  0.000073  0.000005
    28 H    -0.000314 -0.000440 -0.000181
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step  20
-------------------------------------
current energy                          -6.76486361 Hartree
abs of energy change              0.00000094     0.00100000    T
constrained gradient max          0.00069804     0.00100000    T
constrained gradient rms          0.00020231     0.00066667    T
gradient max                      0.00069804
gradient rms                      0.00020231
cart. step max                    0.00943665     0.01000000    T
cart. step rms                    0.00259440     0.00666667    T


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

Pauli Repulsion
  Kinetic (Delta T^0):              76.580293555060095      2083.8558        48054.86        201061.53
  Delta V^Pauli Coulomb:           -39.463376310301427     -1073.8531       -24763.65       -103611.08
  Delta V^Pauli LDA-XC:             -9.484196161372429      -258.0781        -5951.42        -24900.75
  Delta V^Pauli GGA-Exchange:        0.545207392670925        14.8358          342.12          1431.44
  Delta V^Pauli GGA-Correlation:    -0.151299229498385        -4.1171          -94.94          -397.24
                                  --------------------    -----------  ----------  -----------
  Total Pauli Repulsion:            28.026629246558777       762.6434        17586.98        73583.90
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  28.026629246558777       762.6434        17586.98        73583.90
  Electrostatic Interaction:        -5.934352360386042      -161.4819        -3723.86       -15580.64
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------    -----------  ----------  -----------
  Total Steric Interaction:         22.092276886172733       601.1614        13863.11        58003.26
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -28.804786981453894      -783.8181       -18075.28       -75626.96
                                  --------------------    -----------  ----------  -----------
  Total Orbital Interactions:      -28.808822018690108      -783.9279       -18077.81       -75637.55
```

```
Alternative Decomposition Orb.Int.
  Kinetic:                        -70.241330125979204      -1911.3638        -44077.10       -184418.59
  Coulomb:                         38.218865569138465       1039.9882         23982.70        100343.62
  XC:                               3.213642538150645         87.4477          2016.59          8437.42
                                  --------------------     -----------       ----------      -----------
  Total Orbital Interactions:     -28.808822018690094       -783.9279        -18077.81        -75637.55

  Residu (E=Steric+OrbInt+Res):     0.000000027038889          0.0000             0.00             0.00
  Dispersion Energy:               -0.048318543332282         -1.3148           -30.32           -126.86

Total Bonding Energy:              -6.764863648810769       -184.0813         -4245.02        -17761.15


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

  Electrostatic Energy:            -5.934352360386042       -161.4819         -3723.86        -15580.64
  Kinetic Energy:                   6.338963429080891        172.4920          3977.76         16642.95
  Coulomb (Steric+OrbInt) Energy:  -1.244510714124075        -33.8649          -780.94         -3267.46
  XC Energy:                       -5.876645460049245       -159.9117         -3687.65        -15429.13
  Dispersion Energy:               -0.048318543332282         -1.3148           -30.32           -126.86
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:            -6.764863648810753       -184.0813         -4245.02        -17761.15


 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:                  -230.014118714909841      -6259.0026       -144336.05       -603901.98
  Exchange GGA:                   -19.441420362845818       -529.0280        -12199.68        -51043.44
  Correlation LDA:                -12.269000588485408       -333.8565         -7698.91        -32212.26
  Correlation GGA:                  5.710013552887338        155.3774          3583.09         14991.64
                                  --------------------     -----------       ----------      -----------
  Total XC:                      -256.014526113353725      -6966.5097       -160651.56       -672166.04

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2           km/mole
             ----------          ----------          ----------
              31.864282           60.651446            0.484421
              50.480844           82.325417            1.041690
              63.357353           56.564035            0.898288
              75.595442            5.375855            0.101864
              90.434099           19.918950            0.451520
              95.026468           18.555091            0.441963
             104.084332           80.908829            2.110860
             112.498054           12.934836            0.364741
             134.499969           87.205150            2.939967
             141.676056           41.223623            1.463931
             190.814630           30.534632            1.460436
             203.710907            2.207553            0.112721
             284.565995           13.217789            0.942801
             319.387936          194.549182           15.574926
             328.766914          126.130084           10.394051
             350.653894           19.616553            1.724167
             367.464217           13.660836            1.258260
             397.005240           82.541492            8.213847
             421.505849           78.508629            8.294669
             441.769946            1.964729            0.217559
             449.354808            9.209309            1.037276
             501.899609           43.506713            5.473324
             506.595733           58.276486            7.400021
             538.616453           19.212037            2.593768
             568.167883           82.052249           11.685445
             571.399122          134.346455           19.241718
             602.890437           28.961338            4.376582
             618.641277            7.130851            1.105754
             646.292373            6.397955            1.036450
             697.686058           16.914510            2.957996
             727.665567          367.467166           67.023706
             743.412634            5.991924            1.116540
             745.619348          189.467482           35.410326
             771.788604           38.891932            7.523778
             800.304646          242.457562           48.637265
             820.217511           33.675411            6.923409
             867.423151           25.145574            5.467271
             875.348833            7.138847            1.566345
```

936.769894	23.478065	5.512813
940.258042	59.384755	13.995876
958.002495	4.716987	1.132686
969.278230	3.026366	0.735272
979.895944	0.535735	0.131585
989.756731	3.489092	0.865603
999.414373	35.508791	8.895278
1008.002654	2.554261	0.645364
1019.314691	9.836909	2.513304
1036.906313	15.440979	4.013215
1055.409586	24.557123	6.496457
1085.844949	4.104504	1.117137
1129.769024	5.347766	1.514398
1138.398717	1.862510	0.531461
1148.430446	0.605302	0.174243
1250.130480	2.971209	0.931036
1268.062276	11.123329	3.535521
1289.036859	7.843698	2.534336
1303.039809	9.491158	3.099952
1334.617465	22.050910	7.376687
1410.688555	8.779737	3.104493
1426.146369	16.190172	5.787535
1448.060814	95.158692	34.539284
1475.581482	14.091807	5.212042
1531.239694	7.433797	2.853198
1554.031535	9.641089	3.755467
1575.924495	18.222316	7.198086
1588.607450	22.562521	8.984259
1895.083349	110.795454	52.629389
1963.312772	1615.027546	794.781036
2008.977154	1255.694292	632.320102
3092.873958	0.721987	0.559718
3097.072134	15.287817	11.867927
3100.986513	1.835699	1.426853
3101.897306	7.024650	5.461729
3110.809815	5.078030	3.959558
3117.431059	1.580487	1.234997
3117.595414	9.658472	7.547554
3123.983176	8.975335	7.028092
3126.437869	5.576201	4.369848

Zero-Point Energy : **0.191288 a.u.**
========== **5.205202 eV**

```
P3

 Geometry CYCLE 17
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ---------------------------------------
     1 O    -0.000181  0.000046  0.000014
     2 O    -0.000011 -0.000135  0.000004
     3 C     0.000221 -0.000082 -0.000162
     4 C     0.000004  0.000220  0.000217
     5 H    -0.000022  0.000055 -0.000004
     6 Ru    0.000027  0.000048 -0.000684
     7 C     0.000112 -0.000110 -0.000041
     8 H    -0.000041  0.000002 -0.000027
     9 N    -0.000068  0.000065  0.000141
    10 H    -0.000016 -0.000105  0.000018
    11 C    -0.000046 -0.000018  0.000024
    12 C    -0.000034 -0.000208  0.000143
    13 C    -0.000016 -0.000015 -0.000028
    14 C    -0.000019  0.000035 -0.000085
    15 C     0.000004  0.000062 -0.000032
    16 C     0.000021  0.000009  0.000110
    17 C     0.000043 -0.000016  0.000049
    18 C     0.000021  0.000141 -0.000052
    19 H     0.000024  0.000117 -0.000055
    20 H    -0.000042 -0.000004  0.000004
    21 C     0.000046  0.000062 -0.000104
    22 H     0.000071 -0.000063 -0.000069
    23 C    -0.000035 -0.000155  0.000025
    24 H     0.000015  0.000065 -0.000037
    25 H    -0.000052 -0.000024  0.000103
    26 Cl    0.000000 -0.000029  0.000098
    27 H    -0.000095  0.000085  0.000483
    28 H     0.000072 -0.000046 -0.000056
 ---------------------------------------

-------------------------------------
Geometry Convergence after Step  17
-------------------------------------
current energy                          -6.77013550 Hartree
abs of energy change              0.00000137     0.00100000    T
constrained gradient max          0.00068415     0.00100000    T
constrained gradient rms          0.00012263     0.00066667    T
gradient max                      0.00068415
gradient rms                      0.00012263
cart. step max                    0.00488538     0.01000000    T
cart. step rms                    0.00151361     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):             77.262294152518734       2102.4140        48482.83        202852.12
  Delta V^Pauli Coulomb:          -39.890948303662952      -1085.4879       -25031.95       -104733.67
  Delta V^Pauli LDA-XC:            -9.563506329080560       -260.2362        -6001.19        -25108.98
  Delta V^Pauli GGA-Exchange:       0.544919447776742         14.8280          341.94          1430.69
  Delta V^Pauli GGA-Correlation:   -0.151238978985826         -4.1154          -94.90          -397.08
                                  --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:           28.201519988566137        767.4024        17696.72         74043.08
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 28.201519988566137        767.4024        17696.72         74043.08
  Electrostatic Interaction:       -5.985052499497008       -162.8616        -3755.68        -15713.75
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------     -----------     ----------     -----------
  Total Steric Interaction:        22.216467489069128        604.5408        13941.05         58329.33
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                              -28.936897326653000       -787.4130       -18158.18        -75973.81
                                  --------------------     -----------     ----------     -----------
  Total Orbital Interactions:     -28.940625295091532       -787.5145       -18160.52        -75983.60
```

Alternative Decomposition Orb.Int.				
Kinetic:	-70.878585013313881	-1928.7044	-44476.99	-186091.70
Coulomb:	38.647328312380893	1051.6473	24251.57	101468.55
XC:	3.290631405841466	89.5426	2064.90	8639.55
Total Orbital Interactions:	-28.940625295091522	-787.5145	-18160.52	-75983.60
Residu (E=Steric+OrbInt+Res):	0.000001152610070	0.0000	0.00	0.00
Dispersion Energy:	-0.045978851379637	-1.2511	-28.85	-120.72
Total Bonding Energy:	-6.770135504791972	-184.2248	-4248.32	-17774.99

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

Electrostatic Energy:	-5.985052499497008	-162.8616	-3755.68	-15713.75
Kinetic Energy:	6.383709139204853	173.7096	4005.84	16760.43
Coulomb (Steric+OrbInt) Energy:	-1.243618838671992	-33.8406	-780.38	-3265.12
XC Energy:	-5.879194454448179	-159.9810	-3689.25	-15435.82
Dispersion Energy:	-0.045978851379637	-1.2511	-28.85	-120.72
Total Bonding Energy:	-6.770135504791963	-184.2248	-4248.32	-17774.99

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:	-230.014149648963553	-6259.0035	-144336.07	-603902.06
Exchange GGA:	-19.441417164273716	-529.0279	-12199.67	-51043.43
Correlation LDA:	-12.269003481999095	-333.8566	-7698.92	-32212.26
Correlation GGA:	5.709984160797609	155.3766	3583.07	14991.56
Total XC:	-256.014586134438787	-6966.5113	-160651.60	-672166.20

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
42.410768	44.508081	0.473144
53.797674	23.805239	0.321007
69.598993	13.243614	0.231040
76.287204	4.478579	0.085639
84.357655	21.549557	0.455660
94.774191	51.779627	1.230062
113.170928	43.757326	1.241263
134.953656	25.244410	0.853941
166.393538	2.532752	0.105635
171.380265	108.241964	4.649803
207.699784	22.967927	1.195738
232.781441	17.110166	0.998345
272.448685	1.290497	0.088129
316.290564	257.405631	20.407150
349.893901	47.106491	4.131381
365.772797	37.726470	3.458881
378.213624	82.831271	7.852529
402.260117	8.253083	0.832149
412.669105	98.080822	10.145282
441.669565	29.174201	3.229792
454.221722	3.216174	0.366172
478.675128	5.466948	0.655940
512.975298	99.506156	12.794534
548.799118	8.670567	1.192721
567.086864	83.351817	11.847937
572.435092	104.861774	15.046016
614.617201	60.022847	9.246968
621.129888	11.227124	1.747950
647.497287	2.202117	0.357402
708.304279	68.928345	12.237587
726.126192	192.899132	35.109160
742.344029	369.542858	68.761937
748.692899	19.117025	3.587584
781.412556	13.022543	2.550670
805.209758	182.012478	36.735695
809.789869	372.211300	75.550956
852.295786	2.060568	0.440205
870.386416	2.303881	0.502632
932.329975	5.198758	1.214919

951.002847	26.186259	6.242138
964.553167	2.849808	0.689001
967.793625	4.407196	1.069112
972.368954	45.354621	11.054286
983.260214	2.904588	0.715865
997.649557	13.313758	3.329329
1011.547451	3.528875	0.894748
1035.812125	7.830272	2.032993
1046.334855	39.717710	10.416767
1093.811481	5.430213	1.488804
1109.752961	4.454293	1.239034
1135.175122	7.545813	2.147074
1147.743639	9.280404	2.669868
1238.025770	3.772085	1.170548
1270.785680	12.738779	4.057684
1280.662759	25.323461	8.128977
1301.576348	7.432102	2.424708
1325.662493	10.932713	3.632779
1399.427416	17.026844	5.972589
1430.176903	26.568722	9.524419
1435.332223	74.559414	26.824584
1459.660611	146.898423	53.746117
1495.381908	111.172618	41.670434
1542.830625	15.064351	5.825682
1560.237293	35.176446	13.756903
1582.929767	76.416012	30.319643
1591.473587	32.107157	12.807942
1916.979002	100.017058	48.058422
1974.198623	1679.394153	831.039280
2035.568520	1069.505410	545.690988
2103.173019	159.817666	84.251541
3083.274877	55.290627	42.730879
3094.011207	0.339888	0.263594
3098.948715	4.322405	3.357514
3101.411482	1.851117	1.439035
3111.040321	4.528097	3.531014
3119.900308	11.490186	8.985574
3121.425384	9.382769	7.341116
3129.285970	6.263939	4.913273

Zero-Point Energy : **0.190458 a.u.**
========== **5.182622 eV**

P3'

Geometry CYCLE 18
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	O	-0.000239	0.000224	-0.000131
2	O	-0.000112	0.000085	0.000035
3	C	0.000511	-0.000567	0.000328
4	C	0.000235	0.000370	0.000126
5	H	-0.000050	-0.000059	0.000025
6	Ru	-0.000602	0.000125	-0.000225
7	C	0.000074	0.000042	-0.000047
8	H	0.000081	-0.000016	-0.000017
9	N	-0.000060	0.000108	0.000334
10	H	-0.000030	0.000009	0.000018
11	C	-0.000010	0.000013	0.000034
12	C	-0.000095	0.000008	-0.000007
13	C	0.000052	-0.000060	0.000029
14	C	0.000045	-0.000281	-0.000468
15	C	-0.000046	-0.000011	-0.000105
16	C	0.000320	0.000102	0.000023
17	C	-0.000006	-0.000095	0.000079
18	C	0.000032	0.000023	-0.000024
19	H	0.000042	0.000025	-0.000032
20	H	0.000014	-0.000052	0.000056
21	C	0.000059	0.000113	-0.000170
22	H	-0.000023	0.000043	-0.000013
23	C	-0.000033	-0.000076	0.000103
24	H	0.000005	0.000004	0.000003
25	H	-0.000043	-0.000060	0.000011
26	Cl	0.000034	0.000151	-0.000039
27	H	-0.000031	-0.000068	0.000047
28	H	0.000010	0.000000	0.000037
29	O	-0.000216	0.000073	0.000035
30	C	0.000111	0.000114	-0.000021
31	C	-0.000039	-0.000117	0.000180
32	C	-0.000005	0.000090	-0.000212
33	C	0.000053	-0.000136	0.000034
34	H	-0.000072	-0.000024	0.000023
35	H	-0.000008	-0.000010	0.000030
36	H	0.000024	0.000080	-0.000085
37	H	0.000125	-0.000092	-0.000025
38	H	-0.000093	-0.000192	-0.000011
39	H	-0.000102	0.000086	0.000109
40	H	0.000069	0.000038	0.000045
41	H	0.000020	-0.000012	-0.000108

Geometry Convergence after Step 18

---

current energy -9.39713963 Hartree

abs of energy change	0.00001416	0.00100000	T
constrained gradient max	0.00060220	0.00100000	T
constrained gradient rms	0.00014384	0.00066667	T
gradient max	0.00060220		
gradient rms	0.00014384		
cart. step max	0.00560085	0.01000000	T
cart. step rms	0.00150482	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	100.327691302913394	2730.0554	62956.58	263410.32
Delta V^Pauli Coulomb:	-51.016347429371507	-1388.2254	-32013.24	-133943.40
Delta V^Pauli LDA-XC:	-12.776958868988840	-347.6787	-8017.66	-33545.90
Delta V^Pauli GGA-Exchange:	0.748277029703068	20.3617	469.55	1964.60
Delta V^Pauli GGA-Correlation:	-0.210766527561137	-5.7352	-132.26	-553.37
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	37.071895506694972	1008.7776	23262.97	97332.25
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	37.071895506694972	1008.7776	23262.97	97332.25

Electrostatic Interaction:	-7.731215596348071	-210.3771	-4851.41	-20298.30
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	29.340679910346900	798.4005	18411.56	77033.94
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-38.654775671089062	-1051.8500	-24256.24	-101488.10
Total Orbital Interactions:	-38.659948889003594	-1051.9907	-24259.49	-101501.68
Alternative Decomposition Orb.Int.				
Kinetic:	-91.462430434613822	-2488.8194	-57393.55	-240134.58
Coulomb:	48.823574904742649	1328.5571	30637.26	128186.28
XC:	3.978906640867541	108.2716	2496.80	10446.62
Total Orbital Interactions:	-38.659948889003630	-1051.9907	-24259.49	-101501.68
Residu (E=Steric+OrbInt+Res):	0.000007532819981	0.0002	0.00	0.02
Dispersion Energy:	-0.077878280695046	-2.1192	-48.87	-204.47
Total Bonding Energy:	-9.397139726531758	-255.7092	-5896.79	-24672.19

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

Electrostatic Energy:	-7.731215596348071	-210.3771	-4851.41	-20298.30
Kinetic Energy:	8.865260868299572	241.2360	5563.04	23275.74
Coulomb (Steric+OrbInt) Energy:	-2.192764991808879	-59.6682	-1375.98	-5757.10
XC Energy:	-8.260541725979369	-224.7808	-5183.57	-21688.05
Dispersion Energy:	-0.077878280695046	-2.1192	-48.87	-204.47
Total Bonding Energy:	-9.397139726531792	-255.7092	-5896.79	-24672.19

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:	-256.380689976517772	-6976.4735	-160881.33	-673127.41
Exchange GGA:	-22.918679845574701	-623.6490	-14381.69	-60172.99
Correlation LDA:	-14.630502662701588	-398.1162	-9180.78	-38412.38
Correlation GGA:	6.964182981116700	189.5051	4370.09	18284.46
Total XC:	-286.965689503677311	-7808.7337	-180073.71	-753428.31

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
7.879027	258.301734	0.510127
24.857742	218.394028	1.360757
49.629045	21.040008	0.261734
50.213245	7.173508	0.090288
57.427078	46.986378	0.676343
71.465516	21.770674	0.389984
72.937977	30.158089	0.551360
87.230228	13.001006	0.284264
88.337662	11.759495	0.260383
96.828593	22.958471	0.557217
100.393018	9.534105	0.239917
105.152905	7.253020	0.191169
115.818347	64.949536	1.885521
158.758044	30.530842	1.214934
175.728692	26.057458	1.147765
177.572334	17.723813	0.788879
200.363225	20.735255	1.041371
204.811606	12.987876	0.666762
217.951738	25.971468	1.418845
285.550050	6.613491	0.473359
312.720636	206.112573	16.156195
323.364397	159.732114	12.946802
341.835689	23.208261	1.988557
349.766182	107.187681	9.397250
392.966200	26.317225	2.592229
406.760534	2.456279	0.250435

424.437565	23.762234	2.528012
442.343919	80.932109	8.973440
454.058204	47.146049	5.365805
519.500424	112.221117	14.612972
529.176884	33.347327	4.423235
543.731395	23.222788	3.165023
570.492978	63.126950	9.026995
583.490088	123.190336	18.017237
598.775907	9.543854	1.432406
615.015887	0.583645	0.089973
625.929134	16.706369	2.621110
638.506516	0.510976	0.081779
675.642971	57.632371	9.760270
692.390795	241.196460	41.860102
741.367554	172.222740	32.003844
744.131494	59.257032	11.052681
749.681703	41.438540	7.786807
771.909447	62.899646	12.170057
774.421743	21.950027	4.260795
826.768438	3.837587	0.795280
831.113155	23.669349	4.930881
840.081279	170.225276	35.844574
865.615794	0.949491	0.206013
874.610765	21.472279	4.707291
876.484925	516.556672	113.485532
899.131061	12.979744	2.925278
901.873885	18.105957	4.093034
913.554381	0.199375	0.045654
928.049687	54.389746	12.652208
947.072136	0.686958	0.163076
950.955019	5.036190	1.200439
971.297169	0.914975	0.222761
974.834312	1.298186	0.317209
988.621610	0.688337	0.170573
993.042928	7.671684	1.909575
1007.181727	30.912981	7.804171
1009.480289	61.677776	15.606468
1012.189580	65.785758	16.690595
1033.302860	2.895058	0.749830
1060.720436	23.951890	6.368231
1062.328247	32.998964	8.786929
1088.533970	1.498611	0.408892
1105.238328	1.022966	0.283397
1131.958609	2.088402	0.592547
1135.763416	10.273406	2.924694
1155.053207	0.093340	0.027024
1163.344026	7.301437	2.129093
1172.855487	10.965531	3.223682
1203.812579	14.069179	4.245274
1226.170395	28.210675	8.670465
1251.939855	9.181918	2.881343
1258.671553	15.129729	4.773332
1270.774811	8.251065	2.628189
1272.893272	15.967526	5.094572
1290.545122	5.407335	1.749180
1297.957603	1.938142	0.630557
1305.572865	2.572502	0.841850
1325.193732	2.885370	0.958427
1328.943654	43.528801	14.499778
1407.308007	37.871588	13.359209
1429.024415	17.141724	6.140055
1433.270062	1.872813	0.672822
1447.438764	24.465067	8.876151
1451.565225	11.253436	4.094490
1458.721709	90.629090	33.137378
1467.096418	12.289003	4.519115
1485.939856	6.772522	2.522492
1546.708523	42.050790	16.302744
1567.054950	1.002831	0.393904
1584.178251	29.170301	11.583053
1595.922634	5.765494	2.306356
1862.037820	59.414075	27.730386
1944.502711	1812.927548	883.623122
1995.238421	1158.128682	579.201512
2931.760597	25.770929	18.938111
2960.530273	15.215207	11.290819
2964.410884	23.588064	17.527047
2975.546925	45.887518	34.224684
3014.284628	6.353003	4.800002
3030.135606	26.203000	19.901745
3047.472870	0.936956	0.715710
3052.397992	10.147395	7.763790
3081.435146	6.523001	5.038236
3092.974663	4.595439	3.562718
3093.577999	6.077166	4.712379

3100.728535	11.863956	9.220858
3113.876129	0.821113	0.640888
3114.151371	13.555928	10.581496
3120.076749	3.680527	2.878414
3133.426502	2.120796	1.665699
3152.931121	14.948336	11.813686

Zero-Point Energy : 0.306597 a.u.
========== 8.342933 eV

```
P4

 Geometry CYCLE 10
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 O     0.000021 -0.000021  0.000133
     2 O    -0.000241 -0.000155  0.000028
     3 C    -0.000214  0.000108 -0.000086
     4 C     0.000803  0.000485 -0.000085
     5 H    -0.000133 -0.000004 -0.000058
     6 Ru    0.000318 -0.000051  0.000062
     7 C     0.000004 -0.000034 -0.000018
     8 H     0.000048  0.000028  0.000023
     9 N    -0.000047  0.000001  0.000072
    10 H    -0.000036 -0.000008 -0.000023
    11 C     0.000045  0.000009 -0.000008
    12 C    -0.000077 -0.000286  0.000712
    13 C    -0.000169 -0.000028 -0.000210
    14 C     0.000044  0.000023  0.000013
    15 C    -0.000074  0.000036  0.000014
    16 C     0.000085  0.000052 -0.000118
    17 C    -0.000034 -0.000006 -0.000020
    18 C     0.000200 -0.000007  0.000018
    19 H     0.000047  0.000039  0.000018
    20 H     0.000026 -0.000057 -0.000025
    21 C    -0.000026  0.000042  0.000022
    22 H    -0.000023  0.000006 -0.000033
    23 C    -0.000099 -0.000069  0.000021
    24 H     0.000065  0.000005  0.000017
    25 H    -0.000096 -0.000004 -0.000062
    26 Cl   -0.000200 -0.000122  0.000050
    27 H    -0.000547 -0.000298 -0.000141
    28 H     0.000311  0.000316 -0.000316
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step  10
-------------------------------------
current energy                          -6.78168500 Hartree
abs of energy change              0.00006813     0.00100000    T
constrained gradient max          0.00080309     0.00100000    T
constrained gradient rms          0.00018095     0.00066667    T
gradient max                      0.00080309
gradient rms                      0.00018095
cart. step max                    0.00675576     0.01000000    T
cart. step rms                    0.00173002     0.00666667    T


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

Pauli Repulsion
  Kinetic (Delta T^0):              77.308817077885138      2103.6799       48512.02       202974.27
  Delta V^Pauli Coulomb:           -40.021469289098583     -1089.0396      -25113.85      -105076.35
  Delta V^Pauli LDA-XC:             -9.558810614972582      -260.1085       -5998.24       -25096.65
  Delta V^Pauli GGA-Exchange:        0.543476268201488        14.7887         341.04         1426.90
  Delta V^Pauli GGA-Correlation:    -0.150912918880764        -4.1065         -94.70         -396.22
                                  --------------------    ----------    ----------    ----------
  Total Pauli Repulsion:            28.121100523134697       765.2141       17646.26        73831.94
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  28.121100523134697       765.2141       17646.26        73831.94
  Electrostatic Interaction:        -5.941127213025312      -161.6663       -3728.11       -15598.43
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------    ----------    ----------    ----------
  Total Steric Interaction:         22.179973310109386       603.5478       13918.14        58233.51
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -28.912611104040423      -786.7522       -18142.94       -75910.05
                                  --------------------    ----------    ----------    ----------
  Total Orbital Interactions:      -28.916077156632781      -786.8465       -18145.11       -75919.15
```

```
Alternative Decomposition Orb.Int.
  Kinetic:                        -70.916500767179599      -1929.7362        -44500.78       -186191.25
  Coulomb:                         38.719694533467361       1053.6165         24296.98        101658.54
  XC:                               3.280729077079462         89.2732          2058.69          8613.55
                                  --------------------     -----------       ----------      -----------
  Total Orbital Interactions:     -28.916077156632774       -786.8465        -18145.11        -75919.15

  Residu (E=Steric+OrbInt+Res):     0.000001494113899          0.0000             0.00             0.00
  Dispersion Energy:               -0.045582659733669         -1.2404           -28.60           -119.68

Total Bonding Energy:              -6.781685012143165       -184.5390         -4255.57        -17805.31


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

  Electrostatic Energy:            -5.941127213025312       -161.6663         -3728.11        -15598.43
  Kinetic Energy:                   6.392316310705539        173.9438          4011.24         16783.02
  Coulomb (Steric+OrbInt) Energy:  -1.301773261517319        -35.4231          -816.88         -3417.81
  XC Energy:                       -5.885518188572397       -160.1531         -3693.22        -15452.43
  Dispersion Energy:               -0.045582659733669         -1.2404           -28.60           -119.68
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:            -6.781685012143157       -184.5390         -4255.57        -17805.31


 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:                  -230.014156102854201      -6259.0036       -144336.08       -603902.08
  Exchange GGA:                   -19.441426454342412       -529.0281        -12199.68        -51043.46
  Correlation LDA:                -12.269004788645029       -333.8566         -7698.92        -32212.27
  Correlation GGA:                  5.709991558470186        155.3768          3583.07         14991.58
                                  --------------------     -----------       ----------      -----------
  Total XC:                      -256.014595787371491      -6966.5116       -160651.60       -672166.23

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2           km/mole
             ----------          ----------          ----------
              42.168973           63.572917            0.671960
              59.196173            0.856007            0.012701
              72.308630           27.028382            0.489878
              86.017944           25.700493            0.554126
              87.887693           11.364502            0.250355
              96.411235            2.602577            0.062894
             115.440576            1.191932            0.034490
             133.107510          110.885041            3.699590
             186.981542           34.350407            1.609936
             198.089345            6.474023            0.321450
             225.433314           98.030333            5.539322
             252.136652           10.990434            0.694591
             277.531492           76.117281            5.295093
             302.029625          256.861775           19.445857
             369.556110           11.186516            1.036223
             381.279737          178.281809           17.038401
             389.888472           82.498451            8.062398
             418.379590           53.205194            5.579594
             443.167508           11.764222            1.306800
             454.616658            3.224493            0.367439
             466.352575          113.932680           13.318054
             468.816189            3.736836            0.439122
             485.121914          121.268102           14.746045
             501.400983           10.181946            1.279658
             529.461500           50.929208            6.758952
             553.098046            9.459686            1.311466
             584.264834          209.336554           30.657228
             596.977854          300.078586           44.902580
             624.849495           48.644133            7.618754
             637.277854          118.872346           18.988372
             641.705356           69.725048           11.215085
             657.467912            2.502410            0.412393
             710.273868           51.629555            9.191836
             723.663811           95.901857           17.395701
             742.143605          354.007284           65.853402
             754.103779            2.786768            0.526757
             784.428322            7.592283            1.492807
             845.123649            0.912663            0.193334
```

863.758554	0.217791	0.047153
902.917745	61.034321	13.813393
922.744251	0.298194	0.068970
962.866917	0.308098	0.074359
968.924298	0.192772	0.046818
986.180047	1.282286	0.316971
996.427244	20.563728	5.136006
1004.365077	84.327886	21.229555
1012.838810	14.673773	3.725291
1041.039738	2.577661	0.672622
1047.818106	70.357531	18.478834
1094.578222	3.347527	0.918436
1105.396888	8.870536	2.457798
1134.154431	14.150876	4.022848
1150.011576	18.335518	5.285346
1238.189982	13.620080	4.227124
1267.374205	69.553958	22.095548
1279.341905	8.650398	2.773964
1303.528814	41.623460	13.599937
1312.765898	31.898856	10.496402
1406.515677	65.079114	22.943743
1423.565928	19.795683	7.063601
1439.569643	6.780996	2.446832
1467.337453	218.612561	80.405024
1481.447452	65.688234	24.392253
1538.011510	33.750505	13.011217
1550.867475	60.968709	23.700623
1570.993039	96.740180	38.094232
1592.217277	135.451307	54.058451
1973.257961	1476.762214	730.419746
2034.614798	1160.876431	592.033474
3073.174119	67.669220	52.126241
3081.336480	1.257156	0.970971
3090.753644	4.348866	3.369136
3097.463332	19.204330	14.910198
3098.416249	5.391447	4.187195
3113.319148	28.810799	22.483142
3123.741151	5.728697	4.485481
3134.796097	4.323889	3.397519
3422.022950	13.792269	11.830326

Zero-Point Energy : 0.189559 a.u.
========== 5.158164 eV

```
P4'

 Geometry CYCLE 13
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 O    -0.000220  0.000294  0.000146
     2 O     0.000149  0.000364  0.000231
     3 C     0.000068 -0.000305 -0.000247
     4 C    -0.000370 -0.000625 -0.000290
     5 Ru    0.000724 -0.000091 -0.000466
     6 Cl    0.000094 -0.000271  0.000467
     7 H    -0.000114  0.000027 -0.000065
     8 O     0.000036  0.000100  0.000177
     9 C    -0.000151  0.000106 -0.000266
    10 C     0.000217 -0.000218  0.000059
    11 C    -0.000184  0.000028  0.000094
    12 C     0.000273 -0.000178 -0.000168
    13 H    -0.000112 -0.000144 -0.000018
    14 H     0.000059 -0.000138  0.000047
    15 H    -0.000204  0.000138  0.000087
    16 H     0.000186  0.000147 -0.000130
    17 H    -0.000003 -0.000039 -0.000142
    18 H     0.000008 -0.000070  0.000013
    19 H    -0.000013  0.000099  0.000047
    20 H    -0.000050  0.000195  0.000034
    21 O    -0.000606  0.000903  0.000398
    22 C     0.000238 -0.000294  0.000055
    23 C    -0.000007  0.000072  0.000037
    24 C    -0.000082  0.000225  0.000045
    25 C    -0.000032 -0.000470  0.000017
    26 H    -0.000036 -0.000002 -0.000068
    27 H     0.000008  0.000061 -0.000093
    28 H     0.000035 -0.000041  0.000027
    29 H    -0.000021 -0.000019 -0.000010
    30 H     0.000017 -0.000011 -0.000007
    31 H    -0.000004 -0.000011 -0.000003
    32 H     0.000077  0.000085  0.000038
    33 H     0.000019  0.000084 -0.000047
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step  13
-------------------------------------
current energy                          -6.92762453 Hartree
abs of energy change              0.00004520     0.00100000    T
constrained gradient max          0.00090250     0.00100000    T
constrained gradient rms          0.00021854     0.00066667    T
gradient max                      0.00090250
gradient rms                      0.00021854
cart. step max                    0.00076932     0.01000000    T
cart. step rms                    0.00026190     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              69.105141226505950       1880.4466        43364.14        181435.52
  Delta V^Pauli Coulomb:           -36.533698176443934       -994.1325       -22925.24        -95919.21
  Delta V^Pauli LDA-XC:             -8.927189191553119       -242.9212        -5601.90        -23438.33
  Delta V^Pauli GGA-Exchange:        0.573183207966451         15.5971          359.68          1504.89
  Delta V^Pauli GGA-Correlation:    -0.179905945657610         -4.8955         -112.89          -472.34
                                  --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:            24.037531120817739        654.0945        15083.78         63110.53
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  24.037531120817739        654.0945        15083.78         63110.53
  Electrostatic Interaction:        -5.220126218703804       -142.0469        -3275.68        -13705.44
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------     -----------     ----------     -----------
  Total Steric Interaction:         18.817404902113935        512.0476        11808.10         49405.09
 (Total Steric Interaction =
  Delta E^0 in the BB paper)
```

```
Orbital Interactions
  A:                              -25.683451229912883       -698.8823        -16116.61        -67431.89
                                  -------------------      -----------      ----------      -----------
  Total Orbital Interactions:     -25.685547302793097       -698.9393        -16117.93        -67437.39

Alternative Decomposition Orb.Int.
  Kinetic:                        -62.611108314773418      -1703.7349        -39289.07       -164385.44
  Coulomb:                         34.402370183007648        936.1361         21587.82         90323.41
  XC:                               2.523190828972694         68.6595          1583.33          6624.64
                                  -------------------      -----------      ----------      -----------
  Total Orbital Interactions:     -25.685547302793076       -698.9393        -16117.93        -67437.39

  Residu (E=Steric+OrbInt+Res):     0.000012914023420          0.0004             0.01             0.03
  Dispersion Energy:               -0.059495586089654         -1.6190            -37.33           -156.21

Total Bonding Energy:              -6.927625072745395       -188.5103         -4347.15        -18188.48


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

  Electrostatic Energy:            -5.220126218703804       -142.0469         -3275.68        -13705.44
  Kinetic Energy:                   6.494032911732532        176.7116          4075.07         17050.08
  Coulomb (Steric+OrbInt) Energy:  -2.131315079412865        -57.9960         -1337.42         -5595.77
  XC Energy:                       -6.010721100271582       -163.5600         -3771.78        -15781.15
  Dispersion Energy:               -0.059495586089654         -1.6190            -37.33           -156.21
                                  -------------------      -----------      ----------      -----------
  Total Bonding Energy:            -6.927625072745372       -188.5103         -4347.15        -18188.48


 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:                  -227.052843694443141      -6178.4222       -142477.83       -596127.16
  Exchange GGA:                   -18.980894164853268       -516.4964        -11910.69        -49834.33
  Correlation LDA:                -12.067970077101474       -328.3862         -7572.77        -31684.45
  Correlation GGA:                  5.593973978124235        152.2198          3510.27         14686.98
                                  -------------------      -----------      ----------      -----------
  Total XC:                      -252.507733958273633      -6871.0850       -158451.01       -662958.96

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2                km/mole
             ----------         ----------          ----------
              41.380481           27.174320            0.281859
              51.105256            7.326131            0.093847
              55.089333           33.600296            0.463969
              60.522949           51.296136            0.778185
              67.553995           25.969727            0.439741
              75.084610           42.104203            0.792418
              78.283806           11.465583            0.224981
              94.932529           69.933856            1.664105
             104.685204           10.660553            0.279733
             114.297630           26.571861            0.761267
             133.779650           62.175039            2.084895
             167.618711            7.256253            0.304869
             173.436319           15.019929            0.652959
             186.739883           12.303233            0.575883
             197.184293            5.547069            0.274166
             205.205849           47.697569            2.453376
             217.492655           21.274020            1.159771
             314.081147           21.421250            1.686416
             326.651620          432.700333           35.428284
             349.756046          248.077507           21.748569
             378.173215           44.661605            4.233535
             418.620191           73.846651            7.748704
             447.737854           45.160211            5.068248
             538.443499           69.673316            9.403395
             557.965400           36.396623            5.090336
             576.405694           26.284285            3.797541
             577.462071          110.496186           15.993695
             612.699827           11.024724            1.693143
             649.576617           59.021054            9.609824
             691.337060           58.954936           10.216169
             774.645339            9.895873            1.921477
             780.772360           52.516325           10.277721
```

815.978377	40.057003	8.192853
824.422796	89.991111	18.596348
836.047108	62.981292	13.198373
857.280377	400.878696	86.141798
866.413801	286.210075	62.156757
869.241483	49.628183	10.813017
874.342270	66.733149	14.625178
882.461547	35.085231	7.760652
904.566572	2.629823	0.596273
911.444782	2.802888	0.640345
932.360391	42.809872	10.004740
933.714439	26.638334	6.234465
994.346525	74.201080	18.493796
1003.631166	142.766753	35.915283
1005.936316	37.918454	9.560909
1013.900828	37.939496	9.641955
1104.643196	0.539001	0.149242
1107.212913	6.154537	1.708066
1158.847111	9.116630	2.648125
1169.711732	11.840484	3.471573
1173.938236	12.384093	3.644077
1178.418812	3.043245	0.898907
1194.605133	11.104182	3.324980
1214.368808	16.468737	5.012899
1224.266517	21.538833	6.609616
1230.709085	10.896448	3.361386
1263.998569	11.302860	3.581071
1268.769653	2.201547	0.700146
1273.827782	2.432592	0.776709
1276.710675	6.532823	2.090602
1310.840992	0.504936	0.165907
1315.051074	17.350603	5.719200
1335.816554	31.067510	10.402347
1339.933016	10.836476	3.639563
1429.302859	10.347532	3.707141
1433.182020	5.022365	1.804212
1442.865217	16.142637	5.838191
1449.188041	12.587751	4.572471
1451.354424	3.220880	1.171726
1456.915866	1.733737	0.633134
1466.289349	4.745212	1.744028
1469.966308	7.546023	2.780376
1861.781743	118.357622	55.233564
1951.749036	1765.345170	863.637869
1998.482570	1241.640965	621.977204
2943.162262	23.091092	17.034789
2950.361682	16.797840	12.422436
2958.228327	15.335239	11.371043
2962.801898	17.004791	12.628506
2963.367327	6.704192	4.979778
2966.938179	36.737310	27.320832
2974.056486	40.278300	30.026065
2974.618773	56.435760	42.078840
3009.802820	5.203593	3.925721
3014.323062	8.946096	6.759295
3024.153321	6.919457	5.245101
3027.652842	10.094092	7.660400
3034.246841	13.889445	10.563647
3042.235003	19.242574	14.673510
3045.557012	16.786788	12.814817
3057.207132	7.462927	5.718895

Zero-Point Energy : **0.255260 a.u.**
========== **6.945983 eV**

TS1

Geometry CYCLE 67
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	O	-0.000165	-0.000641	0.000122
2	O	-0.000133	0.000104	-0.000018
3	C	0.000283	0.000952	-0.000120
4	C	-0.000116	-0.000139	0.000125
5	H	0.000014	0.000014	0.000007
6	Ru	0.000603	-0.000289	-0.000107
7	C	0.000001	0.000039	-0.000002
8	H	-0.000017	0.000018	0.000008
9	N	0.000020	-0.000060	0.000055
10	H	0.000000	0.000009	0.000010
11	C	0.000000	-0.000015	0.000002
12	C	-0.000042	-0.000056	0.000087
13	C	0.000016	0.000025	-0.000017
14	C	0.000014	0.000010	0.000002
15	C	0.000024	0.000001	-0.000020
16	C	0.000003	0.000018	0.000000
17	C	-0.000017	-0.000025	-0.000008
18	C	-0.000001	0.000013	-0.000003
19	H	0.000026	0.000004	0.000013
20	H	-0.000044	0.000024	0.000041
21	C	-0.000009	-0.000015	-0.000009
22	H	-0.000024	-0.000020	-0.000024
23	C	-0.000007	-0.000007	0.000027
24	H	0.000002	-0.000004	-0.000021
25	H	0.000018	0.000033	-0.000012
26	Cl	0.000030	-0.000042	-0.000052
27	N	0.000041	0.000058	-0.000067
28	H	0.000039	-0.000020	0.000010
29	H	-0.000043	-0.000027	0.000033
30	H	-0.000049	-0.000126	-0.000132
31	B	0.000147	0.000003	0.000159
32	H	-0.000038	0.000039	-0.000035
33	H	-0.000617	0.000162	-0.000026
34	H	0.000041	-0.000039	-0.000028

Geometry Convergence after Step 67

current energy	-7.86149493 Hartree		
abs of energy change	0.00001003	0.00100000	T
constrained gradient max	0.00095207	0.00100000	T
constrained gradient rms	0.00015794	0.00066667	T
gradient max	0.00095207		
gradient rms	0.00015794		
cart. step max	0.00489459	0.01000000	T
cart. step rms	0.00104854	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	86.480135185964542	2353.2442	54267.11	227053.56
Delta V^Pauli Coulomb:	-44.268067071747851	-1204.5954	-27778.63	-116225.79
Delta V^Pauli LDA-XC:	-10.882419465514218	-296.1257	-6828.82	-28571.79
Delta V^Pauli GGA-Exchange:	0.613837575539364	16.7034	385.19	1611.63
Delta V^Pauli GGA-Correlation:	-0.169884102451499	-4.6228	-106.60	-446.03
Total Pauli Repulsion:	31.773602121790340	864.6037	19938.24	83421.58
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	31.773602121790340	864.6037	19938.24	83421.58
Electrostatic Interaction:	-6.629447029374708	-180.3964	-4160.04	-17405.61
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	25.144155092415630	684.2073	15778.20	66015.97
(Total Steric Interaction = Delta E^0 in the BB paper)				

Orbital Interactions				
A:	-32.937263392173044	-896.2685	-20668.45	-86476.77
Total Orbital Interactions:	-32.940709694921388	-896.3623	-20670.61	-86485.82
Alternative Decomposition Orb.Int.				
Kinetic:	-79.104783669362916	-2152.5507	-49639.01	-207689.58
Coulomb:	42.589060818647482	1158.9073	26725.04	111817.56
XC:	3.575013155794016	97.2811	2243.35	9386.20
Total Orbital Interactions:	-32.940709694921416	-896.3623	-20670.61	-86485.82
Residu (E=Steric+OrbInt+Res):	-0.000003673924012	-0.0001	0.00	-0.01
Dispersion Energy:	-0.064936674546025	-1.7670	-40.75	-170.49
Total Bonding Energy:	-7.861494950975795	-213.9222	-4933.16	-20640.35

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

Electrostatic Energy:	-6.629447029374708	-180.3964	-4160.04	-17405.61
Kinetic Energy:	7.375351516601626	200.6935	4628.10	19363.98
Coulomb (Steric+OrbInt) Energy:	-1.679009927024381	-45.6882	-1053.59	-4408.24
XC Energy:	-6.863452836632336	-186.7641	-4306.88	-18019.99
Dispersion Energy:	-0.064936674546025	-1.7670	-40.75	-170.49
Total Bonding Energy:	-7.861494950975825	-213.9222	-4933.16	-20640.35

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:	-239.772731226645277	-6524.5480	-150459.68	-629523.22
Exchange GGA:	-20.772127557038345	-565.2384	-13034.71	-54537.21
Correlation LDA:	-13.181963892561200	-358.6995	-8271.81	-34609.24
Correlation GGA:	6.202767335458613	168.7859	3892.30	16285.36
Total XC:	-267.524055340786219	-7279.6999	-167873.90	-702384.31

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-507.567834	2147.711526	-273.242412
45.341829	58.016041	0.659364
53.127693	28.145050	0.374801
63.168362	57.292552	0.907143
70.509379	2.424353	0.042847
85.411096	5.357298	0.114693
87.272952	35.617237	0.779144
95.556487	3.118006	0.074682
104.104666	83.409105	2.176515
120.577873	21.163198	0.639627
133.966746	9.022975	0.302988
143.553582	182.023673	6.549678
155.473314	87.855957	3.423774
193.947214	62.461036	3.036483
206.338133	10.715551	0.554207
231.929060	56.942212	3.310302
261.643697	43.250111	2.836453
309.356630	248.182124	19.244560
316.798622	223.345553	17.735305
334.722532	66.337531	5.565732
361.684633	18.110689	1.641886
389.544270	28.316695	2.764887
408.325414	10.351200	1.059437
421.699574	2.525424	0.266941
448.704961	25.482806	2.866066
457.967217	4.544197	0.521638
462.261388	123.353864	14.292837
491.303254	21.241373	2.615835
503.917032	74.714190	9.437136
525.945645	68.281010	9.001583
545.160724	2.302142	0.314583
567.072018	96.919831	13.776184
576.754034	234.319746	33.874867
606.279472	266.564345	40.509137

619.799425	10.151031	1.577028
625.244546	71.140712	11.149264
648.455633	8.114951	1.318998
699.508496	141.604406	24.828348
722.637765	37.697888	6.828350
727.472442	179.915250	32.806703
739.718022	4.409270	0.817544
742.622413	263.900735	49.123208
763.965401	43.372626	8.305532
782.089015	8.625120	1.690828
855.576225	12.168601	2.609621
867.861506	2.604999	0.566678
893.602363	478.461241	107.168991
924.626834	323.267653	74.921560
934.394666	14.185685	3.322452
953.428734	22.983738	5.492714
970.089005	47.718619	11.603193
971.634471	805.467122	196.168288
976.639882	10.758965	2.633801
995.154640	20.749845	5.175872
1011.490666	5.974765	1.514819
1018.606401	231.084622	59.000476
1033.146352	45.010762	11.656181
1045.954958	61.734694	16.185285
1082.713735	26.879794	7.294872
1089.442492	10.420190	2.845496
1097.512521	19.702821	5.420208
1134.074862	7.649031	2.174334
1138.401820	6.807571	1.942521
1146.753273	564.662887	162.307020
1189.714437	169.549312	50.561137
1192.311170	47.452779	14.181734
1257.196791	12.522988	3.946293
1276.456024	1.510511	0.483290
1293.291802	31.419367	10.185258
1302.314652	15.336018	5.006182
1345.069005	28.232781	9.518671
1406.920132	41.491305	14.632031
1432.367070	26.286949	9.437839
1446.947801	91.506900	33.188282
1469.055452	24.907395	9.171589
1539.165988	3.673707	1.417320
1552.188968	14.994756	5.833942
1557.023826	62.762377	24.494733
1570.508956	11.020238	4.338199
1589.833646	36.923312	14.713988
1724.205298	1303.240945	563.237759
1897.435522	713.261774	339.229839
1974.967111	1950.069542	965.357193
2026.519900	1812.378527	920.614585
2450.343498	112.413543	69.043640
2490.905675	225.235327	140.628020
3087.742894	1.076913	0.833489
3093.319649	2.777141	2.153282
3097.969557	9.153798	7.108149
3103.557471	5.143802	4.001494
3107.305852	20.852199	16.241044
3114.489973	20.717936	16.173779
3121.034774	2.422496	1.895134
3126.910930	9.882203	7.745463
3439.684005	14.516719	12.515987
3531.989637	8.939988	7.914700

Zero-Point Energy : **0.236476 a.u.**
========== **6.434828 eV**
(imaginary frequencies were excluded from the summation)

TS2

Geometry CYCLE 39
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	O	-0.000163	0.000203	0.000163
2	O	-0.000064	0.000060	0.000073
3	C	0.000103	-0.000093	0.000050
4	C	0.000215	-0.000178	-0.000238
5	H	0.000020	0.000047	0.000007
6	Ru	-0.000063	0.000024	-0.000514
7	C	0.000258	0.000009	0.000016
8	H	-0.000135	-0.000023	-0.000060
9	N	-0.000160	0.000146	0.000060
10	H	0.000013	0.000009	0.000002
11	C	-0.000077	0.000003	-0.000128
12	C	0.000307	0.000096	0.000209
13	C	-0.000176	-0.000059	-0.000136
14	C	-0.000156	-0.000098	-0.000108
15	C	0.000166	0.000066	0.000070
16	C	0.000192	0.000059	0.000083
17	C	-0.000092	0.000058	-0.000078
18	C	0.000073	0.000026	0.000047
19	H	0.000031	0.000003	0.000001
20	H	0.000052	0.000046	0.000022
21	C	0.000103	-0.000082	0.000121
22	H	0.000019	0.000054	-0.000090
23	C	-0.000059	-0.000060	-0.000070
24	H	0.000137	-0.000078	0.000076
25	H	-0.000090	-0.000061	-0.000062
26	Cl	-0.000136	0.000056	0.000212
27	H	-0.000409	-0.000278	0.000393
28	H	0.000088	0.000047	-0.000121

Geometry Convergence after Step 39

current energy	-6.76269434 Hartree		
abs of energy change	0.00000024	0.00100000	T
constrained gradient max	0.00051408	0.00100000	T
constrained gradient rms	0.00014021	0.00066667	T
gradient max	0.00051408		
gradient rms	0.00014021		
cart. step max	0.00926447	0.01000000	T
cart. step rms	0.00232943	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	77.406486745885104	2106.3377	48573.31	203230.70
Delta V^Pauli Coulomb:	-40.064954273333186	-1090.2229	-25141.14	-105190.52
Delta V^Pauli LDA-XC:	-9.583754501284497	-260.7872	-6013.90	-25162.14
Delta V^Pauli GGA-Exchange:	0.546776093103102	14.8785	343.11	1435.56
Delta V^Pauli GGA-Correlation:	-0.152419555163154	-4.1475	-95.64	-400.18
Total Pauli Repulsion:	28.152134509207372	766.0586	17665.73	73913.42
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	28.152134509207372	766.0586	17665.73	73913.42
Electrostatic Interaction:	-6.007824225597014	-163.4812	-3769.97	-15773.54
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	22.144310283610359	602.5773	13895.77	58139.88
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-28.856877597819103	-785.2356	-18107.97	-75763.72
Total Orbital Interactions:	-28.860769507144280	-785.3415	-18110.41	-75773.94

Alternative Decomposition Orb.Int.				
Kinetic:	-71.059032353025955	-1933.6147	-44590.22	-186565.46
Coulomb:	38.871182768785459	1057.7387	24392.04	102056.28
XC:	3.327080077096205	90.5345	2087.77	8735.25
Total Orbital Interactions:	-28.860769507144290	-785.3415	-18110.41	-75773.94
Residu (E=Steric+OrbInt+Res):	0.000001166946479	0.0000	0.00	0.00
Dispersion Energy:	-0.046236298872018	-1.2582	-29.01	-121.39
Total Bonding Energy:	-6.762694355459459	-184.0223	-4243.66	-17755.45

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

Electrostatic Energy:	-6.007824225597014	-163.4812	-3769.97	-15773.54
Kinetic Energy:	6.347454392859149	172.7230	3983.09	16665.24
Coulomb (Steric+OrbInt) Energy:	-1.193770337601244	-32.4841	-749.10	-3134.24
XC Energy:	-5.862317886248344	-159.5218	-3678.66	-15391.51
Dispersion Energy:	-0.046236298872018	-1.2582	-29.01	-121.39
Total Bonding Energy:	-6.762694355459471	-184.0223	-4243.66	-17755.45

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:	-230.014143782017499	-6259.0033	-144336.07	-603902.05
Exchange GGA:	-19.441417986470121	-529.0279	-12199.68	-51043.44
Correlation LDA:	-12.269002586999616	-333.8565	-7698.92	-32212.26
Correlation GGA:	5.709976244428359	155.3764	3583.06	14991.54
Total XC:	-256.014588111058913	-6966.5114	-160651.60	-672166.21

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-970.761434	1093.569390	-266.095133
43.405518	71.697474	0.780058
57.869568	13.069982	0.189585
68.374098	31.074593	0.532568
79.924942	14.353828	0.287560
86.810363	39.528653	0.860125
93.100576	53.057123	1.238152
111.093113	15.347161	0.427359
136.757485	95.090031	3.259599
174.978713	7.460737	0.327224
194.873129	12.658838	0.618335
224.271166	63.091898	3.546705
244.698268	56.853545	3.487117
278.815850	11.538764	0.806408
313.619406	291.181117	22.889916
360.093516	105.237302	9.498676
383.168597	391.654737	37.615892
388.545367	17.079803	1.663423
412.702427	13.520488	1.398645
442.957926	7.253320	0.805337
457.032560	9.345398	1.070590
467.077448	4.497835	0.526587
484.022083	13.146520	1.594976
512.717055	68.313316	8.779326
551.766857	5.732625	0.792843
564.607161	14.199278	2.009513
593.008771	166.921010	24.811338
622.587697	17.755962	2.770913
637.233874	152.508876	24.359706
649.543710	64.315136	10.471277
688.289783	629.546285	108.611812
710.038413	37.222075	6.624613
725.017576	93.687750	17.025874
743.033048	424.728610	79.103867
753.182254	11.806379	2.228922
768.834782	268.097289	51.665842
785.740953	20.095395	3.957801

850.384997	3.940614	0.839958
866.840421	0.242051	0.052592
927.017089	31.907540	7.414112
929.090330	7.842365	1.826346
965.479102	0.532817	0.128943
969.101465	0.507706	0.123327
989.669400	0.088026	0.021836
994.526695	24.272529	6.050755
997.715586	13.590641	3.398793
1010.894090	3.670163	0.929970
1038.273001	4.160065	1.082654
1045.826520	44.768353	11.735696
1093.657148	7.376946	2.022255
1106.077900	9.186335	2.546866
1134.422010	10.036937	2.854000
1149.385232	16.860463	4.857504
1233.932916	3.561250	1.101469
1270.254166	42.380909	13.493946
1278.850981	14.568292	4.669890
1303.039364	27.314383	8.921276
1316.179750	9.403996	3.102457
1404.377339	50.276574	17.698137
1426.617664	30.741396	10.992823
1441.361139	4.481994	1.619281
1467.445000	134.979556	49.648702
1540.435012	18.691857	7.217286
1552.877238	32.923742	12.815170
1571.023567	35.293968	13.898286
1591.987221	68.482970	27.327521
1828.854299	40.362812	18.502849
1971.625480	1277.882119	631.528981
1992.894731	768.639633	383.959311
2044.260325	930.936758	477.017650
3067.285959	76.519647	58.830873
3088.705876	0.379677	0.293947
3096.164096	7.268422	5.640819
3097.959794	1.337303	1.038445
3104.762492	10.805516	8.409148
3116.243791	21.221169	16.575964
3122.304838	6.293228	4.925233
3133.964052	4.423935	3.475208

Zero-Point Energy : 0.186677 a.u.
========== 5.079729 eV
(imaginary frequencies were excluded from the summation)

2-phenylpyridine

Geometry CYCLE 10
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	H	-0.000080	0.000072	-0.000062
2	C	-0.000222	0.000331	-0.000151
3	H	-0.000093	-0.000078	-0.000043
4	N	0.000913	-0.000070	-0.000028
5	H	0.000030	-0.000123	0.000086
6	C	0.000228	-0.000028	0.000016
7	C	-0.000639	-0.000080	0.000465
8	C	-0.000016	0.000615	0.000287
9	C	0.000052	0.000160	0.000041
10	C	-0.000179	0.000105	-0.000162
11	C	0.001144	-0.000093	-0.001314
12	C	-0.000735	-0.000321	0.000741
13	C	-0.000304	0.000476	-0.000175
14	H	-0.000012	0.000000	-0.000048
15	H	-0.000031	-0.000070	-0.000037
16	C	-0.001345	-0.000218	0.000842
17	H	0.000535	-0.000570	0.000020
18	C	0.000154	-0.000174	-0.000132
19	H	-0.000029	0.000007	-0.000159
20	H	0.000002	-0.000008	0.000121
21	H	0.000628	0.000069	-0.000307

Geometry Convergence after Step 10

current energy	-5.07426174 Hartree		
abs of energy change	0.00015693	0.00100000	T
constrained gradient max	0.00134452	0.01000000	T
constrained gradient rms	0.00041207	0.00666667	T
gradient max	0.00134452		
gradient rms	0.00041207		
cart. step max	0.00928195	0.01000000	T
cart. step rms	0.00360907	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	53.750943427442877	1462.6376	33729.23	141123.08
Delta V^Pauli Coulomb:	-25.337236283534395	-689.4613	-15899.36	-66522.90
Delta V^Pauli LDA-XC:	-6.889786016223458	-187.4806	-4323.41	-18089.13
Delta V^Pauli GGA-Exchange:	0.341997090253770	9.3062	214.61	897.91
Delta V^Pauli GGA-Correlation:	-0.076419058426816	-2.0795	-47.95	-200.64
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	21.789499159511980	592.9224	13673.12	57208.32
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	21.789499159511980	592.9224	13673.12	57208.32
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-4.250868290679326	-115.6720	-2667.46	-11160.65
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	17.538630868832655	477.2504	11005.66	46047.67
Orbital Interactions				
A:	-22.589648662702398	-614.6956	-14175.22	-59309.11
Total Orbital Interactions:	-22.592967857816575	-614.7859	-14177.30	-59317.83
Alternative Decomposition Orb.Int.				
Kinetic:	-49.003265054692001	-1333.4467	-30750.02	-128658.05
Coulomb:	24.379391397076809	663.3970	15298.30	64008.08
XC:	2.030905799798620	55.2638	1274.41	5332.14
Total Orbital Interactions:	-22.592967857816571	-614.7859	-14177.30	-59317.83

Residu (E=Steric+OrbInt+Res):	-0.000001155231089	0.0000	0.00	0.00
Dispersion Energy:	-0.019923605248032	-0.5421	-12.50	-52.31
Total Bonding Energy:	-5.074261749463041	-138.0777	-3184.15	-13322.47

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

Electrostatic Energy:	-4.250868290679326	-115.6720	-2667.46	-11160.65
Kinetic Energy:	4.747678372750876	129.1909	2979.21	12465.03
Coulomb (Steric+OrbInt) Energy:	-0.957846041688676	-26.0643	-601.06	-2514.82
XC Energy:	-4.593302184597884	-124.9901	-2882.34	-12059.71
Dispersion Energy:	-0.019923605248032	-0.5421	-12.50	-52.31
Total Bonding Energy:	-5.074261749463042	-138.0777	-3184.15	-13322.47

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:	-55.694381000244476	-1515.5212	-34948.76	-146225.58
Exchange GGA:	-7.415011738029785	-201.7727	-4652.99	-19468.11
Correlation LDA:	-4.924027758487175	-133.9896	-3089.87	-12928.03
Correlation GGA:	2.624283520981801	71.4104	1646.76	6890.06
Total XC:	-65.409136975779631	-1779.8732	-41044.86	-171731.66

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
60.966518	80.540165	1.230784
86.652233	78.204115	1.698586
145.673327	48.387298	1.766808
243.504815	7.337695	0.447863
323.935154	0.379930	0.030849
380.028512	26.013306	2.477934
400.477488	9.766874	0.980419
405.135117	12.065469	1.225243
466.240966	34.520411	4.034265
543.418576	5.375337	0.732181
607.334171	22.887383	3.484191
618.769439	34.215301	5.306734
632.762008	25.013990	3.967358
684.784203	184.459975	31.661680
728.541748	350.307637	63.970850
731.089056	80.508195	14.753275
749.063935	1.253239	0.235305
788.779001	21.628306	4.276179
824.543500	2.349649	0.485618
868.657522	1.465259	0.319037
904.662115	3.545737	0.804028
942.336470	0.478715	0.113074
952.101276	2.553131	0.609304
967.813276	2.497334	0.605824
970.943841	0.691736	0.168350
973.280170	10.145281	2.475027
989.385150	0.056221	0.013942
1008.912094	48.436135	12.249007
1030.942639	2.989883	0.772621
1047.915192	3.373903	0.886210
1072.863169	29.169681	7.844298
1081.168036	17.030442	4.615271
1131.899449	8.423080	2.389774
1137.004328	2.266749	0.646017
1167.106044	15.311677	4.479310
1258.218728	9.362917	2.952877
1269.068349	26.755248	8.510833
1287.262825	15.759541	5.084976
1305.132507	1.376808	0.450408
1331.123125	1.212357	0.404508
1403.847930	51.872312	18.252978
1432.238903	68.344761	24.535718
1450.153498	67.220867	24.434089
1480.791873	4.993744	1.853525
1548.500107	46.213732	17.937435
1568.822854	33.117420	13.022923
1573.290431	157.270762	62.020457

1590.661928	5.919574	2.360187
3061.736760	27.340666	20.982393
3082.389800	1.383800	1.069151
3086.582595	5.359213	4.146264
3090.627173	11.627141	9.007362
3099.321073	28.270635	21.962420
3105.042737	7.456810	5.803617
3108.825610	19.905120	15.510980
3116.090259	7.650091	5.975231
3120.301670	4.678401	3.659081

Zero-Point Energy : 0.164116 a.u.
========== 4.465831 eV

in THF (COSMO, Klamt's adjustment for van der Waals radii)

NH_3BH3

Geometry CYCLE 5
==========

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

Atom	Cartesian (a.u./angstrom) X	Y	Z
1 N	0.000002	0.000358	-0.000349
2 H	0.000079	-0.000089	0.000085
3 H	-0.000042	-0.000116	0.000056
4 H	-0.000031	-0.000074	0.000053
5 B	-0.000018	-0.000037	0.000133
6 H	-0.000002	0.000099	0.000095
7 H	0.000144	-0.000069	-0.000022
8 H	-0.000132	-0.000072	-0.000053

Geometry Convergence after Step 5

current energy	-1.35971512 Hartree		
abs of energy change	0.00000445	0.00100000	T
constrained gradient max	0.00035756	0.00100000	T
constrained gradient rms	0.00012714	0.00066667	T
gradient max	0.00035756		
gradient rms	0.00012714		
cart. step max	0.00013643	0.01000000	T
cart. step rms	0.00008052	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	9.578333233235185	260.6397	6010.50	25147.91
Delta V^Pauli Coulomb:	-4.298219657933766	-116.9605	-2697.17	-11284.97
Delta V^Pauli LDA-XC:	-1.342114981681921	-36.5208	-842.19	-3523.72
Delta V^Pauli GGA-Exchange:	0.060272982455995	1.6401	37.82	158.25
Delta V^Pauli GGA-Correlation:	-0.013959113847257	-0.3798	-8.76	-36.65
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	3.984312462228236	108.4187	2500.19	10460.81
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	3.984312462228236	108.4187	2500.19	10460.81
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-0.682550218650939	-18.5731	-428.31	-1792.04
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	3.301762243577297	89.8455	2071.89	8668.78
Orbital Interactions				
A:	-4.633701989692250	-126.0894	-2907.69	-12165.78
Total Orbital Interactions:	-4.633861506869699	-126.0938	-2907.79	-12166.20
Alternative Decomposition Orb.Int.				
Kinetic:	-8.354691956024656	-227.3427	-5242.65	-21935.24
Coulomb:	3.596657776549654	97.8700	2256.94	9443.02
XC:	0.124172672605301	3.3789	77.92	326.02
Total Orbital Interactions:	-4.633861506869701	-126.0938	-2907.79	-12166.20
Residu (E=Steric+OrbInt+Res):	0.000000067859353	0.0000	0.00	0.00
Solvation Energy (el):	-0.025562558540520	-0.6956	-16.04	-67.11
Dispersion Energy:	-0.004613073683357	-0.1255	-2.89	-12.11
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.002559705827860	0.0697	1.61	6.72
Total Bonding Energy:	-1.359715121829066	-36.9997	-853.23	-3569.93

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

Electrostatic Energy:	-0.682550218650939	-18.5731	-428.31	-1792.04
Kinetic Energy:	1.223641277210529	33.2970	767.85	3212.67
Coulomb (Steric+OrbInt) Energy:	-0.701561813524759	-19.0905	-440.24	-1841.95
XC Energy:	-1.171628440467882	-31.8816	-735.21	-3076.11
Solvation:	-0.023002852712660	-0.6259	-14.43	-60.39
Dispersion Energy:	-0.004613073683357	-0.1255	-2.89	-12.11
Total Bonding Energy:	-1.359715121829068	-36.9997	-853.23	-3569.93

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:	-10.155392078725320	-276.3423	-6372.61	-26662.98
Exchange GGA:	-1.418172567525287	-38.5904	-889.92	-3723.41
Correlation LDA:	-0.992813020778647	-27.0158	-623.00	-2606.63
Correlation GGA:	0.540448767116546	14.7064	339.14	1418.95
Total XC:	-12.025928899912710	-327.2422	-7546.39	-31574.07

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
240.181751	0.057122	0.003439
622.236017	12.062508	1.881355
623.881118	10.778379	1.685518
695.049555	22.144284	3.857940
1040.431032	113.055507	29.483775
1040.686680	111.686674	29.133954
1164.809061	410.738948	119.921954
1171.885730	10.447570	3.068871
1172.425983	10.115206	2.972612
1321.094255	239.811877	79.411347
1619.803991	57.988635	23.544172
1620.725357	58.773494	23.876409
2392.991674	94.369024	56.604208
2401.290056	397.279892	239.121858
2402.135589	395.753105	238.286764
3339.430214	0.166262	0.139169
3439.206065	35.598052	30.687570
3440.305437	35.639986	30.733540

Zero-Point Energy : 0.067772 a.u.
========== 1.844176 eV

```
NH2BH2

 Geometry CYCLE 5
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 N     0.000250  0.000208 -0.000567
     2 H     0.000062 -0.000363  0.000124
     3 H    -0.000214  0.000245  0.000212
     4 B    -0.000288 -0.000248  0.000679
     5 H    -0.000131  0.000018 -0.000323
     6 H     0.000322  0.000140 -0.000124
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step   5
-------------------------------------
current energy                          -1.09453802 Hartree
abs of energy change                0.00000281     0.00100000    T
constrained gradient max            0.00067908     0.00100000    T
constrained gradient rms            0.00029779     0.00066667    T
gradient max                        0.00067908
gradient rms                        0.00029779
cart. step max                      0.00220744     0.01000000    T
cart. step rms                      0.00093890     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):               8.332834058559401        226.7480         5228.93         21877.85
  Delta V^Pauli Coulomb:            -3.789447231158996       -103.1161        -2377.91         -9949.19
  Delta V^Pauli LDA-XC:             -1.105158697861239        -30.0729         -693.50         -2901.59
  Delta V^Pauli GGA-Exchange:        0.043066613630098          1.1719           27.02           113.07
  Delta V^Pauli GGA-Correlation:    -0.007760612150041         -0.2112           -4.87           -20.38
                                   --------------------     -----------     ----------      -----------
  Total Pauli Repulsion:             3.473534131019223         94.5197         2179.68         9119.76
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):   3.473534131019223         94.5197         2179.68         9119.76
  Electrostatic Interaction:        -0.583616033854117        -15.8810         -366.22        -1532.28
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                   --------------------     -----------     ----------      -----------
  Total Steric Interaction:          2.889918097165106         78.6387         1813.45         7587.48
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                                -3.978107461419179       -108.2498        -2496.30        -10444.52
                                   --------------------     -----------     ----------      -----------
  Total Orbital Interactions:       -3.979213163097453       -108.2799        -2496.99        -10447.42

Alternative Decomposition Orb.Int.
  Kinetic:                          -7.331935286040679       -199.5121        -4600.86        -19249.99
  Coulomb:                           3.233269337615498         87.9817         2028.91         8488.95
  XC:                                0.119452785327727          3.2505           74.96          313.62
                                   --------------------     -----------     ----------      -----------
  Total Orbital Interactions:       -3.979213163097454       -108.2799        -2496.99        -10447.42

  Residu (E=Steric+OrbInt+Res):      0.000000054269767          0.0000            0.00            0.00


  Solvation Energy (el):            -0.005759564470140         -0.1567           -3.61           -15.12
  Dispersion Energy:                -0.001973975207514         -0.0537           -1.24            -5.18

Post-SCF Solvation Energies
  Solvation Energy (cd):             0.002486317400511          0.0677            1.56            6.53

Total Bonding Energy:               -1.094542233939723        -29.7840         -686.84         -2873.72


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

Electrostatic Energy:	-0.583616033854117	-15.8810	-366.22	-1532.28
Kinetic Energy:	1.000898772518722	27.2358	628.07	2627.86
Coulomb (Steric+OrbInt) Energy:	-0.556177839273731	-15.1344	-349.01	-1460.24
XC Energy:	-0.950399911053455	-25.8617	-596.39	-2495.27
Solvation:	-0.003273247069629	-0.0891	-2.05	-8.59
Dispersion Energy:	-0.001973975207514	-0.0537	-1.24	-5.18
Total Bonding Energy:	-1.094542233939724	-29.7840	-686.84	-2873.72

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:	-9.758669988090588	-265.5469	-6123.66	-25621.38
Exchange GGA:	-1.330698961091227	-36.2102	-835.03	-3493.75
Correlation LDA:	-0.912972661612320	-24.8433	-572.90	-2397.01
Correlation GGA:	0.492783341635344	13.4093	309.23	1293.80
Total XC:	-11.509558269158791	-313.1910	-7222.36	-30218.34

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
583.882743	1729.878409	253.174108
701.379111	0.768776	0.135155
829.569159	0.412421	0.085757
954.159172	140.325570	33.561063
1075.916850	224.980139	60.673767
1117.903632	1.721549	0.482394
1314.897856	214.441610	70.677169
1556.008929	317.429806	123.804907
2506.277834	232.477122	146.045273
2552.701915	389.838858	249.438393
3453.181345	65.180513	56.417681
3552.465387	87.952278	78.316815

Zero-Point Energy : 0.046015 a.u.
1.252138 eV

```
THF

 Geometry CYCLE 5
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ---------------------------------------
     1 O     0.000001  0.000080 -0.000009
     2 C    -0.000013 -0.000247 -0.000269
     3 C    -0.000077  0.000311  0.000251
     4 C    -0.000229  0.000132  0.000099
     5 C     0.000270 -0.000053 -0.000192
     6 H    -0.000048  0.000008  0.000138
     7 H     0.000063  0.000094  0.000027
     8 H     0.000004 -0.000003 -0.000076
     9 H     0.000132 -0.000118 -0.000019
    10 H    -0.000004 -0.000060 -0.000052
    11 H     0.000014 -0.000160 -0.000001
    12 H    -0.000041  0.000071 -0.000026
    13 H    -0.000072 -0.000056  0.000129
 ---------------------------------------

-------------------------------------
Geometry Convergence after Step   5
-------------------------------------
current energy                          -2.61574372 Hartree
abs of energy change                0.00000779     0.00100000    T
constrained gradient max            0.00031061     0.00100000    T
constrained gradient rms            0.00012759     0.00066667    T
gradient max                        0.00031061
gradient rms                        0.00012759
cart. step max                      0.00107247     0.01000000    T
cart. step rms                      0.00043968     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              22.795242261208546        620.2901        14304.23        59848.90
  Delta V^Pauli Coulomb:           -10.986849917738530       -298.9674        -6894.35       -28845.97
  Delta V^Pauli LDA-XC:             -3.091722927067142        -84.1301        -1940.09        -8117.32
  Delta V^Pauli GGA-Exchange:        0.175246912809191          4.7687          109.97          460.11
  Delta V^Pauli GGA-Correlation:    -0.048906985974652         -1.3308          -30.69         -128.41
                                   --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:            8.843009343237414        240.6305         5549.07        23217.32
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  8.843009343237414        240.6305         5549.07        23217.32
  Electrostatic Interaction:       -1.774611127339901        -48.2896        -1113.59        -4659.24
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                   --------------------     -----------     ----------     -----------
  Total Steric Interaction:         7.068398215897512        192.3409         4435.49        18558.08
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -9.668077393500647       -263.0818        -6066.81       -25383.53
                                   --------------------     -----------     ----------     -----------
  Total Orbital Interactions:      -9.669740393666121       -263.1270        -6067.85       -25387.90

Alternative Decomposition Orb.Int.
  Kinetic:                        -20.390350147741888       -554.8497       -12795.14       -53534.86
  Coulomb:                         10.114883350759772        275.2400         6347.19        26556.62
  XC:                               0.605726403315997         16.4827          380.10         1590.33
                                   --------------------     -----------     ----------     -----------
  Total Orbital Interactions:      -9.669740393666119       -263.1270        -6067.85       -25387.90

  Residu (E=Steric+OrbInt+Res):     0.000000585965072          0.0000            0.00            0.00


  Solvation Energy (el):           -0.006781716441528         -0.1845           -4.26           -17.81
  Dispersion Energy:               -0.010518110295366         -0.2862           -6.60           -27.62

Post-SCF Solvation Energies
  Solvation Energy (cd):            0.002897708019752          0.0789            1.82            7.61
```

Total Bonding Energy:	**-2.615743710520678**	**-71.1780**	**-1641.40**	**-6867.63**

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

Electrostatic Energy:	**-1.774611127339901**	**-48.2896**	**-1113.59**	**-4659.24**
Kinetic Energy:	**2.404892113466659**	**65.4404**	**1509.09**	**6314.04**
Coulomb (Steric+OrbInt) Energy:	**-0.871965981013686**	**-23.7274**	**-547.17**	**-2289.35**
XC Energy:	**-2.359656596916605**	**-64.2095**	**-1480.71**	**-6195.28**
Solvation:	**-0.003884008421777**	**-0.1057**	**-2.44**	**-10.20**
Dispersion Energy:	**-0.010518110295366**	**-0.2862**	**-6.60**	**-27.62**
Total Bonding Energy:	**-2.615743710520676**	**-71.1780**	**-1641.40**	**-6867.63**

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:	**-26.366660279493701**	**-717.4733**	**-16545.33**	**-69225.66**
Exchange GGA:	**-3.477285504494469**	**-94.6218**	**-2182.03**	**-9129.61**
Correlation LDA:	**-2.361507049692932**	**-64.2599**	**-1481.87**	**-6200.14**
Correlation GGA:	**1.254082082242942**	**34.1253**	**786.95**	**3292.59**
Total XC:	**-30.951370751438159**	**-842.2297**	**-19422.28**	**-81262.81**

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
21.855804	21.253197	0.116431
275.586454	206.665817	14.275936
604.395886	46.194302	6.998226
623.533059	26.913492	4.206371
762.563836	59.207259	11.316946
826.423602	56.641876	11.733252
866.193448	133.681869	29.024548
883.527004	233.925510	51.805454
893.556563	10.336047	2.315019
911.272850	42.697409	9.752771
996.616420	23.696150	5.919485
1012.934259	443.667539	112.646314
1098.184728	6.340686	1.745379
1150.851264	37.662867	10.864523
1171.140263	15.954364	4.683456
1199.508876	36.673271	11.026335
1209.679954	36.823422	11.165359
1250.406457	13.676030	4.286367
1263.075030	4.061320	1.285803
1298.595306	0.469558	0.152842
1329.504786	13.984738	4.660390
1415.316194	12.029075	4.267404
1424.845340	41.274025	14.740853
1433.433780	1.516433	0.544852
1440.338123	4.043245	1.459730
2881.905609	128.471034	92.803219
2889.134375	136.290073	98.698383
2958.918684	50.947499	37.786265
2968.892790	55.976948	41.656407
3005.449815	34.259876	25.809128
3013.128901	5.311986	4.011924
3016.957686	19.325132	14.614022
3026.686382	90.419272	68.597217

Zero-Point Energy : **0.111914 a.u.**
3.045325 eV

```
H2

 Geometry CYCLE 4
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 H     0.000000  0.000000  0.000250
     2 H     0.000000  0.000000 -0.000250
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step   4
-------------------------------------
current energy                          -0.24537743 Hartree
abs of energy change               0.00000003     0.00100000    T
constrained gradient max           0.00024982     0.00100000    T
constrained gradient rms           0.00014423     0.00066667    T
gradient max                       0.00024982
gradient rms                       0.00014423
cart. step max                     0.00010004     0.01000000    T
cart. step rms                     0.00005776     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              0.585917215084310         15.9436          367.67          1538.33
  Delta V^Pauli Coulomb:           -0.124022409024830         -3.3748          -77.83          -325.62
  Delta V^Pauli LDA-XC:            -0.093537992820664         -2.5453          -58.70          -245.58
  Delta V^Pauli GGA-Exchange:      -0.002576452444738         -0.0701           -1.62            -6.76
  Delta V^Pauli GGA-Correlation:    0.001749756938793          0.0476            1.10             4.59
                                  --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:            0.367530117732872         10.0010          230.63          964.95
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  0.367530117732872         10.0010          230.63          964.95
  Electrostatic Interaction:        0.008957703470661          0.2438            5.62           23.52
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------     -----------     ----------     -----------
  Total Steric Interaction:         0.376487821203533         10.2448          236.25          988.47
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  SIGMA.g:                         -0.478126745568888        -13.0105         -300.03         -1255.32
  SIGMA.u:                         -0.145241229367401         -3.9522          -91.14          -381.33
  PI.g:                             0.000000000000000          0.0000            0.00            0.00
  PI.u:                             0.000000000000000          0.0000            0.00            0.00
                                  --------------------     -----------     ----------     -----------
  Total Orbital Interactions:      -0.623496371334037        -16.9662         -391.25         -1636.99

Alternative Decomposition Orb.Int.
  Kinetic:                         -0.348501058707706         -9.4832         -218.69          -914.99
  Coulomb:                         -0.186601353353172         -5.0777         -117.09          -489.92
  XC:                              -0.088393959273159         -2.4053          -55.47          -232.08
                                  --------------------     -----------     ----------     -----------
  Total Orbital Interactions:      -0.623496371334037        -16.9662         -391.25         -1636.99

  Residu (E=Steric+OrbInt+Res):     0.000000007373625          0.0000            0.00            0.00


  Solvation Energy (el):           -0.000451849712643         -0.0123           -0.28           -1.19
  Dispersion Energy:               -0.000001165736921          0.0000            0.00            0.00

Post-SCF Solvation Energies
  Solvation Energy (cd):            0.002084128264735          0.0567            1.31            5.47

Total Bonding Energy:              -0.245377429941709         -6.6771         -153.98          -644.24


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

  Electrostatic Energy:             0.008957703470661          0.2438            5.62           23.52
```

Kinetic Energy:	0.237416156376605	6.4604	148.98	623.34
Coulomb (Steric+OrbInt) Energy:	-0.310623755004378	-8.4525	-194.92	-815.54
XC Energy:	-0.182758647599767	-4.9731	-114.68	-479.83
Solvation:	0.001632278552092	0.0444	1.02	4.29
Dispersion Energy:	-0.000001165736921	0.0000	0.00	0.00
Total Bonding Energy:	-0.245377429941708	-6.6771	-153.98	-644.24

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:	-0.396722097371877	-10.7954	-248.95	-1041.59
Exchange GGA:	-0.087472208659961	-2.3802	-54.89	-229.66
Correlation LDA:	-0.079840340638723	-2.1726	-50.10	-209.62
Correlation GGA:	0.047665891697241	1.2971	29.91	125.15
Total XC:	-0.516368754973320	-14.0511	-324.03	-1355.73

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
4282.634665	0.000000	0.000000

Zero-Point Energy : 0.009757 a.u.
0.265490 eV

S1

Geometry CYCLE 19
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	C	-0.000010	0.000032	-0.000086
2	H	-0.000030	-0.000043	0.000019
3	C	-0.000160	0.000073	-0.000175
4	C	-0.000031	0.000024	0.000125
5	Cl	-0.000339	0.000122	-0.000144
6	N	0.000453	-0.000032	0.000103
7	O	0.000072	0.000282	-0.000002
8	C	-0.000077	-0.000082	0.000031
9	O	-0.000001	-0.000060	0.000014
10	H	-0.000012	0.000009	-0.000012
11	C	0.000462	-0.000210	-0.000174
12	C	-0.000235	-0.000177	-0.000071
13	C	0.000146	0.000220	-0.000179
14	Ru	-0.000168	-0.000108	-0.000012
15	H	-0.000036	0.000007	0.000031
16	Ru	0.000382	-0.000315	-0.000146
17	C	-0.000063	-0.000052	0.000070
18	C	0.000056	0.000078	0.000175
19	C	-0.000056	-0.000149	-0.000147
20	C	-0.000041	-0.000069	0.000027
21	H	-0.000031	0.000002	0.000050
22	H	-0.000023	0.000025	0.000013
23	C	-0.000008	0.000043	-0.000017
24	O	0.000103	-0.000038	-0.000141
25	N	-0.000222	0.000191	0.000101
26	H	-0.000027	0.000052	-0.000040
27	C	0.000053	-0.000006	0.000049
28	C	0.000102	0.000114	0.000003
29	H	-0.000008	0.000009	-0.000026
30	C	-0.000191	-0.000103	0.000144
31	C	-0.000033	0.000013	0.000041
32	C	-0.000123	-0.000021	-0.000040
33	C	0.000033	-0.000017	0.000028
34	H	0.000000	-0.000001	0.000029
35	C	0.000083	0.000080	0.000069
36	C	-0.000011	0.000012	0.000040
37	H	0.000018	0.000010	0.000039
38	C	0.000059	0.000164	-0.000038
39	C	0.000009	-0.000009	0.000038
40	C	-0.000069	0.000005	0.000069
41	H	-0.000009	-0.000019	0.000018
42	H	0.000020	0.000015	0.000023
43	C	-0.000067	-0.000036	-0.000011
44	H	0.000035	0.000033	-0.000056
45	C	0.000042	-0.000003	-0.000036
46	H	-0.000036	0.000013	0.000072
47	H	-0.000035	-0.000006	0.000016
48	H	-0.000040	-0.000047	-0.000006
49	H	-0.000018	-0.000041	-0.000008
50	Cl	0.000131	-0.000163	-0.000119
51	C	0.000007	0.000394	0.000118
52	O	-0.000055	-0.000216	0.000131

Geometry Convergence after Step 19

---

current energy -13.14710742 Hartree

abs of energy change	0.00011518	0.00100000	T
constrained gradient max	0.00046214	0.00100000	T
constrained gradient rms	0.00011617	0.00066667	T
gradient max	0.00046214		
gradient rms	0.00011617		
cart. step max	0.00798654	0.01000000	T
cart. step rms	0.00253911	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	153.657393021075791	4181.2304	96421.48	403427.43

```
  Delta V^Pauli Coulomb:          -80.212982627452675      -2182.7063       -50334.41       -210599.16
  Delta V^Pauli LDA-XC:           -18.943905522961973       -515.4899       -11887.48        -49737.22
  Delta V^Pauli GGA-Exchange:       1.109374169956176         30.1876          696.14          2912.66
  Delta V^Pauli GGA-Correlation:   -0.312653784333063         -8.5077          -196.19          -820.87
                                  --------------------     -----------      ----------      -----------
  Total Pauli Repulsion:           55.297225256284257       1504.7141        34699.54        145182.84
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 55.297225256284257       1504.7141        34699.54        145182.84
  Electrostatic Interaction:      -11.803180345373027       -321.1809        -7406.61        -30989.25
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------     -----------      ----------      -----------
  Total Steric Interaction:        43.494044910911228       1183.5332        27292.93        114193.60
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                              -56.500491336221586      -1537.4566       -35454.60       -148342.02
                                  --------------------     -----------      ----------      -----------
  Total Orbital Interactions:     -56.507528169396551      -1537.6481       -35459.01       -148360.49

Alternative Decomposition Orb.Int.
  Kinetic:                       -141.290918202773526      -3844.7215       -88661.40       -370959.25
  Coulomb:                         78.075238519674713       2124.5353        48992.96        204986.51
  XC:                               6.708151513702091        182.5381         4209.43         17612.25
                                  --------------------     -----------      ----------      -----------
  Total Orbital Interactions:     -56.507528169396721      -1537.6481       -35459.01       -148360.49

  Residu (E=Steric+OrbInt+Res):    -0.000011802390465         -0.0003          -0.01           -0.03


  Solvation Energy (el):           -0.032582984434513         -0.8866          -20.45           -85.55
  Dispersion Energy:               -0.107159425122269         -2.9160          -67.24          -281.35

Post-SCF Solvation Energies
  Solvation Energy (cd):            0.006126897640164          0.1667            3.84            16.09

Total Bonding Energy:             -13.147110572792405       -357.7511        -8249.94        -34517.73


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

  Electrostatic Energy:           -11.803180345373027       -321.1809        -7406.61        -30989.25
  Kinetic Energy:                  12.366474818302265        336.5089         7760.08         32468.18
  Coulomb (Steric+OrbInt) Energy:  -2.137755910168423        -58.1713        -1341.46         -5612.68
  XC Energy:                      -11.439033623636773       -311.2719        -7178.10        -30033.18
  Solvation:                       -0.026456086794349         -0.7199          -16.60          -69.46
  Dispersion Energy:               -0.107159425122269         -2.9160          -67.24          -281.35
                                  --------------------     -----------      ----------      -----------
  Total Bonding Energy:           -13.147110572792576       -357.7511        -8249.94        -34517.73


 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:                  -459.234117614289175      -12496.3962      -288173.79      -1205719.01
  Exchange GGA:                   -38.707704673560812       -1053.2902       -24289.45        -101627.06
  Correlation LDA:                -24.378241141102887        -663.3657       -15297.58         -64005.06
  Correlation GGA:                 11.324523941743802         308.1560         7106.25          29732.53
                                  --------------------     -----------      ----------      -----------
  Total XC:                      -510.995539487209044      -13904.8961      -320654.58      -1341618.60

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2           km/mole
             ----------         ----------          ----------
             15.454937          753.513643            2.919016
             21.837753          665.719027            3.643988
             38.031836            1.971337            0.018793
             40.566705           59.937131            0.609458
             55.597403           11.877243            0.165519
             61.652152           96.870711            1.496990
             66.389933           13.522584            0.225030
             68.528028           29.192494            0.501438
```

74.057476	317.894303	5.901056
82.102517	26.560877	0.546609
86.637164	1.744560	0.037885
87.648310	17.932957	0.393979
93.929965	0.208810	0.004916
102.659947	34.340815	0.883669
104.580411	0.254069	0.006660
111.130978	13.176192	0.367031
121.599725	0.451459	0.013760
136.901749	0.511434	0.017550
149.718935	105.658871	3.965160
180.569081	200.046631	9.054255
195.268664	1.891219	0.092566
197.535184	23.809109	1.178869
200.063759	1.679639	0.084229
211.333795	583.248530	30.895887
215.798289	1.704896	0.092220
250.802759	116.799475	7.342624
252.189135	31.304898	1.978868
257.568516	0.389300	0.025134
262.475437	131.831922	8.673359
265.988512	0.448426	0.029897
277.736630	1288.129860	89.674896
289.149732	10.684894	0.774410
290.555664	77.212583	5.623355
369.240141	0.145478	0.013464
370.639828	74.112317	6.885263
409.251563	296.706608	30.436565
410.920198	4.609468	0.474773
420.102406	6.565389	0.691343
420.433418	2.548024	0.268521
463.202108	1.025983	0.119121
463.825901	32.949251	3.830704
466.591825	9.276763	1.084955
467.023872	38.545111	4.512180
484.609643	5.968242	0.724964
484.786035	11.986518	1.456536
509.579028	0.857311	0.109504
511.301028	149.212032	19.123113
517.038458	43.693508	5.662625
518.127921	279.298632	36.273033
540.697460	6.348752	0.860440
541.178772	101.345956	13.747548
553.443108	17.984917	2.494936
554.634664	0.237742	0.033052
589.046283	208.923224	30.847091
589.311212	268.035406	39.592684
620.371612	33.526172	5.213315
621.140388	99.234196	15.450025
630.795650	549.739701	86.920829
631.853807	6.910013	1.094394
640.356854	42.487913	6.819704
640.837501	25.558565	4.105466
656.105792	7.824572	1.286804
656.740775	33.554429	5.523596
712.229325	174.847633	31.214593
713.239712	0.624364	0.111622
719.575145	760.632333	137.192069
720.080177	47.364400	8.548914
736.074396	1490.717158	275.039476
737.118357	2.658374	0.491169
750.504069	0.919804	0.173032
750.803822	10.967827	2.064073
778.955768	31.751601	6.199498
779.457180	16.447462	3.213433
841.609901	4.337700	0.915058
842.166418	0.887598	0.187367
863.991370	17.031832	3.688492
864.589582	5.916523	1.282197
921.955579	7.104819	1.641879
922.485563	3.337303	0.771673
956.569882	40.093811	9.613292
957.366136	0.579052	0.138955
959.285795	3.856303	0.927251
961.042824	0.406897	0.098018
976.018794	0.915125	0.223881
977.376226	1.913676	0.468822
994.385385	11.673210	2.909532
994.624963	14.012749	3.493500
1001.212170	12.060229	3.026633
1001.503832	364.587352	91.523429
1012.098515	6.342130	1.608926
1012.404647	16.751856	4.251039
1041.249303	5.803453	1.514674
1041.674563	3.729273	0.973720

1045.778867	195.336422	51.203678
1046.424697	39.114425	10.259425
1087.360895	18.976148	5.172016
1087.993710	18.244183	4.975410
1097.411913	17.916376	4.928309
1098.679045	11.720843	3.227808
1119.283802	3.511396	0.985140
1120.194549	49.093475	13.784636
1136.483536	37.491737	10.680136
1138.341046	41.920000	11.961117
1233.857858	35.226919	10.894765
1234.300619	66.077481	20.443370
1264.110829	157.481623	49.899145
1264.845706	12.145168	3.850518
1281.254936	28.327825	9.097600
1281.588965	14.142033	4.542957
1299.095592	71.597057	23.313869
1299.395628	42.602818	13.875793
1310.296759	24.185527	7.943342
1310.391295	139.988459	45.980247
1401.383350	10.164849	3.570557
1401.575396	290.060906	101.902241
1415.676633	16.768827	5.950382
1415.946244	140.011471	49.692226
1436.942566	0.686111	0.247122
1437.348158	35.487950	12.785596
1463.062083	34.294078	12.576505
1463.608409	741.609100	272.068346
1531.819171	25.232885	9.688409
1532.227112	58.745725	22.561994
1546.017600	162.939863	63.142220
1546.371752	112.535537	43.619599
1562.334658	305.922002	119.801664
1562.621593	47.320513	18.534520
1588.718931	219.273542	87.319527
1589.020792	294.762401	117.403146
1910.157241	0.875193	0.419036
1910.529296	5939.965097	2844.563708
1982.813262	5268.646276	2618.538281
1990.468491	0.577814	0.288285
3081.164563	0.025480	0.019679
3088.118139	0.765846	0.592807
3096.231384	0.495705	0.384711
3096.528761	0.088812	0.068933
3100.552907	0.794664	0.617591
3102.070521	36.367537	28.277671
3103.886199	1.485177	1.155479
3108.261516	10.167452	7.921506
3112.456221	2.888874	2.253772
3114.128944	70.381527	54.938064
3117.807353	35.699319	27.898913
3117.951639	12.192262	9.528658
3130.162269	3.474289	2.725906
3131.526740	3.812822	2.992821
3137.210923	2.031904	1.597810
3138.552222	3.020850	2.376493

Zero-Point Energy : **0.347155 a.u.**
========== **9.446557 eV**

A1

Geometry CYCLE 67
==========

Energy gradients wrt nuclear displacements
==

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	O	0.000133	-0.000036	-0.000012
2	O	0.000013	-0.000011	0.000009
3	C	-0.000299	0.000063	0.000048
4	C	-0.000192	0.000010	0.000183
5	H	0.000086	-0.000065	-0.000048
6	Ru	0.000382	-0.000015	-0.000548
7	C	-0.000012	0.000100	0.000049
8	H	0.000024	0.000008	0.000020
9	N	-0.000248	0.000043	0.000124
10	H	-0.000010	0.000041	0.000001
11	C	-0.000041	0.000029	0.000074
12	C	-0.000032	-0.000007	0.000027
13	C	-0.000070	0.000094	0.000065
14	C	0.000167	-0.000026	-0.000033
15	C	0.000055	-0.000031	-0.000038
16	C	0.000056	0.000052	-0.000102
17	C	-0.000181	0.000013	-0.000026
18	C	0.000080	-0.000108	-0.000071
19	H	-0.000009	-0.000039	-0.000018
20	H	0.000013	-0.000017	-0.000016
21	C	0.000073	-0.000094	0.000048
22	H	-0.000023	0.000030	-0.000003
23	C	-0.000052	0.000031	0.000009
24	H	0.000038	0.000016	0.000010
25	H	-0.000001	0.000051	0.000037
26	Cl	0.000118	-0.000201	0.000195
27	N	-0.000337	-0.000058	-0.000474
28	H	0.000208	0.000145	0.000095
29	H	0.000013	-0.000133	0.000042
30	H	-0.000111	0.000073	0.000115
31	B	0.000492	0.000005	0.000252
32	H	-0.000042	0.000008	-0.000042
33	H	-0.000195	0.000022	-0.000016
34	H	-0.000096	0.000009	0.000042

Geometry Convergence after Step 67

current energy	-7.93754718 Hartree		
abs of energy change	0.00000387	0.00100000	T
constrained gradient max	0.00054788	0.00100000	T
constrained gradient rms	0.00013366	0.00066667	T
gradient max	0.00054788		
gradient rms	0.00013366		
cart. step max	0.00659538	0.01000000	T
cart. step rms	0.00195614	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	86.946612620765634	2365.9377	54559.83	228278.30
Delta V^Pauli Coulomb:	-44.634942764996289	-1214.5786	-28008.85	-117189.03
Delta V^Pauli LDA-XC:	-10.924500017280753	-297.2708	-6855.23	-28682.27
Delta V^Pauli GGA-Exchange:	0.618826292214109	16.8391	388.32	1624.73
Delta V^Pauli GGA-Correlation:	-0.171930428459481	-4.6785	-107.89	-451.40
Total Pauli Repulsion:	31.834065702243223	866.2490	19976.18	83580.33
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	31.834065702243223	866.2490	19976.18	83580.33
Electrostatic Interaction:	-6.636085748858866	-180.5771	-4164.21	-17423.04
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	25.197979953384355	685.6719	15811.97	66157.29
(Total Steric Interaction =				

```
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                              -33.040071439139588       -899.0661        -20732.96        -86746.70
                                  -------------------     -----------      ----------      -----------
  Total Orbital Interactions:     -33.042886374670374       -899.1427        -20734.73        -86754.09

Alternative Decomposition Orb.Int.
  Kinetic:                        -79.507900780156518      -2163.5201        -49891.97       -208747.96
  Coulomb:                         42.883197942332835       1166.9112         26909.62        112589.82
  XC:                               3.581816463153244         97.4662          2247.62          9404.06
                                  -------------------     -----------      ----------      -----------
  Total Orbital Interactions:     -33.042886374670438       -899.1427        -20734.73        -86754.09

  Residu (E=Steric+OrbInt+Res):    -0.000001735724702          0.0000             0.00             0.00


  Solvation Energy (el):           -0.033077701161116         -0.9001           -20.76           -86.85
  Dispersion Energy:               -0.064211111814565         -1.7473           -40.29          -168.59

Post-SCF Solvation Energies
  Solvation Energy (cd):            0.004650058957698          0.1265             2.92            12.21

Total Bonding Energy:              -7.937546911028705       -215.9916         -4980.89        -20840.03


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

  Electrostatic Energy:            -6.636085748858866       -180.5771         -4164.21        -17423.04
  Kinetic Energy:                   7.438711840609116        202.4176          4667.86         19530.34
  Coulomb (Steric+OrbInt) Energy:  -1.751746558388156        -47.6674         -1099.24         -4599.21
  XC Energy:                       -6.895787690372881       -187.6439         -4327.17        -18104.89
  Solvation:                       -0.028427642203418         -0.7736           -17.84           -74.64
  Dispersion Energy:               -0.064211111814565         -1.7473           -40.29          -168.59
                                  -------------------     -----------      ----------      -----------
  Total Bonding Energy:            -7.937546911028770       -215.9916         -4980.89        -20840.03


 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:                   -239.772788141621220       -6524.5495       -150459.71       -629523.37
  Exchange GGA:                    -20.772112115001235         -565.2379        -13034.70        -54537.17
  Correlation LDA:                 -13.181972010595377         -358.6997         -8271.81        -34609.26
  Correlation GGA:                   6.202763018649623          168.7858          3892.29         16285.35
                                  -------------------     -----------      ----------      -----------
  Total XC:                       -267.524109248568152       -7279.7014       -167873.93       -702384.45

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2           km/mole
             ----------         ----------          ----------
              33.191872         1201.591098            9.996927
              36.488797          271.387747            2.482149
              62.865563          141.696263            2.232797
              74.874090          458.051597            8.596547
              83.783660           88.004561            1.848173
              85.651933           15.904809            0.341463
              90.176876           39.699682            0.897347
              98.253943          337.214908            8.304908
             110.613109          521.972579           14.472127
             125.773556           48.200794            1.519573
             139.282173          571.077565           19.937408
             162.494576          305.064237           12.425339
             190.784899          395.852846           18.930228
             195.588982          172.777154            8.470495
             202.849720          129.899580            6.604808
             221.632242          724.274331           40.235936
             241.458991          699.943169           42.362758
             263.182288           58.666649            3.870134
             268.032547          294.531658           19.787803
             291.961083          122.297253            8.949932
             369.722092           68.631783            6.360317
             410.355216          164.088743           16.877838
             418.528235            5.894119            0.618332
             453.180771          217.840130           24.744998
             466.209301           15.806758            1.847148
```

469.795132	21.903877	2.579334
493.507952	86.463186	10.695558
509.976112	174.516278	22.308165
514.791037	55.768527	7.196117
546.438121	98.349414	13.470721
554.417440	27.971071	3.887085
592.051135	267.669629	39.722483
620.097614	61.053329	9.489591
626.585963	397.118050	62.370376
639.328666	27.201420	4.359070
656.137387	20.609946	3.389610
709.856821	112.092276	19.944563
715.634500	106.185386	19.047329
721.284408	337.740032	61.061456
736.795371	790.886498	146.062631
750.295144	2.193581	0.412538
762.250411	52.661003	10.061549
779.880288	21.267149	4.157337
800.341975	103.232048	20.709433
842.052713	4.640063	0.979357
862.788877	1.065592	0.230448
921.574719	4.411892	1.019139
946.704031	160.439935	38.071920
956.830278	11.757236	2.819799
960.552502	1.165147	0.280530
974.976578	2.473776	0.604550
992.699401	27.509506	6.845081
1002.234192	175.007873	43.964777
1010.934553	29.463073	7.465848
1017.172736	694.938319	177.181772
1038.276004	6.080297	1.582398
1044.683750	137.489724	36.002541
1049.872931	307.575708	80.940678
1085.391093	4.653270	1.265968
1097.373032	15.708581	4.320851
1118.776494	24.396070	6.841342
1136.441929	33.398617	9.513795
1160.362327	146.909429	42.728865
1196.737960	384.404857	115.309743
1233.293563	74.412358	23.003271
1260.146196	89.145682	28.157839
1278.751823	27.407240	8.784755
1299.300813	80.779047	26.307920
1312.592532	110.757532	36.440243
1357.006916	556.613713	189.327645
1399.296585	167.738837	58.833065
1415.465768	64.779960	22.983603
1434.321358	11.742866	4.221810
1460.965821	534.908368	195.883348
1529.650742	67.844348	26.012616
1542.656474	119.198756	46.091306
1552.439004	85.514007	33.275905
1563.566549	214.498884	84.065825
1586.791818	272.645565	108.441736
1592.353640	239.255144	95.494614
1909.523992	2772.995405	1327.248794
1985.661806	2490.725097	1239.678728
2152.335862	2889.739638	1559.002556
2450.594313	309.985795	190.410671
2522.437575	295.678517	186.946900
3031.251374	858.972740	652.648591
3082.827569	1.882378	1.454569
3092.481866	1.024729	0.794318
3099.257684	28.707681	22.301489
3105.023800	54.431296	42.363485
3108.401107	0.707501	0.551242
3113.339232	28.936115	22.581081
3128.105260	4.934742	3.869224
3138.457223	0.629030	0.494841
3379.632404	94.551492	80.096940
3445.365008	166.079726	143.426674

Zero-Point Energy : **0.242115 a.u.**
========== **6.588280 eV**

A2

Geometry CYCLE 17
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	O	0.000157	0.000001	-0.000034
2	O	-0.000053	-0.000035	0.000070
3	C	-0.000064	0.000036	0.000060
4	C	-0.000078	-0.000368	-0.000088
5	H	0.000003	-0.000001	0.000001
6	Ru	-0.000112	0.000244	0.000030
7	C	0.000039	0.000054	0.000020
8	H	0.000002	0.000010	0.000014
9	N	-0.000003	0.000005	0.000041
10	H	0.000016	0.000020	-0.000014
11	C	-0.000027	0.000026	0.000048
12	C	0.000027	-0.000054	-0.000010
13	C	0.000025	0.000021	-0.000009
14	C	-0.000009	-0.000047	-0.000033
15	C	-0.000007	-0.000002	-0.000027
16	C	-0.000011	0.000064	0.000029
17	C	0.000021	0.000002	0.000014
18	C	0.000002	-0.000012	-0.000010
19	H	-0.000007	-0.000003	-0.000012
20	H	-0.000009	0.000014	0.000010
21	C	-0.000026	0.000005	-0.000044
22	H	-0.000001	-0.000002	0.000002
23	C	0.000026	0.000014	0.000001
24	H	-0.000007	0.000003	-0.000013
25	H	0.000007	-0.000004	0.000004
26	Cl	0.000091	0.000065	-0.000092
27	N	0.000149	0.000067	-0.000032
28	H	0.000002	0.000004	0.000047
29	H	-0.000053	0.000057	0.000028
30	H	-0.000054	-0.000111	0.000011
31	B	-0.000119	-0.000211	0.000101
32	H	0.000026	0.000007	0.000025
33	H	0.000045	0.000106	-0.000130
34	H	0.000001	0.000025	-0.000008

Geometry Convergence after Step 17

current energy	-7.92974513 Hartree		
abs of energy change	0.00000254	0.00100000	T
constrained gradient max	0.00036762	0.00100000	T
constrained gradient rms	0.00006799	0.00066667	T
gradient max	0.00036762		
gradient rms	0.00006799		
cart. step max	0.00477522	0.01000000	T
cart. step rms	0.00109058	0.00066667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	86.661777654206318	2358.1870	54381.09	227530.47
Delta V^Pauli Coulomb:	-44.428764747686365	-1208.9682	-27879.47	-116647.71
Delta V^Pauli LDA-XC:	-10.888131703046760	-296.2811	-6832.41	-28586.79
Delta V^Pauli GGA-Exchange:	0.616742640331513	16.7824	387.01	1619.26
Delta V^Pauli GGA-Correlation:	-0.171174271119875	-4.6579	-107.41	-449.42
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	31.790449572684832	865.0621	19948.81	83465.81
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	31.790449572684832	865.0621	19948.81	83465.81
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-6.629574595953757	-180.3999	-4160.12	-17405.95

Total Steric Interaction:	25.160874976731073	684.6622	15788.69	66059.87
(Total Steric Interaction = Delta E^0 in the BB paper)				
Orbital Interactions				
A:	-32.986530593300756	-897.6092	-20699.36	-86606.12
Total Orbital Interactions:	-32.990678374676605	-897.7220	-20701.97	-86617.01
Alternative Decomposition Orb.Int.				
Kinetic:	-79.243104633062956	-2156.3146	-49725.80	-208052.74
Coulomb:	42.700545085533875	1161.9410	26795.00	112110.27
XC:	3.551881172852443	96.6516	2228.84	9325.46
Total Orbital Interactions:	-32.990678374676641	-897.7220	-20701.97	-86617.01
Residu (E=Steric+OrbInt+Res):	0.000008434273668	0.0002	0.01	0.02
Solvation Energy (el):	-0.040655934798634	-1.1063	-25.51	-106.74
Dispersion Energy:	-0.063948102126499	-1.7401	-40.13	-167.90
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.004649070957629	0.1265	2.92	12.21
Total Bonding Energy:	-7.929749929639369	-215.7795	-4975.99	-20819.56

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

Electrostatic Energy:	-6.629574595953757	-180.3999	-4160.12	-17405.95
Kinetic Energy:	7.418673021143363	201.8724	4655.29	19477.72
Coulomb (Steric+OrbInt) Energy:	-1.728211227878823	-47.0270	-1084.47	-4537.42
XC Energy:	-6.890682160982680	-187.5050	-4323.97	-18091.48
Solvation:	-0.036006863841006	-0.9798	-22.59	-94.54
Dispersion Energy:	-0.063948102126499	-1.7401	-40.13	-167.90
Total Bonding Energy:	-7.929749929639402	-215.7795	-4975.99	-20819.56

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:	-239.772123012376255	-6524.5314	-150459.29	-629521.62
Exchange GGA:	-20.771815684510845	-565.2299	-13034.51	-54536.39
Correlation LDA:	-13.181904104994603	-358.6979	-8271.77	-34609.08
Correlation GGA:	6.202739683513089	168.7851	3892.28	16285.29
Total XC:	-267.523103118368624	-7279.6740	-167873.30	-702381.81

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
33.976016	422.247173	3.595980
57.131702	410.711049	5.881548
67.060677	101.738845	1.710144
76.989742	190.196450	3.670400
84.196149	14.573301	0.307559
93.826693	19.992513	0.470188
99.314660	27.774528	0.691414
113.754396	68.405443	1.950459
122.969244	337.178206	10.392836
139.611631	95.780735	3.351798
181.254471	132.202925	6.006312
197.341669	17.715424	0.876291
211.459664	198.885106	10.541632
221.177424	842.387931	46.701518
230.219626	505.176806	29.151695
268.679998	370.283842	24.937228
278.281099	319.999786	22.320888
292.194666	250.446301	18.342772
368.163140	52.316965	4.827929
410.018614	117.498875	12.075784
422.073053	13.224198	1.399056
464.257702	24.795425	2.885418
469.943877	45.739532	5.387854

479.220795	28.348413	3.405199
493.436391	40.138668	4.964462
514.205291	124.856413	16.092572
538.668254	61.228144	8.267050
553.700253	10.682396	1.482591
568.530682	357.378796	50.928485
587.670092	338.575377	49.873177
620.304175	53.958217	8.389583
629.472319	200.175186	31.583841
638.427251	30.533238	4.886100
654.818190	20.056956	3.292030
680.405882	183.291415	31.259948
716.859606	186.258371	33.467863
717.874818	110.582013	19.898085
723.655864	317.924456	57.667894
737.758714	724.780755	134.029091
749.484107	4.097587	0.769784
780.021987	84.737673	16.567671
782.762149	14.462813	2.837662
846.829804	4.411011	0.936294
864.714910	1.333173	0.288960
924.312601	6.972639	1.615452
933.233984	185.451630	43.380971
960.547757	1.556144	0.374668
963.154511	6.107075	1.474373
978.382873	2.015526	0.494283
992.650123	22.494932	5.597047
1002.031905	140.985235	35.410597
1009.520874	2.514812	0.636354
1037.374484	1.397240	0.363316
1042.542874	106.182048	27.747451
1043.852869	349.353209	91.407556
1085.246689	13.875986	3.774595
1096.001353	91.643370	25.176202
1098.790969	664.037766	182.888304
1118.802762	18.668392	5.235263
1135.570649	24.107599	6.861928
1152.231714	105.283486	30.407320
1230.321630	71.876813	22.165909
1259.054977	95.192676	30.041824
1277.889800	28.651752	9.177463
1295.512734	34.521558	11.210117
1306.702835	86.000269	28.167916
1310.617310	89.602191	29.435580
1344.644484	421.455862	142.048824
1397.948230	145.525346	50.992676
1414.394063	73.712118	26.132887
1432.474275	18.243469	6.550468
1459.624369	429.751053	157.230257
1528.857230	53.874525	20.645645
1544.144584	116.772463	45.196674
1560.426871	209.093267	81.782718
1562.574585	76.560265	29.986257
1580.624125	195.000393	77.257769
1585.942982	199.513923	79.311990
1908.204906	2676.747864	1280.296456
1986.223087	2490.237454	1239.786368
2162.590495	1939.212285	1051.181511
2443.421295	314.083902	192.363249
2523.175321	202.149436	127.849205
3086.603944	0.912530	0.706002
3096.930900	0.984625	0.764330
3098.777773	74.626212	57.964207
3101.463495	15.870022	12.337361
3105.173658	0.064833	0.050461
3112.336004	31.894298	24.881559
3125.829070	3.155663	2.472487
3133.981760	1.850094	1.453343
3294.833850	92.259954	76.194710
3397.318888	188.756250	160.736951
3439.640922	124.903153	107.687323

Zero-Point Energy : **0.242546 a.u.**
========== **6.600003 eV**

```
P1

 Geometry CYCLE 10
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 O    -0.000120  0.000178 -0.000174
     2 O    -0.000117  0.000343 -0.000190
     3 C     0.000112 -0.000365  0.000382
     4 C     0.000291 -0.000793  0.000394
     5 H    -0.000004 -0.000069  0.000000
     6 Ru   -0.000326  0.000812 -0.000601
     7 C    -0.000020 -0.000121 -0.000061
     8 H    -0.000070 -0.000040 -0.000042
     9 N    -0.000002 -0.000028  0.000102
    10 H    -0.000004 -0.000011 -0.000005
    11 C    -0.000027  0.000014 -0.000004
    12 C     0.000023 -0.000030 -0.000036
    13 C     0.000004  0.000002 -0.000048
    14 C    -0.000033 -0.000118 -0.000075
    15 C     0.000073  0.000064  0.000058
    16 C    -0.000148 -0.000021 -0.000090
    17 C     0.000001  0.000014  0.000022
    18 C     0.000021  0.000056 -0.000028
    19 H     0.000014  0.000018  0.000078
    20 H    -0.000001 -0.000003 -0.000020
    21 C     0.000045  0.000009  0.000145
    22 H     0.000007  0.000019 -0.000011
    23 C    -0.000026  0.000046 -0.000029
    24 H     0.000015  0.000003 -0.000025
    25 H    -0.000005 -0.000010 -0.000035
    26 Cl   -0.000048  0.000092  0.000056
    27 N     0.000118  0.000204 -0.000004
    28 H    -0.000093 -0.000137 -0.000048
    29 H     0.000150  0.000115  0.000054
    30 H     0.000093  0.000181 -0.000031
    31 B     0.000038 -0.000068  0.000083
    32 H    -0.000018  0.000066 -0.000003
    33 H     0.000145 -0.000167  0.000155
    34 H    -0.000087 -0.000256  0.000031
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Geometry Convergence after Step  10
-------------------------------------
current energy                          -7.88823413 Hartree
abs of energy change              0.00002475     0.00100000    T
constrained gradient max          0.00081249     0.00100000    T
constrained gradient rms          0.00017238     0.00066667    T
gradient max                      0.00081249
gradient rms                      0.00017238
cart. step max                    0.00785528     0.01000000    T
cart. step rms                    0.00274279     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              85.850013701953714       2336.0977        53871.70        225399.18
  Delta V^Pauli Coulomb:           -43.833455946310593      -1192.7690       -27505.91       -115084.72
  Delta V^Pauli LDA-XC:            -10.779625025509761       -293.3285        -6764.32        -28301.90
  Delta V^Pauli GGA-Exchange:        0.608438484002487         16.5565           381.80          1597.46
  Delta V^Pauli GGA-Correlation:    -0.167313740046859         -4.5528          -104.99          -439.28
                                   --------------------     -----------     ----------      -----------
  Total Pauli Repulsion:            31.678057474088988        862.0038        19878.28        83170.73
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  31.678057474088988        862.0038        19878.28        83170.73
  Electrostatic Interaction:        -6.567625991329886       -178.7142        -4121.25       -17243.30
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                   --------------------     -----------     ----------      -----------
  Total Steric Interaction:         25.110431482759100        683.2896        15757.04        65927.43
 (Total Steric Interaction =
  Delta E^0 in the BB paper)
```

Orbital Interactions				
A:	-32.902929010286584	-895.3343	-20646.90	-86386.63
Total Orbital Interactions:	-32.907317368662781	-895.4537	-20649.66	-86398.15
Alternative Decomposition Orb.Int.				
Kinetic:	-78.489519600697037	-2135.8085	-49252.92	-206074.20
Coulomb:	42.099836249406344	1145.5948	26418.05	110533.10
XC:	3.482365982627930	94.7600	2185.22	9142.95
Total Orbital Interactions:	-32.907317368662760	-895.4537	-20649.66	-86398.15
Residu (E=Steric+OrbInt+Res):	0.000000963283979	0.0000	0.00	0.00
Solvation Energy (el):	-0.031455622264134	-0.8560	-19.74	-82.59
Dispersion Energy:	-0.064541384479097	-1.7563	-40.50	-169.45
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.004647788007275	0.1265	2.92	12.20
Total Bonding Energy:	-7.888234141355658	-214.6498	-4949.94	-20710.56

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

Electrostatic Energy:	-6.567625991329886	-178.7142	-4121.25	-17243.30
Kinetic Energy:	7.360494101256677	200.2892	4618.78	19324.97
Coulomb (Steric+OrbInt) Energy:	-1.733618733620268	-47.1742	-1087.86	-4551.62
XC Energy:	-6.856134298926202	-186.5649	-4302.29	-18000.78
Solvation:	-0.026807834256858	-0.7295	-16.82	-70.38
Dispersion Energy:	-0.064541384479097	-1.7563	-40.50	-169.45
Total Bonding Energy:	-7.888234141355635	-214.6498	-4949.94	-20710.56

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:	-239.772821476299896	-6524.5504	-150459.73	-629523.45
Exchange GGA:	-20.772122435027267	-565.2382	-13034.70	-54537.20
Correlation LDA:	-13.181976717267531	-358.6998	-8271.82	-34609.27
Correlation GGA:	6.202756447320331	168.7856	3892.29	16285.33
Total XC:	-267.524164181274386	-7279.7029	-167873.97	-702384.59

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
17.441177	1808.027659	7.904218
33.268015	174.338802	1.453781
52.097298	193.427013	2.525867
55.896820	180.896578	2.534519
61.139440	190.349609	2.917101
75.997170	3.867372	0.073670
83.702769	421.703997	8.847603
88.903656	34.246101	0.763148
93.499058	358.886141	8.410891
100.562171	353.061563	8.899450
116.235174	55.698618	1.622782
133.444759	424.546610	14.200544
146.025235	1113.654273	40.762083
156.450414	632.585146	24.806973
193.142270	464.248749	22.475333
216.302397	141.701906	7.682722
272.600357	837.965504	57.257269
283.361546	39.240765	2.787125
307.493075	876.532660	67.558736
326.924968	27.929647	2.288714
358.558763	355.421846	31.943502
366.387717	291.763698	26.794782
412.032499	2023.508332	208.984723
420.288594	671.329238	70.723091
430.263004	175.606312	18.938789
441.153275	2232.405419	246.854271

461.208055	90.068178	10.412292
475.116237	3857.675261	459.413347
500.929422	69.262677	8.696688
506.718005	366.096405	46.498599
538.326668	83.870193	11.317008
566.166521	234.356514	33.258242
576.285049	262.794406	37.960466
602.299118	21.534602	3.251076
614.102743	4.226025	0.650506
644.610495	2.050559	0.331320
657.891806	41.807956	6.894321
702.409351	73.563803	12.951872
728.155706	733.944990	133.957131
740.778911	456.566109	84.775498
744.505022	35.656629	6.654049
769.015394	288.002022	55.514782
770.821970	37.132071	7.174330
828.593130	438.848268	91.145197
851.543689	95.239576	20.328365
871.650966	151.327175	33.062646
874.638551	2788.429950	611.316932
898.921641	1022.567945	230.405096
947.552970	3.592558	0.853268
948.494013	13.038246	3.099787
968.595987	156.192852	37.921184
977.884433	22.505950	5.516491
979.458354	5.264868	1.292562
994.587878	39.297375	9.796812
1005.358455	21.467613	5.409819
1008.859749	97.938414	24.766346
1019.224029	23.762924	6.070823
1036.643570	54.239409	14.093617
1048.945234	19.292485	5.072465
1056.917290	35.763204	9.474482
1079.306490	17.007692	4.601170
1082.899262	128.641869	34.917928
1113.019091	13.599908	3.794169
1123.137773	2.834125	0.797866
1134.130033	10.713145	3.045495
1228.985421	319.997041	98.575903
1244.588559	16.409299	5.119103
1267.787357	10.108956	3.212409
1290.194064	29.704316	9.606223
1299.339340	40.743248	13.269553
1337.517818	111.663548	37.435968
1402.985404	26.710153	9.393071
1421.924626	56.681140	20.201947
1442.473143	282.324800	102.078631
1473.527229	25.439925	9.396196
1532.787876	40.615656	15.604635
1546.139188	67.195792	26.041664
1548.523804	119.149429	46.247464
1568.650492	121.521882	47.781386
1587.136826	74.798294	29.756656
1803.115743	516.730276	233.542317
1914.904119	3678.801247	1765.759000
1976.324326	3040.015220	1505.955172
2450.057036	238.555389	146.501981
2484.428416	469.718167	292.510807
3087.911623	73.716699	57.056984
3101.219978	1.914721	1.488388
3106.220283	0.165216	0.128636
3110.135294	2.175261	1.695777
3116.394185	2.060948	1.609895
3119.338058	8.571640	6.702000
3124.387049	18.369522	14.386023
3126.234007	6.386173	5.004264
3130.150717	5.455150	4.280062
3450.591876	56.453635	48.827397
3551.474709	45.412573	40.426199

Zero-Point Energy : **0.238156 a.u.**
========== **6.480550 eV**

```
P2

 Geometry CYCLE 18
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 O     0.000031  0.000075 -0.000115
     2 O    -0.000067 -0.000044 -0.000052
     3 C     0.000478 -0.000259  0.000030
     4 C     0.000020  0.000196  0.000140
     5 H     0.000019  0.000012 -0.000006
     6 Ru   -0.000336 -0.000177  0.000588
     7 C     0.000014  0.000187  0.000074
     8 H    -0.000026  0.000038  0.000024
     9 N     0.000109 -0.000365 -0.000188
    10 H    -0.000081  0.000040 -0.000059
    11 C     0.000052  0.000006 -0.000013
    12 C    -0.000199  0.000855 -0.000486
    13 C     0.000416  0.000407 -0.000710
    14 C    -0.000348  0.000173  0.000102
    15 C    -0.000070 -0.000071 -0.000051
    16 C     0.000200 -0.000281  0.000026
    17 C     0.000100  0.000020 -0.000008
    18 C    -0.000374 -0.000611  0.000396
    19 H     0.000039 -0.000065 -0.000014
    20 H    -0.000106 -0.000008  0.000020
    21 C    -0.000039  0.000139 -0.000209
    22 H     0.000042  0.000010  0.000078
    23 C     0.000135 -0.000035  0.000009
    24 H    -0.000048 -0.000036 -0.000043
    25 H    -0.000082 -0.000009  0.000039
    26 Cl    0.000039 -0.000191  0.000222
    27 H     0.000025 -0.000069  0.000215
    28 H     0.000054  0.000062 -0.000009
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step  18
-------------------------------------
current energy                          -6.78439363 Hartree
abs of energy change              0.00005451     0.00100000    T
constrained gradient max          0.00085466     0.00100000    T
constrained gradient rms          0.00022375     0.00066667    T
gradient max                      0.00085466
gradient rms                      0.00022375
cart. step max                    0.00876331     0.01000000    T
cart. step rms                    0.00173213     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):             76.411046746351758       2079.2504        47948.66        200617.17
  Delta V^Pauli Coulomb:          -39.376368541834651      -1071.4855       -24709.05       -103382.64
  Delta V^Pauli LDA-XC:            -9.466783612994247       -257.6043        -5940.50        -24855.04
  Delta V^Pauli GGA-Exchange:       0.543926759927519         14.8010           341.32          1428.08
  Delta V^Pauli GGA-Correlation:   -0.150789388528797         -4.1032           -94.62          -395.90
                                  --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:           27.961031962921581        760.8584        17545.81        73411.68
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli): 27.961031962921581        760.8584        17545.81        73411.68
  Electrostatic Interaction:       -5.915414081496593       -160.9666        -3711.98       -15530.92
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------     -----------     ----------     -----------
  Total Steric Interaction:        22.045617881424988         599.8918        13833.84        57880.76
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                              -28.752062006059763        -782.3834       -18042.19       -75488.53
                                  --------------------     -----------     ----------     -----------
  Total Orbital Interactions:     -28.756256833774408        -782.4976       -18044.83       -75499.54
```

```
Alternative Decomposition Orb.Int.
  Kinetic:                        -70.097410953647497      -1907.4476        -43986.79       -184040.73
  Coulomb:                         38.138902120590956       1037.8123         23932.52         100133.67
  XC:                               3.202251999282123         87.1377          2009.44           8407.51
                                  -------------------     -----------       ----------      -----------
  Total Orbital Interactions:     -28.756256833774419       -782.4976        -18044.83        -75499.54

  Residu (E=Steric+OrbInt+Res):    -0.000000380539911          0.0000             0.00             0.00


  Solvation Energy (el):           -0.029773514518873         -0.8102           -18.68           -78.17
  Dispersion Energy:               -0.048379706086047         -1.3165           -30.36          -127.02

Post-SCF Solvation Energies
  Solvation Energy (cd):            0.004397429249231          0.1197             2.76            11.55

Total Bonding Energy:              -6.784395124245020       -184.6128         -4257.27        -17812.43


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

  Electrostatic Energy:            -5.915414081496593       -160.9666         -3711.98        -15530.92
  Kinetic Energy:                   6.313635792704261        171.8028          3961.87         16576.45
  Coulomb (Steric+OrbInt) Energy:  -1.237466801783604        -33.6732          -776.52         -3248.97
  XC Energy:                       -5.871394242313402       -159.7688         -3684.36        -15415.34
  Solvation:                       -0.025376085269642         -0.6905           -15.92           -66.62
  Dispersion Energy:               -0.048379706086047         -1.3165           -30.36          -127.02
                                  -------------------     -----------       ----------      -----------
  Total Bonding Energy:            -6.784395124245027       -184.6128         -4257.27        -17812.43


 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:                   -230.014086923651007      -6259.0018       -144336.03       -603901.90
  Exchange GGA:                    -19.441419751636779        -529.0279        -12199.68        -51043.44
  Correlation LDA:                -12.268996968032374        -333.8564         -7698.91        -32212.25
  Correlation GGA:                  5.710012400272075         155.3773          3583.09         14991.64
                                  -------------------     -----------       ----------      -----------
  Total XC:                       -256.014491243048042      -6966.5088       -160651.54       -672165.95

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1          1e-40 esu2 cm2           km/mole
             ----------          ----------          ----------
              33.604897           50.954324            0.429202
              53.643418          428.746225            5.764940
              58.594115          215.889698            3.170765
              70.008651           44.676816            0.783993
              80.455450           60.856583            1.227273
              87.347344           62.145475            1.360621
              95.954450          197.723028            4.755547
             110.904561           15.461064            0.429800
             130.988728          300.102824            9.853308
             138.139848           81.219511            2.812273
             186.590388           73.936997            3.458033
             212.467459            2.669260            0.142155
             279.440550           42.990105            3.011175
             305.369645          875.398201           67.005366
             327.123797           17.286448            1.417412
             351.608334           42.952718            3.785540
             368.644615           39.882381            3.685251
             402.554928          177.675233           17.927929
             422.820678          280.037911           29.679127
             442.103300           44.230602            4.901451
             452.037197            8.134429            0.921678
             497.954222           68.241965            8.517635
             510.113235          114.199725           14.601912
             535.407493           80.022162           10.739221
             567.738091          196.179233           27.917668
             570.889851          295.130838           42.232324
             602.094189           28.340574            4.277117
             614.382012            9.664008            1.488243
             643.044871            6.388816            1.029769
             700.598238           74.330125           13.053049
             734.632036          664.087156          122.284951
             740.365786          640.757007          118.909835
             743.324630           38.243611            7.125502
             773.725252          146.398516           28.392361
```

797.261421	430.318442	85.994124
817.299815	192.704865	39.477728
873.481182	33.730810	7.385134
879.428775	162.241227	35.763496
929.982516	40.199204	9.370663
948.218570	18.510611	4.399540
955.417180	9.244493	2.213881
979.796770	0.459157	0.112765
982.711922	3.763663	0.927075
990.068031	11.271060	2.797099
994.905869	18.217572	4.543082
1003.975157	12.332409	3.103480
1017.580427	11.088807	2.828340
1032.023798	34.375067	8.892243
1048.816097	43.670894	11.480730
1078.903019	15.525037	4.198490
1115.071592	13.383329	3.740632
1128.151424	11.920061	3.370730
1135.099905	0.957316	0.272375
1242.530825	9.172782	2.856843
1262.571705	14.341365	4.538628
1286.846769	46.506501	15.000943
1296.139969	13.101526	4.256492
1341.871374	93.561716	31.469304
1405.921845	35.393993	12.472939
1423.696589	58.327846	20.814762
1439.105368	315.417716	113.777594
1473.853251	13.541201	5.002528
1531.536551	24.822085	9.528920
1544.763598	8.546275	3.309154
1579.200416	114.424296	45.293259
1588.161635	68.229352	27.160891
1858.731237	545.576699	254.185330
1918.947671	3237.696877	1557.318305
1975.363786	2696.754555	1335.262274
3038.365403	1.748607	1.331712
3103.368484	9.429549	7.335037
3103.428485	17.242236	13.412613
3108.505375	2.408679	1.876759
3114.315350	3.618925	2.825012
3115.404071	20.802277	16.244387
3120.980870	6.435277	5.034269
3123.043328	6.618887	5.181328
3130.065663	3.497998	2.744423

Zero-Point Energy : **0.190636 a.u.**
========== **5.187473 eV**

```
P3

 Geometry CYCLE 15
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ----------------------------------------
     1 O     0.000026 -0.000092 -0.000059
     2 O    -0.000024  0.000070  0.000079
     3 C    -0.000063  0.000069  0.000013
     4 C     0.000087  0.000089 -0.000055
     5 H    -0.000038  0.000010 -0.000027
     6 Ru    0.000119 -0.000201 -0.000380
     7 C     0.000051 -0.000053 -0.000069
     8 H    -0.000016 -0.000015 -0.000025
     9 N    -0.000104  0.000012  0.000016
    10 H     0.000008 -0.000004  0.000043
    11 C     0.000025 -0.000061 -0.000066
    12 C    -0.000063  0.000026  0.000424
    13 C    -0.000017 -0.000051 -0.000010
    14 C     0.000037  0.000077  0.000061
    15 C     0.000023  0.000032  0.000038
    16 C    -0.000037  0.000019 -0.000076
    17 C    -0.000067 -0.000058 -0.000027
    18 C     0.000021  0.000005 -0.000067
    19 H     0.000025  0.000031  0.000006
    20 H    -0.000064  0.000027 -0.000011
    21 C     0.000027  0.000031  0.000041
    22 H    -0.000018 -0.000066 -0.000003
    23 C    -0.000022 -0.000025 -0.000004
    24 H     0.000033  0.000028  0.000004
    25 H     0.000009  0.000005  0.000020
    26 Cl   -0.000037 -0.000011  0.000199
    27 H     0.000132  0.000074  0.000011
    28 H    -0.000052  0.000030 -0.000076
 ----------------------------------------

-------------------------------------
Geometry Convergence after Step  15
-------------------------------------
current energy                          -6.78728185 Hartree
abs of energy change          0.00001444     0.00100000    T
constrained gradient max      0.00042389     0.00100000    T
constrained gradient rms      0.00008447     0.00066667    T
gradient max                  0.00042389
gradient rms                  0.00008447
cart. step max                0.00711757     0.01000000    T
cart. step rms                0.00179224     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):           77.076846959820642    2097.3677      48366.46      202365.23
  Delta V^Pauli Coulomb:        -39.780945724157696   -1082.4946     -24962.92     -104444.86
  Delta V^Pauli LDA-XC:          -9.543836622298651    -259.7010      -5988.85      -25057.34
  Delta V^Pauli GGA-Exchange:     0.543573686927136      14.7914        341.10        1427.15
  Delta V^Pauli GGA-Correlation: -0.150678323361173      -4.1002        -94.55        -395.61
                                ------------------    ----------    ----------    ----------
  Total Pauli Repulsion:         28.144959976930259     765.8633      17661.23      73894.58
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  28.144959976930259   765.8633      17661.23      73894.58
  Electrostatic Interaction:        -5.966683419642836  -162.3617      -3744.15      -15665.53
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                ------------------    ----------    ----------    ----------
  Total Steric Interaction:         22.178276557287425   603.5016      13917.08      58229.06
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -28.893104670104108  -786.2214     -18130.70     -75858.84
                                ------------------    ----------    ----------    ----------
  Total Orbital Interactions:      -28.897080917737465  -786.3296     -18133.19     -75869.28
```

Alternative Decomposition Orb.Int.				
Kinetic:	**-70.708975459506945**	**-1924.0891**	**-44370.56**	**-185646.39**
Coulomb:	**38.539508800826262**	**1048.7134**	**24183.91**	**101185.47**
XC:	**3.272385740943210**	**89.0461**	**2053.45**	**8591.65**
Total Orbital Interactions:	**-28.897080917737473**	**-786.3296**	**-18133.19**	**-75869.28**
Residu (E=Steric+OrbInt+Res):	**0.000000439274358**	**0.0000**	**0.00**	**0.00**
Solvation Energy (el):	**-0.026757495700882**	**-0.7281**	**-16.79**	**-70.25**
Dispersion Energy:	**-0.046166751547916**	**-1.2563**	**-28.97**	**-121.21**
Post-SCF Solvation Energies				
Solvation Energy (cd):	**0.004446544521971**	**0.1210**	**2.79**	**11.67**
Total Bonding Energy:	**-6.787281623902508**	**-184.6913**	**-4259.08**	**-17820.01**

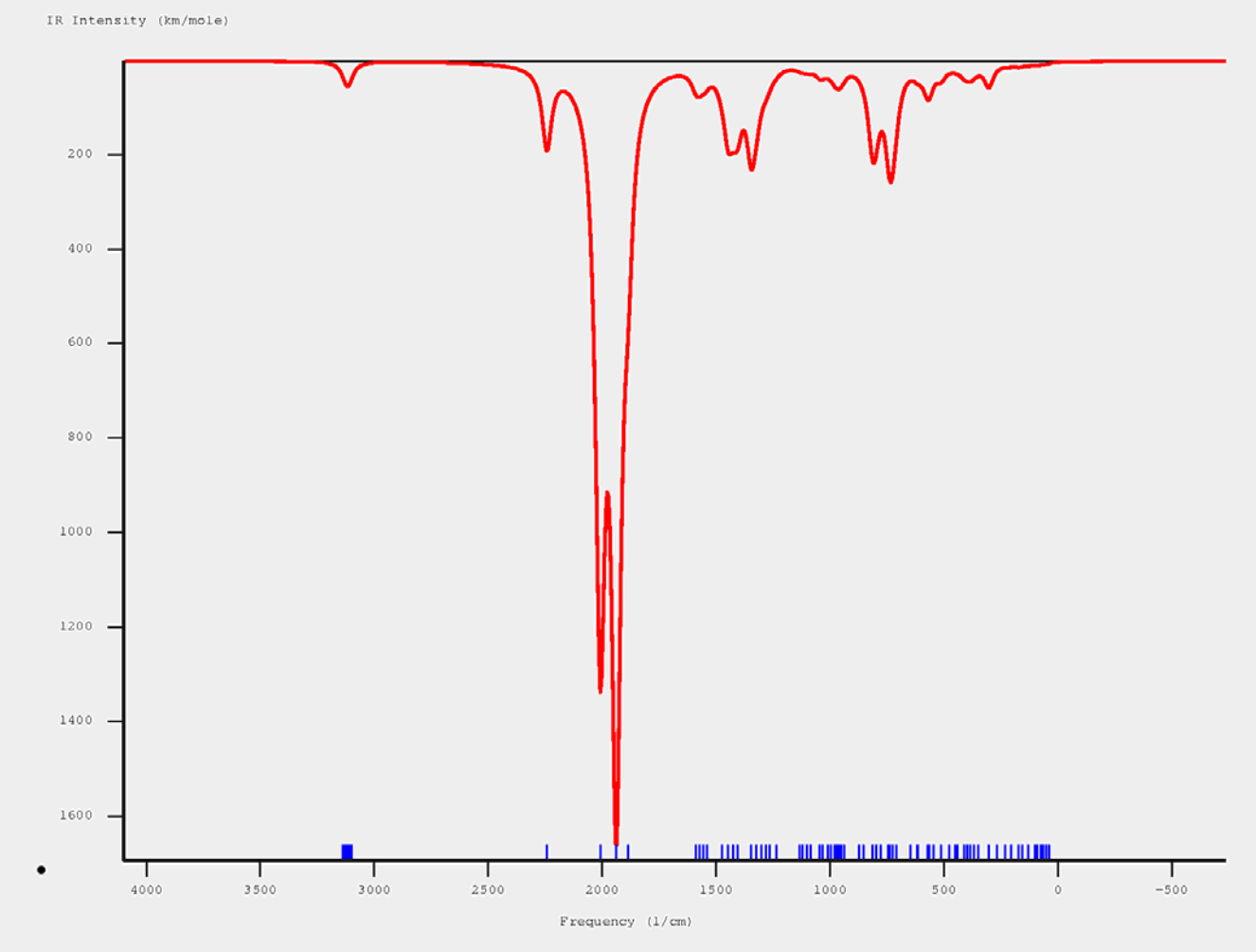
Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Electrostatic Energy:	**-5.966683419642836**	**-162.3617**	**-3744.15**	**-15665.53**
Kinetic Energy:	**6.367871500313697**	**173.2786**	**3995.90**	**16718.84**
Coulomb (Steric+OrbInt) Energy:	**-1.241436484057076**	**-33.7812**	**-779.01**	**-3259.39**
XC Energy:	**-5.878555517789479**	**-159.9636**	**-3688.85**	**-15434.15**
Solvation:	**-0.022310951178911**	**-0.6071**	**-14.00**	**-58.58**
Dispersion Energy:	**-0.046166751547916**	**-1.2563**	**-28.97**	**-121.21**
Total Bonding Energy:	**-6.787281623902521**	**-184.6913**	**-4259.08**	**-17820.01**

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:	**-230.014142088686469**	**-6259.0033**	**-144336.07**	**-603902.04**
Exchange GGA:	**-19.441416099461748**	**-529.0278**	**-12199.67**	**-51043.43**
Correlation LDA:	**-12.269002697508277**	**-333.8566**	**-7698.92**	**-32212.26**
Correlation GGA:	**5.709982425062107**	**155.3765**	**3583.07**	**14991.56**
Total XC:	**-256.014578460594407**	**-6966.5111**	**-160651.59**	**-672166.18**



```
P3'

 Geometry CYCLE 18
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ---------------------------------------
     1 O     0.000021 -0.000091 -0.000073
     2 O    -0.000135 -0.000017  0.000112
     3 C    -0.000194  0.000286  0.000327
     4 C     0.000348  0.000021 -0.000220
     5 H     0.000011 -0.000033  0.000018
     6 Ru   -0.000247  0.000583 -0.000831
     7 C     0.000015 -0.000001  0.000066
     8 H     0.000003  0.000048  0.000038
     9 N    -0.000275  0.000051  0.000138
    10 H     0.000002  0.000040 -0.000045
    11 C     0.000004  0.000069 -0.000014
    12 C     0.000026 -0.000098 -0.000073
    13 C     0.000055  0.000054  0.000093
    14 C     0.000034 -0.000003 -0.000192
    15 C     0.000060 -0.000046  0.000001
    16 C    -0.000052  0.000085  0.000167
    17 C    -0.000009 -0.000118 -0.000091
    18 C     0.000072 -0.000032  0.000021
    19 H     0.000037 -0.000019  0.000015
    20 H    -0.000006 -0.000012  0.000018
    21 C     0.000054  0.000067 -0.000131
    22 H    -0.000002  0.000050  0.000000
    23 C    -0.000083  0.000002  0.000070
    24 H     0.000031  0.000059 -0.000016
    25 H    -0.000029 -0.000082  0.000017
    26 Cl    0.000151 -0.000279  0.000176
    27 H    -0.000017 -0.000047 -0.000010
    28 H     0.000066  0.000004  0.000071
    29 O    -0.000246 -0.000567  0.000220
    30 C     0.000035  0.000118  0.000090
    31 C    -0.000004 -0.000112  0.000100
    32 C     0.000045 -0.000030 -0.000169
    33 C     0.000096 -0.000065  0.000025
    34 H    -0.000003 -0.000009 -0.000013
    35 H     0.000032 -0.000017  0.000028
    36 H     0.000046  0.000057 -0.000056
    37 H     0.000046 -0.000037 -0.000014
    38 H    -0.000046 -0.000073 -0.000004
    39 H    -0.000054  0.000124  0.000151
    40 H     0.000070  0.000077  0.000047
    41 H     0.000043 -0.000007 -0.000054
 ---------------------------------------

-------------------------------------
Geometry Convergence after Step  18
-------------------------------------
current energy                          -9.42046502 Hartree
abs of energy change              0.00006772     0.00100000    T
constrained gradient max          0.00083074     0.00100000    T
constrained gradient rms          0.00014505     0.00066667    T
gradient max                      0.00083074
gradient rms                      0.00014505
cart. step max                    0.00676361     0.01000000    T
cart. step rms                    0.00205083     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):             100.193694570014827       2726.4091        62872.50        263058.51
  Delta V^Pauli Coulomb:           -50.965983262647889      -1386.8550       -31981.64       -133811.17
  Delta V^Pauli LDA-XC:            -12.764925762563845       -347.3513        -8010.11        -33514.31
  Delta V^Pauli GGA-Exchange:        0.747642560671622         20.3444          469.15          1962.94
  Delta V^Pauli GGA-Correlation:    -0.210630299668880         -5.7315          -132.17          -553.01
                                  --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:           36.999797805805841       1006.8157        23217.73        97142.96
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  36.999797805805841       1006.8157        23217.73        97142.96
```

Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-7.715163343534382	-209.9403	-4841.34	-20256.16
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	29.284634462271459	796.8754	18376.39	76886.80
Orbital Interactions				
A:	-38.591177988472595	-1050.1194	-24216.33	-101321.12
Total Orbital Interactions:	-38.596403297164372	-1050.2616	-24219.61	-101334.84
Alternative Decomposition Orb.Int.				
Kinetic:	-91.348607027871736	-2485.7221	-57322.12	-239835.73
Coulomb:	48.782280369864836	1327.4334	30611.35	128077.86
XC:	3.969923360842534	108.0271	2491.16	10423.03
Total Orbital Interactions:	-38.596403297164365	-1050.2616	-24219.61	-101334.84
Residu (E=Steric+OrbInt+Res):	0.000016407978253	0.0004	0.01	0.04
Solvation Energy (el):	-0.035593830133443	-0.9686	-22.34	-93.45
Dispersion Energy:	-0.078080366396544	-2.1247	-49.00	-205.00
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.004964174249672	0.1351	3.12	13.03
Total Bonding Energy:	-9.420462449194975	-256.3438	-5911.43	-24733.42

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

Electrostatic Energy:	-7.715163343534382	-209.9403	-4841.34	-20256.16
Kinetic Energy:	8.845087542143091	240.6871	5550.38	23222.77
Coulomb (Steric+OrbInt) Energy:	-2.183686484804802	-59.4211	-1370.28	-5733.27
XC Energy:	-8.257990140718569	-224.7113	-5181.97	-21681.35
Solvation:	-0.030629655883771	-0.8335	-19.22	-80.42
Dispersion Energy:	-0.078080366396544	-2.1247	-49.00	-205.00
Total Bonding Energy:	-9.420462449194977	-256.3438	-5911.43	-24733.42

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:	-256.380798736800898	-6976.4765	-160881.40	-673127.69
Exchange GGA:	-22.918693271995100	-623.6494	-14381.70	-60173.02
Correlation LDA:	-14.630517455362350	-398.1166	-9180.79	-38412.42
Correlation GGA:	6.964190613630675	189.5053	4370.10	18284.48
Total XC:	-286.965818850527683	-7808.7372	-180073.79	-753428.65

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
13.078465	973.073028	3.189924
17.373846	34.590906	0.150639
45.207586	39.144268	0.443565
50.811063	108.135565	1.377225
54.745987	150.995713	2.072025
62.249750	16.268609	0.253844
71.006546	107.799838	1.918645
79.163017	39.007537	0.774014
79.823184	51.314128	1.026701
97.160026	21.791957	0.530716
100.439237	143.311858	3.607976
106.481614	169.518522	4.524492
149.049787	50.320221	1.879975
170.065756	3.265008	0.139181
180.178483	41.849619	1.890047
197.537808	56.370825	2.791147
209.632104	79.177808	4.160441
217.193339	16.734813	0.911057
279.803839	6.698024	0.469763
297.647992	800.394445	59.715228

318.308391	18.416822	1.469403
327.382720	128.182805	10.518737
348.843512	105.791967	9.250419
387.040670	38.716955	3.756089
403.195772	5.576336	0.563564
424.937156	93.999452	10.012167
443.280025	195.376342	21.708420
447.555457	99.570409	11.170053
519.344809	183.322286	23.864324
524.993944	107.853420	14.192741
540.147100	97.986103	13.266446
572.995217	96.481638	13.857144
580.496923	271.734439	39.538726
601.851266	12.730769	1.920533
611.953653	1.532353	0.235047
622.339329	30.469304	4.753000
636.635572	2.460087	0.392572
668.737328	50.886095	8.529681
687.620970	642.549542	110.747467
738.021735	411.018640	76.034158
741.998894	192.333812	35.771485
745.736082	43.180638	8.071463
770.721151	115.143085	22.244017
773.790189	36.348179	7.049916
818.878760	48.531160	9.961353
825.177907	21.773808	4.503602
848.226915	412.271278	87.654294
863.682829	850.814212	184.190442
868.332202	102.496648	22.308668
870.456088	13.599595	2.967228
897.810788	67.128766	15.106768
903.424978	52.548218	11.899485
915.263664	1.796452	0.412135
924.347513	36.215836	8.390964
949.413466	1.482197	0.352728
952.588097	15.842108	3.782650
972.750023	4.951726	1.207358
978.508311	2.562883	0.628596
985.509476	13.879278	3.428513
990.251982	11.841659	2.939249
993.881119	229.640395	57.208531
1005.763502	41.798050	10.537315
1007.637083	42.272433	10.676759
1031.042111	1.310933	0.338794
1056.697491	70.115868	18.571418
1058.020628	57.373928	15.215520
1081.249460	11.868781	3.216696
1095.894067	7.509101	2.062693
1119.399789	8.992239	2.523081
1120.017358	14.962803	4.200643
1147.727946	4.830911	1.389780
1153.478428	17.623113	5.095305
1165.463935	26.353153	7.698560
1193.787604	47.517165	14.218561
1215.593050	55.321054	16.856085
1247.339139	20.523514	6.416739
1250.901237	51.009203	15.993725
1265.512387	49.953653	15.845711
1268.203311	13.240223	4.208838
1283.925773	9.930813	3.195971
1297.146901	5.166334	1.679770
1304.190258	20.938672	6.844916
1321.604980	6.205527	2.055694
1324.171716	52.099397	17.292392
1399.368839	63.595327	22.306708
1418.650524	33.719939	11.990582
1424.322903	45.001180	16.066099
1429.010023	32.780833	11.741764
1437.559165	40.935504	14.750405
1445.733385	15.329787	5.555234
1450.559273	264.950821	96.333828
1479.770741	12.406982	4.601916
1540.578442	69.880882	26.984866
1560.407258	6.204407	2.426701
1580.018248	73.677709	29.179395
1589.680906	22.708693	9.048574
1856.002578	813.285919	378.355367
1911.599467	3050.567202	1461.690982
1972.533207	2640.748439	1305.657973
2944.566929	39.093528	28.853890
2961.808397	40.268769	29.895332
2968.689898	29.167375	21.704023
2979.419759	44.905392	33.535768
3024.122013	5.130850	3.889257
3036.812600	24.920041	18.969016

3047.390561	14.277944	10.906160
3055.067373	15.628864	11.968130
3089.479303	2.447205	1.895107
3093.170196	2.603651	2.018667
3101.811246	3.815402	2.966428
3104.865842	2.354731	1.832577
3113.511616	10.867155	8.480949
3118.742127	0.049849	0.038969
3124.369025	0.825726	0.646661
3139.988725	8.408333	6.617837
3156.453140	14.191605	11.228169

Zero-Point Energy : 0.305379 a.u.
========== 8.309787 eV

```
P4

 Geometry CYCLE 12
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ---------------------------------------
     1 O    -0.000096 -0.000166 -0.000031
     2 O     0.000040 -0.000162  0.000018
     3 C    -0.000045  0.000450  0.000254
     4 C     0.000126  0.000530  0.000124
     5 H    -0.000089  0.000131  0.000040
     6 Ru   -0.000057 -0.000554 -0.000903
     7 C    -0.000008 -0.000265 -0.000123
     8 H     0.000007  0.000044  0.000006
     9 N     0.000113  0.000114  0.000135
    10 H    -0.000045 -0.000074  0.000032
    11 C     0.000055  0.000063  0.000018
    12 C     0.000111  0.000081  0.000068
    13 C    -0.000004  0.000058 -0.000136
    14 C    -0.000048  0.000137 -0.000116
    15 C    -0.000074  0.000086 -0.000023
    16 C    -0.000021 -0.000146 -0.000058
    17 C     0.000064 -0.000150 -0.000025
    18 C     0.000048 -0.000018  0.000132
    19 H     0.000083 -0.000007  0.000027
    20 H    -0.000058 -0.000034 -0.000040
    21 C     0.000030  0.000109  0.000046
    22 H    -0.000001  0.000022  0.000098
    23 C    -0.000080 -0.000128 -0.000010
    24 H     0.000056  0.000000 -0.000013
    25 H    -0.000054  0.000012 -0.000042
    26 Cl   -0.000154 -0.000048  0.000050
    27 H     0.000219  0.000018  0.000421
    28 H    -0.000119 -0.000103  0.000051
 ---------------------------------------

-------------------------------------
Geometry Convergence after Step  12
-------------------------------------
current energy                          -6.79684192 Hartree
abs of energy change              0.00000483     0.00100000    T
constrained gradient max          0.00090278     0.00100000    T
constrained gradient rms          0.00017120     0.00066667    T
gradient max                      0.00090278
gradient rms                      0.00017120
cart. step max                    0.00581096     0.01000000    T
cart. step rms                    0.00124723     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              77.123609498182375       2098.6402        48395.80        202488.01
  Delta V^Pauli Coulomb:           -39.915672308527448      -1086.1607       -25047.47       -104798.58
  Delta V^Pauli LDA-XC:             -9.539160298017411       -259.5738        -5985.91        -25045.06
  Delta V^Pauli GGA-Exchange:        0.542125042290998         14.7520          340.19          1423.35
  Delta V^Pauli GGA-Correlation:    -0.150407049092260         -4.0928          -94.38          -394.89
                                  --------------------     -----------     ----------      -----------
  Total Pauli Repulsion:            28.060494884836253        763.5649        17608.23        73672.82
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  28.060494884836253        763.5649        17608.23        73672.82
  Electrostatic Interaction:        -5.925250022781407       -161.2343        -3718.15       -15556.74
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------     -----------     ----------      -----------
  Total Steric Interaction:         22.135244862054847        602.3307        13890.08        58116.08
 (Total Steric Interaction =
  Delta E^0 in the BB paper)

Orbital Interactions
  A:                               -28.863499969291258       -785.4158       -18112.12       -75781.11
                                  --------------------     -----------     ----------      -----------
  Total Orbital Interactions:      -28.867231876942803       -785.5173       -18114.46       -75790.91

Alternative Decomposition Orb.Int.
```

Kinetic:	-70.755195845497454	-1925.3468	-44399.56	-185767.74
Coulomb:	38.623062539688227	1050.9870	24236.34	101404.84
XC:	3.264901428866414	88.8425	2048.76	8572.00
Total Orbital Interactions:	-28.867231876942814	-785.5173	-18114.46	-75790.91
Residu (E=Steric+OrbInt+Res):	-0.000000086530315	0.0000	0.00	0.00
Solvation Energy (el):	-0.023653528729480	-0.6436	-14.84	-62.10
Dispersion Energy:	-0.045634428021853	-1.2418	-28.64	-119.81
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.004433335385971	0.1206	2.78	11.64
Total Bonding Energy:	-6.796841722783634	-184.9515	-4265.08	-17845.11

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

Electrostatic Energy:	-5.925250022781407	-161.2343	-3718.15	-15556.74
Kinetic Energy:	6.368413652684922	173.2934	3996.24	16720.27
Coulomb (Steric+OrbInt) Energy:	-1.292609855369534	-35.1737	-811.13	-3393.75
XC Energy:	-5.882540875952259	-160.0721	-3691.35	-15444.61
Solvation:	-0.019220193343509	-0.5230	-12.06	-50.46
Dispersion Energy:	-0.045634428021853	-1.2418	-28.64	-119.81
Total Bonding Energy:	-6.796841722783641	-184.9515	-4265.08	-17845.11

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:	-230.014124633296035	-6259.0028	-144336.06	-603902.00
Exchange GGA:	-19.441423369082109	-529.0280	-12199.68	-51043.45
Correlation LDA:	-12.269000534921709	-333.8565	-7698.91	-32212.26
Correlation GGA:	5.709988502065416	155.3767	3583.07	14991.57
Total XC:	-256.014560035234467	-6966.5106	-160651.58	-672166.13

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
34.710496	236.061022	2.053824
47.541324	48.018931	0.572218
66.367805	116.521319	1.938389
77.983539	34.346756	0.671377
83.754745	13.390034	0.281105
92.967081	11.017515	0.256738
103.923160	4.732819	0.123285
125.432178	349.127585	10.976685
181.527875	101.817282	4.632793
196.553642	15.127026	0.745268
220.492981	471.481650	26.057793
249.570506	40.921371	2.559891
270.938540	329.658090	22.387861
292.919347	306.889587	22.532443
338.486907	14.199423	1.204733
367.197278	24.868340	2.288887
373.976173	255.382211	23.939366
385.027202	219.001353	21.135683
416.316406	156.849196	16.367558
442.374679	35.977717	3.989348
464.104281	200.997876	23.382186
465.773104	27.690652	3.232851
485.509779	192.057848	23.372658
497.597747	19.537972	2.436890
530.764978	110.417817	14.689922
550.308011	29.502946	4.069577
578.143707	505.712659	73.285440
595.713289	657.153472	98.125564
620.541829	84.125299	13.085061
632.210251	343.655347	54.458128
639.145014	72.806338	11.663977
654.847473	4.110593	0.674719

710.029905	95.500929	16.996610
720.661902	339.174635	61.267901
736.906799	727.760605	134.424731
749.757008	1.436420	0.269948
780.316154	15.196787	2.972353
843.029308	1.611174	0.340458
864.263765	3.376017	0.731356
916.949193	201.265591	46.258642
922.823948	4.675612	1.081522
959.849173	2.464046	0.592830
961.926420	4.022418	0.969856
977.963063	0.217652	0.053354
993.272484	15.689877	3.906304
1000.583904	163.179142	40.925710
1011.120867	11.753233	2.978780
1039.353254	3.034859	0.790642
1045.871183	122.046468	31.994953
1085.793091	11.064228	3.011246
1096.345985	21.891098	6.015798
1121.032581	23.729751	6.667906
1137.431213	34.808818	9.924131
1232.021169	49.021813	15.138596
1261.087624	84.239703	26.628099
1278.204652	38.431910	12.313186
1299.028877	61.768558	20.112420
1309.447050	83.120011	27.281711
1400.148352	148.153371	51.995249
1415.792070	83.143875	29.505828
1431.847887	138.016317	49.534227
1436.261263	2.483616	0.894120
1461.403884	470.701455	172.422472
1532.707512	59.275110	22.772448
1545.328661	111.991977	43.379630
1563.010221	156.783060	61.424132
1587.073331	255.513811	101.645801
1937.613870	3083.730818	1497.689434
2011.062833	2253.221811	1135.815148
3083.588979	2.808066	2.170410
3097.720739	3.529247	2.740327
3101.229984	18.198982	14.146830
3104.868746	67.067932	52.195881
3108.422115	3.826062	2.981055
3111.167359	29.473304	22.984246
3129.526766	3.477129	2.727580
3137.636268	0.623680	0.490504
3468.484151	12.935353	11.245948

Zero-Point Energy : **0.188638 a.u.**
========== **5.133112 eV**

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P4'

 Geometry CYCLE 14
 ==============

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

     Atom      Cartesian (a.u./angstrom)
                 X         Y         Z
 ---------------------------------------
     1 O     0.000000 -0.000014 -0.000033
     2 O     0.000076  0.000025  0.000106
     3 C    -0.000019  0.000226  0.000027
     4 C    -0.000268 -0.000223 -0.000074
     5 Ru    0.000153 -0.000187  0.000228
     6 Cl    0.000036  0.000042 -0.000072
     7 H    -0.000022 -0.000045 -0.000031
     8 O     0.000133  0.000060 -0.000305
     9 C    -0.000343  0.000009  0.000149
    10 C     0.000071 -0.000045 -0.000111
    11 C    -0.000030 -0.000007 -0.000081
    12 C     0.000141  0.000144  0.000159
    13 H    -0.000008 -0.000046  0.000001
    14 H     0.000068 -0.000013  0.000016
    15 H    -0.000057  0.000029 -0.000006
    16 H     0.000059  0.000029 -0.000023
    17 H    -0.000036 -0.000004 -0.000010
    18 H    -0.000007 -0.000015 -0.000009
    19 H     0.000004  0.000001  0.000027
    20 H    -0.000011 -0.000044 -0.000010
    21 O     0.000046 -0.000009  0.000027
    22 C    -0.000049  0.000075  0.000073
    23 C     0.000021 -0.000070 -0.000098
    24 C     0.000027  0.000031  0.000046
    25 C    -0.000035 -0.000066 -0.000009
    26 H     0.000023  0.000033 -0.000014
    27 H     0.000026  0.000021 -0.000043
    28 H     0.000021 -0.000060  0.000015
    29 H    -0.000012  0.000040  0.000050
    30 H    -0.000027  0.000068 -0.000016
    31 H     0.000007 -0.000018 -0.000032
    32 H    -0.000009  0.000026  0.000021
    33 H     0.000023  0.000006  0.000032
 ---------------------------------------

-------------------------------------
Geometry Convergence after Step  14
-------------------------------------
current energy                          -6.94162867 Hartree
abs of energy change              0.00000809     0.00100000    T
constrained gradient max          0.00034318     0.00100000    T
constrained gradient rms          0.00008710     0.00066667    T
gradient max                      0.00034318
gradient rms                      0.00008710
cart. step max                    0.00254932     0.01000000    T
cart. step rms                    0.00086827     0.00666667    T

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

Pauli Repulsion
  Kinetic (Delta T^0):              69.047565868834511       1878.8799        43328.01        181284.36
  Delta V^Pauli Coulomb:           -36.505541946131878       -993.3663       -22907.58        -95845.29
  Delta V^Pauli LDA-XC:             -8.923359589595830       -242.8170        -5599.49        -23428.28
  Delta V^Pauli GGA-Exchange:        0.572855365846699         15.5882          359.47          1504.03
  Delta V^Pauli GGA-Correlation:    -0.179752862438548         -4.8913         -112.80          -471.94
                                  --------------------     -----------     ----------     -----------
  Total Pauli Repulsion:            24.011766836514955        653.3934        15067.61         63042.88
 (Total Pauli Repulsion =
  Delta E^Pauli in BB paper)

Steric Interaction
  Pauli Repulsion (Delta E^Pauli):  24.011766836514955        653.3934        15067.61         63042.88
  Electrostatic Interaction:        -5.211050656519714       -141.7999        -3269.98        -13681.61
 (Electrostatic Interaction =
  Delta V_elstat in the BB paper)
                                  --------------------     -----------     ----------     -----------
  Total Steric Interaction:         18.800716179995241        511.5935        11797.63         49361.27
 (Total Steric Interaction =
  Delta E^0 in the BB paper)
```

```
Orbital Interactions
  A:                              -25.660068067771761       -698.2460        -16101.94        -67370.50
                                  -------------------     -----------      ----------      -----------
  Total Orbital Interactions:     -25.662042619927533       -698.2997        -16103.18        -67375.68

Alternative Decomposition Orb.Int.
  Kinetic:                        -62.590445175154322      -1703.1727        -39276.10       -164331.19
  Coulomb:                         34.406234870718350        936.2413         21590.24         90333.56
  XC:                               2.522167684508428         68.6317          1582.68          6621.95
                                  -------------------     -----------      ----------      -----------
  Total Orbital Interactions:     -25.662042619927544       -698.2997        -16103.18        -67375.68

  Residu (E=Steric+OrbInt+Res):     0.000000134464032          0.0000             0.00             0.00


  Solvation Energy (el):           -0.024821998188544         -0.6754           -15.58           -65.17
  Dispersion Energy:               -0.059888927670338         -1.6297           -37.58          -157.24

Post-SCF Solvation Energies
  Solvation Energy (cd):            0.004407846187832          0.1199             2.77            11.57

Total Bonding Energy:               -6.941629385139309       -188.8913         -4355.94        -18225.25


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

  Electrostatic Energy:             -5.211050656519714       -141.7999         -3269.98        -13681.61
  Kinetic Energy:                    6.457120693680189        175.7072          4051.90         16953.17
  Coulomb (Steric+OrbInt) Energy:   -2.099306940949496        -57.1250         -1317.34         -5511.73
  XC Energy:                        -6.008089401679250       -163.4884         -3770.13        -15774.24
  Solvation:                        -0.020414152000711         -0.5555           -12.81           -53.60
  Dispersion Energy:                -0.059888927670338         -1.6297           -37.58          -157.24
                                    -------------------     -----------      ----------      -----------
  Total Bonding Energy:             -6.941629385139322       -188.8913         -4355.94        -18225.25


 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:                   -227.053057340647797      -6178.4281       -142477.96       -596127.72
  Exchange GGA:                    -18.980968726729962       -516.4984        -11910.74        -49834.53
  Correlation LDA:                 -12.067984619475835       -328.3866         -7572.78        -31684.49
  Correlation GGA:                   5.593849268109887        152.2164          3510.19         14686.65
                                  -------------------     -----------      ----------      -----------
  Total XC:                       -252.508161418743697      -6871.0967       -158451.28       -662960.08


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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2                km/mole
             ----------        ----------            ----------
              42.293442          207.758100            2.202465
              53.546357           17.854378            0.239636
              60.593214          204.010332            3.098519
              65.579218          108.055298            1.776194
              75.799654           53.727194            1.020797
              82.397865           85.568061            1.767281
              96.637620           51.773669            1.254103
             104.052576           17.447988            0.455068
             115.320366          177.693615            5.136365
             160.501134           18.454939            0.742453
             173.030347           28.607176            1.240724
             186.851614           22.610537            1.058975
             200.867538           11.498832            0.578951
             209.948484          105.185824            5.535387
             225.731238           22.232450            1.257932
             303.273596          527.922687           40.131279
             320.659830          390.797968           31.410505
             333.908942          380.742280           31.866710
             375.518144           60.518367            5.696344
             418.849891          187.801615           19.716771
             440.138229           67.931582            7.494435
             538.109304          156.817863           21.151643
             563.171032           65.496272            9.245597
             573.047014            0.970425            0.139390
             577.625202          295.255299           42.748601
```

608.608735	12.787340	1.950727
650.829860	81.987183	13.374930
688.262196	73.475795	12.675826
767.760047	18.754322	3.609150
777.381836	56.908836	11.088994
810.938188	96.569137	19.629271
819.687609	218.318409	44.855613
823.793739	82.821618	17.101739
832.685801	849.530840	177.312102
859.501008	817.183088	176.053162
864.532055	55.592695	12.046944
870.690355	7.260033	1.584457
879.122462	15.041322	3.314465
904.303794	4.973929	1.127436
911.376026	7.270928	1.660984
924.904109	42.833569	9.930224
927.568333	28.012590	6.512943
979.977402	151.107916	37.117725
985.939286	324.528159	80.201156
1004.045944	37.349400	9.399728
1009.561368	53.101030	13.437353
1095.305852	6.251588	1.716342
1098.858484	11.853569	3.264893
1147.491874	19.380909	5.574447
1157.968135	21.263183	6.171674
1162.442539	24.735717	7.207324
1170.610348	10.866822	3.188548
1183.115110	22.261982	6.601899
1201.670019	50.923157	15.338349
1213.506743	47.130523	14.335819
1224.896307	20.316345	6.237678
1252.978475	22.003457	6.910550
1262.744477	21.731365	6.878291
1267.305275	0.654584	0.207934
1268.706718	4.530308	1.440678
1304.503237	11.652209	3.810057
1311.566409	49.606136	16.308114
1325.096326	23.389709	7.768736
1332.625231	22.984683	7.677585
1412.095134	20.517135	7.262042
1418.775269	11.073696	3.938078
1428.013144	29.182072	10.445432
1430.604684	32.633005	11.701857
1436.817325	1.043915	0.375963
1443.101397	8.700874	3.147298
1447.314622	23.605396	8.563520
1454.153900	16.031471	5.843349
1854.223826	1156.183151	537.361891
1914.161642	2694.105417	1292.621171
1977.697461	2614.083132	1295.857722
2953.881507	30.691069	22.723915
2958.984431	20.035199	14.859850
2962.306652	43.988977	32.662690
2967.637442	33.554093	24.959415
2969.465580	29.397745	21.881162
2972.200345	19.660207	14.646850
2978.706773	31.088674	23.211757
2981.017431	62.558997	46.744699
3019.122540	4.551934	3.444727
3022.117511	6.496637	4.921279
3030.625196	3.135172	2.381616
3032.521041	14.345130	10.904013
3039.872444	24.899275	18.972306
3050.168864	15.790992	12.072893
3050.926442	25.914410	19.817603
3062.052041	12.049284	9.248086

Zero-Point Energy : **0.253899 a.u.**
========== **6.908950 eV**

TS1

Geometry CYCLE 56
==========

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

Atom		Cartesian (a.u./angstrom) X	Y	Z
1	O	-0.000026	-0.000525	0.000028
2	O	-0.000368	0.000442	0.000058
3	C	0.000338	0.000606	-0.000196
4	C	0.000282	-0.000840	0.000335
5	H	-0.000023	0.000115	0.000091
6	Ru	-0.000167	0.000146	-0.000764
7	C	0.000026	0.000012	0.000082
8	H	-0.000035	-0.000010	-0.000017
9	N	-0.000083	0.000534	-0.000194
10	H	-0.000027	0.000166	0.000158
11	C	0.000021	0.000061	-0.000092
12	C	-0.000079	-0.000038	0.000695
13	C	0.000090	-0.000008	-0.000092
14	C	0.000008	0.000091	0.000003
15	C	-0.000131	-0.000070	0.000110
16	C	0.000080	-0.000100	0.000080
17	C	-0.000043	-0.000060	0.000007
18	C	0.000120	0.000112	-0.000110
19	H	0.000063	0.000047	-0.000013
20	H	-0.000081	-0.000124	-0.000089
21	C	-0.000003	0.000014	-0.000138
22	H	-0.000114	-0.000057	-0.000023
23	C	-0.000021	-0.000043	-0.000054
24	H	0.000022	-0.000045	0.000031
25	H	0.000005	0.000039	-0.000111
26	Cl	0.000089	-0.000231	0.000307
27	N	0.000110	-0.000199	0.000193
28	H	0.000040	0.000012	0.000037
29	H	-0.000047	0.000073	0.000041
30	H	-0.000120	-0.000234	-0.000059
31	B	0.000948	-0.000646	-0.000038
32	H	-0.000158	0.000110	-0.000201
33	H	-0.000737	0.000486	-0.000017
34	H	0.000020	0.000166	-0.000047

Geometry Convergence after Step 56

current energy	-7.88183747 Hartree		
abs of energy change	0.00001377	0.00100000	T
constrained gradient max	0.00094778	0.00100000	T
constrained gradient rms	0.00024923	0.00066667	T
gradient max	0.00094778		
gradient rms	0.00024923		
cart. step max	0.00687972	0.01000000	T
cart. step rms	0.00260610	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	86.280597247238134	2347.8145	54141.90	226529.68
Delta V^Pauli Coulomb:	-44.165690594529778	-1201.8096	-27714.39	-115957.00
Delta V^Pauli LDA-XC:	-10.858181814007342	-295.4662	-6813.61	-28508.15
Delta V^Pauli GGA-Exchange:	0.612065446041431	16.6551	384.08	1606.98
Delta V^Pauli GGA-Correlation:	-0.169091421723855	-4.6012	-106.11	-443.95
Total Pauli Repulsion:	31.699698863018590	862.5927	19891.86	83227.55
(Total Pauli Repulsion = Delta E^Pauli in BB paper)				
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	31.699698863018590	862.5927	19891.86	83227.55
Electrostatic Interaction:	-6.607050054129642	-179.7870	-4145.99	-17346.81
(Electrostatic Interaction = Delta V_elstat in the BB paper)				
Total Steric Interaction:	25.092648808888946	682.8057	15745.88	65880.74

(Total Steric Interaction =
Delta E^0 in the BB paper)

Orbital Interactions				
A:	-32.877952320340270	-894.6546	-20631.23	-86321.05
Total Orbital Interactions:	-32.881688552911896	-894.7563	-20633.57	-86330.86
Alternative Decomposition Orb.Int.				
Kinetic:	-78.936062856570857	-2147.9596	-49533.13	-207246.60
Coulomb:	42.499084350506450	1156.4589	26668.58	111581.33
XC:	3.555289953152499	96.7444	2230.98	9334.41
Total Orbital Interactions:	-32.881688552911911	-894.7563	-20633.57	-86330.86
Residu (E=Steric+OrbInt+Res):	-0.000002965701866	-0.0001	0.00	-0.01
Solvation Energy (el):	-0.032566181550544	-0.8862	-20.44	-85.50
Dispersion Energy:	-0.064898199046327	-1.7660	-40.72	-170.39
Post-SCF Solvation Energies				
Solvation Energy (cd):	0.004666956783644	0.1270	2.93	12.25
Total Bonding Energy:	-7.881840133538044	-214.4758	-4945.93	-20693.77

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

Electrostatic Energy:	-6.607050054129642	-179.7870	-4145.99	-17346.81
Kinetic Energy:	7.344534390667278	199.8549	4608.77	19283.07
Coulomb (Steric+OrbInt) Energy:	-1.666609209725195	-45.3507	-1045.81	-4375.68
XC Energy:	-6.859917836537266	-186.6679	-4304.66	-18010.71
Solvation:	-0.027899224766901	-0.7592	-17.51	-73.25
Dispersion Energy:	-0.064898199046327	-1.7660	-40.72	-170.39
Total Bonding Energy:	-7.881840133538054	-214.4758	-4945.93	-20693.77

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:	-239.772747576091319	-6524.5484	-150459.69	-629523.26
Exchange GGA:	-20.772135849882787	-565.2386	-13034.71	-54537.23
Correlation LDA:	-13.181966062016789	-358.6995	-8271.81	-34609.25
Correlation GGA:	6.202774550181566	168.7861	3892.30	16285.38
Total XC:	-267.524074937809303	-7279.7005	-167873.91	-702384.36

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-340.986765	4197.413603	-358.754501
31.813326	86.661819	0.691059
37.911637	110.291128	1.048072
57.024493	122.565988	1.751901
64.740869	70.091004	1.137415
75.668355	80.288219	1.522805
81.005920	38.349369	0.778669
91.630107	124.239457	2.853486
98.187227	372.561018	9.169180
113.688249	355.099617	10.119146
117.646434	152.961465	4.510647
130.233552	212.396142	6.933421
140.846428	122.806752	4.335570
189.984121	78.719066	3.748654
200.228831	98.391472	4.938126
243.594132	99.298156	6.062979
261.672927	267.934269	17.573778
298.627680	1156.259174	86.549253
307.379638	225.988392	17.411625
331.997586	86.246598	7.177199
375.845804	62.974351	5.932688
391.015732	163.588202	16.033350
411.607868	43.249708	4.462158
430.647009	21.917292	2.365846

449.801485	69.390151	7.823423
459.142124	17.676656	2.034348
479.746528	476.942164	57.352933
492.718763	57.209862	7.065584
503.821835	247.114788	31.207127
518.299060	103.194373	13.406472
541.856730	4.116933	0.559160
557.481464	215.650950	30.134215
575.736016	557.216243	80.412810
605.490527	661.771322	100.436915
613.950680	91.625777	14.100328
619.698252	118.486192	18.404587
645.223488	27.031096	4.371715
709.176554	141.284928	25.114716
718.000041	69.969813	12.592537
728.494852	385.993692	70.483062
739.049524	551.751061	102.210330
742.030743	120.306062	22.376259
778.241148	31.647444	6.173492
788.664304	456.429967	90.228639
862.580826	15.082149	3.260927
872.359592	25.618270	5.601746
877.085211	1527.431636	335.800733
934.697044	1057.681919	247.801551
945.827176	32.801194	7.776416
951.707011	5.828638	1.390428
960.642793	999.764828	240.734233
977.709060	6.559516	1.607532
978.932705	5.066898	1.243292
992.791224	20.643595	5.137139
1008.593504	9.891291	2.500617
1017.567088	236.356142	60.284826
1033.337661	114.703412	29.709590
1042.899869	170.049668	44.452529
1069.843718	153.005262	41.030308
1078.714317	20.826670	5.631244
1088.566121	88.457417	24.136102
1110.186586	1278.833032	355.867143
1117.545675	30.097589	8.430922
1123.391547	17.933465	5.049791
1176.283373	548.910533	161.842133
1183.471476	26.989619	8.006314
1251.178514	12.880796	4.039616
1272.540037	13.292906	4.240035
1291.636265	101.310223	32.799828
1300.842697	102.951845	33.568890
1353.801396	174.226755	59.121831
1399.451427	88.000202	30.868787
1425.682126	74.406291	26.589516
1441.148290	395.934137	143.024253
1467.232740	32.048563	11.786521
1531.429610	18.143394	6.964559
1532.657287	132.039750	50.725673
1545.656474	13.509865	5.234100
1563.766677	142.736656	55.948126
1585.075233	73.399729	29.162342
1735.624866	3905.594608	1699.108437
1885.301889	1215.754020	574.519385
1945.562176	5013.303628	2444.821706
1991.133429	3958.374575	1975.583191
2424.779778	337.487081	205.119772
2452.670213	467.931182	287.673074
3098.320947	0.161525	0.125442
3101.796853	0.359171	0.279250
3109.265833	1.247052	0.971897
3111.800794	4.036576	3.148495
3118.787459	14.829607	11.592937
3121.056943	7.143320	5.588302
3127.978987	16.897942	13.248775
3132.267430	8.738987	6.861167
3436.931130	54.131177	46.633324
3530.470930	45.272727	40.063360

Zero-Point Energy : 0.235654 a.u.
========== 6.412475 eV
(imaginary frequencies were excluded from the summation)

TS2

Geometry CYCLE 24
==========

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

Atom	Cartesian (a.u./angstrom) X	Y	Z
1 O	-0.000091	0.000191	0.000077
2 O	0.000183	-0.000246	-0.000238
3 C	0.000190	-0.000155	-0.000207
4 C	-0.000349	0.000500	0.000233
5 H	0.000010	-0.000013	0.000012
6 Ru	-0.000005	-0.000597	0.000690
7 C	0.000009	-0.000022	-0.000052
8 H	0.000069	-0.000008	0.000066
9 N	0.000065	0.000206	-0.000019
10 H	0.000307	-0.000017	0.000021
11 C	0.000017	-0.000062	0.000107
12 C	-0.000347	-0.000071	-0.000264
13 C	0.000045	0.000062	0.000151
14 C	-0.000003	0.000019	0.000008
15 C	-0.000057	0.000041	0.000073
16 C	-0.000046	0.000170	0.000033
17 C	0.000058	-0.000095	-0.000340
18 C	0.000170	0.000024	-0.000118
19 H	0.000104	-0.000056	0.000041
20 H	0.000128	0.000030	0.000020
21 C	-0.000027	-0.000274	-0.000322
22 H	0.000053	0.000277	-0.000072
23 C	-0.000272	0.000220	0.000146
24 H	-0.000151	-0.000183	0.000346
25 H	-0.000133	-0.000077	0.000003
26 Cl	-0.000222	0.000002	-0.000077
27 H	0.000289	0.000023	-0.000229
28 H	0.000007	0.000111	-0.000089

Geometry Convergence after Step 24

current energy	-6.77828716 Hartree		
abs of energy change	0.00000458	0.00100000	T
constrained gradient max	0.00069036	0.00100000	T
constrained gradient rms	0.00018980	0.00066667	T
gradient max	0.00069036		
gradient rms	0.00018980		
cart. step max	0.00917931	0.01000000	T
cart. step rms	0.00299673	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	77.212190855203346	2101.0506	48451.39	202720.58
Delta V^Pauli Coulomb:	-39.937339396385063	-1086.7503	-25061.06	-104855.47
Delta V^Pauli LDA-XC:	-9.565594854856148	-260.2931	-6002.50	-25114.47
Delta V^Pauli GGA-Exchange:	0.545109085912838	14.8332	342.06	1431.18
Delta V^Pauli GGA-Correlation:	-0.151746367884987	-4.1292	-95.22	-398.41
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	28.102619321989987	764.7112	17634.66	73783.42
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	28.102619321989987	764.7112	17634.66	73783.42
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-5.992886968661976	-163.0748	-3760.59	-15734.32
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	22.109732353328013	601.6364	13874.07	58049.09
Orbital Interactions				
A:	-28.817292628419015	-784.1584	-18083.13	-75659.79
Total Orbital Interactions:	-28.821422463954608	-784.2708	-18085.72	-75670.63

```
Alternative Decomposition Orb.Int.
  Kinetic:                        -70.882077706959080      -1928.7995        -44479.18       -186100.87
  Coulomb:                         38.751584728065112       1054.4843         24316.99        101742.27
  XC:                               3.309070514939364         90.0444          2076.47          8687.96
                                  --------------------     -----------       ----------      -----------
  Total Orbital Interactions:     -28.821422463954605       -784.2708        -18085.72        -75670.63

  Residu (E=Steric+OrbInt+Res):     0.000000988092721          0.0000             0.00             0.00


  Solvation Energy (el):           -0.024750264005796         -0.6735           -15.53           -64.98
  Dispersion Energy:               -0.046302903682096         -1.2600           -29.06          -121.57

Post-SCF Solvation Energies
  Solvation Energy (cd):            0.004441476382430          0.1209             2.79            11.66

Total Bonding Energy:              -6.778300813839335       -184.4469         -4253.45        -17796.43


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

  Electrostatic Energy:            -5.992886968661976       -163.0748         -3760.59        -15734.32
  Kinetic Energy:                   6.330113148244266        172.2511          3972.21         16619.71
  Coulomb (Steric+OrbInt) Energy:  -1.185753680227229        -32.2660          -744.07         -3113.20
  XC Energy:                       -5.863161621888932       -159.5447         -3679.19        -15393.73
  Solvation:                       -0.020308787623366         -0.5526           -12.74           -53.32
  Dispersion Energy:               -0.046302903682096         -1.2600           -29.06          -121.57
                                  --------------------     -----------       ----------      -----------
  Total Bonding Energy:            -6.778300813839333       -184.4469         -4253.45        -17796.43


 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:                   -230.014145824632408      -6259.0034       -144336.07       -603902.05
  Exchange GGA:                    -19.441423905678629       -529.0281        -12199.68        -51043.45
  Correlation LDA:                 -12.269003163208856       -333.8566         -7698.92        -32212.26
  Correlation GGA:                   5.709982362420276        155.3765          3583.07         14991.56
                                  --------------------     -----------       ----------      -----------
  Total XC:                       -256.014590531099657      -6966.5115       -160651.60       -672166.21

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

              Frequency       Dipole Strength        Absorption Intensity (degeneracy not counted)
                cm-1           1e-40 esu2 cm2                km/mole
             ----------          ----------          ----------
            -988.565462         3165.830906         -784.460749
              36.906686          213.812953            1.977958
              50.168984            8.827832            0.111011
              63.576502          145.624088            2.320641
              74.136415           56.990516            1.059040
              78.059090           17.122828            0.335025
              89.568646           40.931093            0.918941
             102.915148           19.374386            0.499787
             130.363448          298.542687            9.755294
             169.398689            2.372218            0.100726
             192.230833            9.764382            0.470485
             220.229132          244.693213           13.507493
             244.320387          137.651631            8.429836
             275.534451          101.711669            7.024651
             300.654569          625.767689           47.158395
             360.888724           23.064009            2.086345
             382.642289           66.385332            6.367122
             392.740030          598.179976           58.886414
             408.938090           81.669982            8.371400
             440.674719           22.148906            2.446518
             453.550939            5.725798            0.650939
             466.374812           14.083153            1.646315
             488.415816           32.204849            3.942658
             510.529058          124.822741           15.973212
             548.326155            3.289494            0.452112
             569.410215           77.131546           11.008683
             589.581376          319.927823           47.279605
             618.514081           41.588915            6.447706
             637.220416          101.264024           16.174205
             649.510046           64.162184           10.445833
             707.152385          129.885975           23.022546
```

719.980913	634.829574	114.566120
733.169692	702.598759	129.118940
738.684083	762.582485	141.196404
749.950790	222.591129	41.842603
765.704974	984.857660	189.022283
781.141225	35.482116	6.947317
850.997417	16.613623	3.543812
868.400429	2.098432	0.456765
931.869895	12.840021	2.999156
940.998382	110.058968	25.959264
962.690294	3.254818	0.785401
966.428882	2.463344	0.596723
978.610099	0.034419	0.008443
990.476384	13.899338	3.450772
995.418147	6.513251	1.625105
1009.950117	16.308696	4.128547
1035.618363	6.623749	1.719419
1043.311707	83.061117	21.721505
1085.078288	29.813007	8.108582
1098.449788	20.444460	5.629035
1119.518872	17.865191	5.013224
1134.582361	27.464181	7.810535
1230.896167	13.039678	4.023151
1264.480168	45.139435	14.306922
1277.815781	58.823597	18.840737
1302.379540	43.130419	14.079892
1315.154330	44.610053	14.705762
1397.976483	82.796143	29.012693
1419.407817	114.128466	40.604974
1438.190452	68.135318	24.562171
1462.998128	253.806814	93.073301
1535.296354	31.176422	11.997660
1546.726934	39.190402	15.193976
1563.912477	34.772534	13.630973
1587.738463	135.221927	53.815101
1794.403983	269.420682	121.179520
1921.200928	1730.394758	833.289767
1945.297447	2494.298364	1216.220975
2014.706546	1921.722211	970.466341
3096.169209	0.544253	0.422380
3102.623914	38.294278	29.781124
3103.248742	22.787758	17.725408
3105.062332	10.982497	8.547705
3110.246102	5.185562	4.042674
3118.569444	18.624187	14.558305
3126.279297	5.224580	4.094088
3135.498016	0.785257	0.617158

Zero-Point Energy : 0.186058 a.u.
========== 5.062885 eV
(imaginary frequencies were excluded from the summation)

2-phenylpyridine

Geometry CYCLE 6
==========

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

Atom	Cartesian (a.u./angstrom) X	Y	Z
1 H	-0.000081	-0.000013	0.000013
2 C	-0.000137	-0.000142	0.000000
3 H	0.000070	0.000087	-0.000009
4 N	0.000398	-0.000020	0.000115
5 H	0.000051	-0.000060	-0.000015
6 C	0.000080	0.000022	-0.000052
7 C	0.000237	-0.000033	0.000122
8 C	-0.000037	0.000042	0.000038
9 C	0.000189	-0.000094	-0.000243
10 C	0.000086	-0.000156	0.000083
11 C	-0.000118	0.000014	0.000025
12 C	-0.000551	0.000463	0.000204
13 C	-0.000045	0.000051	-0.000029
14 H	-0.000017	-0.000054	0.000013
15 H	-0.000107	0.000002	-0.000023
16 C	-0.000077	-0.000148	0.000056
17 H	0.000215	-0.000244	-0.000046
18 C	-0.000003	0.000000	-0.000052
19 H	-0.000129	0.000140	-0.000058
20 H	0.000085	0.000013	0.000025
21 H	-0.000110	0.000129	-0.000168

Geometry Convergence after Step 6

current energy	-5.08466851 Hartree		
abs of energy change	0.00002407	0.00100000	T
constrained gradient max	0.00055069	0.01000000	T
constrained gradient rms	0.00014401	0.00666667	T
gradient max	0.00055069		
gradient rms	0.00014401		
cart. step max	0.00570863	0.01000000	T
cart. step rms	0.00253871	0.00666667	T

	hartree	eV	kcal/mol	kJ/mol
Pauli Repulsion				
Kinetic (Delta T^0):	53.622855224889022	1459.1521	33648.85	140786.79
Delta V^Pauli Coulomb:	-25.292902378933206	-688.2549	-15871.54	-66406.51
Delta V^Pauli LDA-XC:	-6.878122208264295	-187.1632	-4316.09	-18058.51
Delta V^Pauli GGA-Exchange:	0.341534241218545	9.2936	214.32	896.70
Delta V^Pauli GGA-Correlation:	-0.076374462258057	-2.0783	-47.93	-200.52
Total Pauli Repulsion: (Total Pauli Repulsion = Delta E^Pauli in BB paper)	21.716990416652010	590.9494	13627.62	57017.95
Steric Interaction				
Pauli Repulsion (Delta E^Pauli):	21.716990416652010	590.9494	13627.62	57017.95
Electrostatic Interaction: (Electrostatic Interaction = Delta V_elstat in the BB paper)	-4.235485733630800	-115.2534	-2657.81	-11120.27
Total Steric Interaction: (Total Steric Interaction = Delta E^0 in the BB paper)	17.481504683021210	475.6959	10969.81	45897.68
Orbital Interactions				
A:	-22.530207530232509	-613.0781	-14137.92	-59153.05
Total Orbital Interactions:	-22.533772049695010	-613.1751	-14140.16	-59162.41
Alternative Decomposition Orb.Int.				
Kinetic:	-48.884484015271077	-1330.2145	-30675.48	-128346.19
Coulomb:	24.329574746654654	662.0414	15267.04	63877.29
XC:	2.021137218921422	54.9979	1268.28	5306.50

Total Orbital Interactions:	-22.533772049695003	-613.1751	-14140.16	-59162.41
Residu (E=Steric+OrbInt+Res):	-0.000002168630106	-0.0001	0.00	-0.01
Solvation Energy (el):	-0.016138669419793	-0.4392	-10.13	-42.37
Dispersion Energy:	-0.019933119969537	-0.5424	-12.51	-52.33

Post-SCF Solvation Energies

Solvation Energy (cd):	0.003672815778144	0.0999	2.30	9.64
Total Bonding Energy:	-5.084668508915091	-138.3609	-3190.68	-13349.80

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

Electrostatic Energy:	-4.235485733630800	-115.2534	-2657.81	-11120.27
Kinetic Energy:	4.738371209617945	128.9376	2973.37	12440.59
Coulomb (Steric+OrbInt) Energy:	-0.963329800908660	-26.2135	-604.50	-2529.22
XC Energy:	-4.591825210382385	-124.9499	-2881.41	-12055.84
Solvation:	-0.012465853641649	-0.3392	-7.82	-32.73
Dispersion Energy:	-0.019933119969537	-0.5424	-12.51	-52.33
Total Bonding Energy:	-5.084668508915087	-138.3609	-3190.68	-13349.80

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:	-55.694388511439058	-1515.5214	-34948.76	-146225.60
Exchange GGA:	-7.415017657590511	-201.7729	-4652.99	-19468.13
Correlation LDA:	-4.924029221850020	-133.9897	-3089.88	-12928.04
Correlation GGA:	2.624287728715931	71.4105	1646.77	6890.07
Total XC:	-65.409147662163662	-1779.8735	-41044.86	-171731.69

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
49.291993	187.487859	2.316475
80.905736	208.480420	4.227880
152.876386	81.102795	3.107809
240.394000	9.947706	0.599411
325.129028	0.916309	0.074675
382.318785	85.740753	8.216578
397.044648	27.569324	2.743744
400.212890	8.955206	0.898348
458.181851	84.171297	9.666739
541.722318	13.321642	1.808892
603.522689	46.993212	7.108972
614.574736	59.862735	9.221665
628.370738	32.911806	5.183770
682.562743	414.323555	70.885968
727.069974	738.761669	134.635204
730.216079	163.555540	29.936066
742.999709	2.613643	0.486758
788.834805	37.023287	7.320472
823.709278	3.037343	0.627113
870.598462	3.062693	0.668343
906.017313	10.881862	2.471256
944.723511	1.844715	0.436830
954.225643	2.863942	0.685004
968.404461	22.756636	5.523863
970.765968	11.869278	2.888131
974.695989	1.459165	0.356493
981.328197	1.237954	0.304507
1001.570253	73.781881	18.522910
1022.911928	5.237718	1.342946
1041.212221	7.303234	1.906042
1063.270305	64.987668	17.320192
1071.755164	36.473276	9.798248
1115.401273	8.009852	2.239410
1122.973845	20.663268	5.816299
1156.742293	18.005684	5.220647
1254.440148	7.263050	2.283742

1265.808485	49.005020	15.548434
1277.658263	42.744552	13.689057
1300.638972	3.545911	1.156013
1326.329281	7.031351	2.337589
1397.471100	98.929203	34.653365
1425.563340	142.242788	50.827043
1445.965391	180.902789	65.566384
1477.480582	6.581207	2.437280
1542.911506	94.821382	36.671221
1561.438318	61.313132	23.996970
1568.301315	235.191679	92.454814
1582.549497	6.798561	2.696822
3072.470199	27.768792	21.385664
3086.254535	1.627876	1.259306
3092.594407	2.979522	2.309658
3094.678134	12.261740	9.511427
3099.818451	14.616838	11.357108
3108.295266	6.541251	5.096373
3110.436085	10.194449	7.948096
3113.820566	13.102252	10.226278
3121.428321	2.034053	1.591453

Zero-Point Energy : 0.163716 a.u.
========== 4.454931 eV

Isotopic effects

P3-{D,H}
Coordinates in Frequency Displacement 0

Atom	X	Y	Z (Angstrom)
1.O	-2.592196	-0.204867	4.871256
2.O	0.163139	-3.823322	4.542926
3.C	-1.448302	-0.423383	4.827113
4.C	0.282948	-2.675597	4.604106
5.H	3.032232	-0.238810	6.365638
6.Ru	0.399978	-0.689996	4.713009
7.C	3.452464	-0.391199	5.372722
8.H	5.505344	-0.140215	5.958227
9.N	2.553609	-0.637043	4.395025
10.H	-1.423026	-0.671414	1.737946
11.C	4.823493	-0.344157	5.133833
12.C	0.629374	-0.731833	2.410130
13.C	-0.405687	-0.976214	1.495649
14.C	2.999805	-0.839638	3.117498
15.C	5.290962	-0.555483	3.832060
16.C	1.967862	-1.082224	2.104676
17.C	4.369171	-0.803104	2.818588
18.C	-0.117039	-1.591557	0.275121
19.H	-0.917520	-1.787149	-0.438495
20.H	6.357249	-0.519048	3.608615
21.C	2.239696	-1.697060	0.872468
22.H	4.697387	-0.955737	1.792705
23.C	1.204895	-1.948563	-0.032904
24.H	3.256528	-2.001179	0.627332
25.H	1.429651	-2.431677	-0.983731
26.Cl	0.630789	-0.779423	7.127182
27.H.D	0.456440	0.179489	3.123062
28.H	0.531776	0.937598	4.904968

Intensities
==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
39.489603	112.135513	1.109952
49.992943	16.667744	0.208864
65.403319	149.227885	2.446402
71.775614	56.773979	1.021420
73.848101	8.770058	0.162338
90.300632	40.135441	0.908441
100.202993	76.325916	1.917038
130.643505	119.749571	3.921388

155.549490	11.220143	0.437467
170.566539	148.103842	6.331961
205.670048	65.258428	3.364230
229.564380	45.733410	2.631577
267.952007	3.903584	0.262179
302.279997	647.317197	49.046116
346.940520	25.819105	2.245299
367.230902	84.703726	7.796861
383.839241	193.739493	18.639987
396.029815	35.578731	3.531802
408.390388	152.947969	15.656594
439.031968	49.893024	5.490527
450.381749	8.927013	1.007778
475.308071	19.921847	2.373465
510.758354	181.568325	23.245219
542.561940	37.162036	5.053903
564.105080	219.880638	31.090311
571.697843	226.853319	32.507963
607.898230	83.915732	12.786519
614.874446	14.733687	2.270785
644.727336	2.501299	0.404222
695.939570	228.829594	39.917358
721.777600	314.603129	56.917329
726.373576	281.688703	51.287029
738.199520	708.248732	131.050184
743.788802	10.883743	2.029112
780.917018	14.320854	2.803186
799.336531	358.355488	71.799561
813.794396	653.654881	133.334112
849.664414	26.105203	5.559716
872.701766	8.587030	1.878395
923.723418	176.264479	40.811713
938.183989	2.923785	0.687561
959.463022	9.193949	2.211100
969.579820	20.450706	4.970155
979.928175	3.058406	0.751221
987.448346	202.507411	50.122576
1002.064475	137.577010	34.555693
1009.883762	25.044818	6.339680
1034.052900	12.917827	3.348192
1043.145356	51.089082	13.358294
1083.817178	25.560208	6.943820
1095.626718	17.855185	4.903487
1119.548369	11.622166	3.261430
1133.119272	20.586563	5.847060
1229.646875	10.829430	3.337829
1264.964738	5.318642	1.686387
1278.871202	57.557628	18.450484
1299.920248	16.360965	5.330939
1324.904469	47.378710	15.734244
1395.319161	126.237707	44.151018
1420.247916	82.918744	29.518545
1438.551440	194.039397	69.967021
1465.792799	114.400411	42.031824
1537.299821	33.068751	12.742494
1548.678572	24.096329	9.353846
1566.184995	8.030934	3.152733
1587.310322	81.381843	32.379298
1677.318968	143.443902	60.308124
1885.126685	512.050302	241.953126
1937.217878	3133.374807	1521.489241
2007.688730	2364.632073	1189.975520
3101.039430	0.265175	0.206119
3109.258626	1.968340	1.534034
3110.647393	10.785504	8.409483
3116.092122	33.838961	26.430500
3117.371150	7.916890	6.186161
3122.350311	12.173177	9.527164
3129.654815	6.426782	5.041597
3136.886635	0.118126	0.092880

Zero-Point Energy : **0.187055 a.u.**

========== 5.090012 eV

TS2-{D,H}

Coordinates in Frequency Displacement 0

Atom	X	Y	Z (Angstrom)
1.O	1.735844	-3.418345	-1.135031
2.O	-2.391373	-1.744990	-1.379085
3.C	1.187183	-2.468216	-0.747788
4.C	-1.378689	-1.412143	-0.933413
5.H	-0.132287	2.135186	-0.559323
6.Ru	0.324606	-0.943757	-0.071908
7.C	-0.597827	2.019065	0.418898
8.H	-1.185182	4.075144	0.641888
9.N	-0.566120	0.769392	0.928882
10.H	0.441855	-3.799315	1.662843
11.C	-1.182509	3.085408	1.096550
12.C	-0.286138	-1.768571	1.834659
13.C	-0.167808	-3.107096	2.243703
14.C	-1.125327	0.525480	2.154559
15.C	-1.750050	2.853562	2.354567
16.C	-1.046676	-0.861387	2.619401
17.C	-1.717867	1.566711	2.884655
18.C	-0.829326	-3.554920	3.392299
19.H	-0.742230	-4.599004	3.694852
20.H	-2.210003	3.666518	2.916920
21.C	-1.705023	-1.323728	3.772868
22.H	-2.145995	1.363407	3.863642
23.C	-1.599544	-2.662806	4.153841
24.H	-2.310413	-0.643435	4.370372
25.H	-2.116396	-3.012164	5.047624
26.Cl	1.063422	0.434494	-1.995219
27.H.D	0.982596	-1.207588	1.452714
28.H	1.742113	-0.531030	0.743129

Intensities

==========

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-748.181445	2068.906241	-387.994718
38.618092	216.290438	2.093660
50.775303	11.371180	0.144723
63.341824	142.891976	2.268697
74.648677	58.273326	1.090360
79.028764	28.170644	0.558033
89.394135	38.006964	0.851629
103.140454	19.098729	0.493755
129.960951	290.082429	9.449577
169.512401	1.281895	0.054467
191.592110	12.964506	0.622604
220.021662	246.862651	13.614412
242.877408	134.072563	8.162160
274.996543	98.327901	6.777696
300.281660	625.107864	47.050240
360.194499	20.765392	1.874801
380.429044	95.487475	9.105382
389.221887	598.047118	58.345951
407.208831	29.123767	2.972643
436.848242	15.835061	1.733917
451.239903	9.553873	1.080600
464.664247	19.526139	2.274226
487.515526	36.554624	4.466927
510.127523	109.738634	14.031897
547.007168	24.712138	3.388297
564.004288	92.245881	13.040897
587.819457	354.815360	52.278659
617.444392	42.859062	6.633131
635.979602	180.547811	28.781504
645.178760	97.019195	15.689742
669.418151	303.425663	50.912903
708.287432	56.843453	10.091787
712.995652	1158.390329	207.023609

723.636118	341.289936	61.904438
737.457901	766.539587	141.693488
750.230344	54.589503	10.265541
781.167790	63.421504	12.418208
790.224601	280.692306	55.597994
849.773601	3.320536	0.707277
868.463821	2.463467	0.536261
931.461767	6.734919	1.572445
963.278043	2.362285	0.570377
966.260444	2.061760	0.499356
979.512588	0.048587	0.011929
988.022973	10.253420	2.539299
994.816503	10.335510	2.577229
1009.858519	14.909181	3.773918
1034.837045	8.060596	2.090823
1042.881158	79.666508	20.825176
1084.691642	35.246381	9.582943
1096.516203	25.370457	6.973028
1117.801507	15.745802	4.411716
1134.405378	34.751853	9.881533
1229.378022	8.578682	2.643529
1263.975259	42.734595	13.539301
1277.397550	56.024225	17.938247
1302.332698	41.978498	13.703355
1314.035135	73.852229	24.324765
1326.191343	228.018754	75.797490
1401.941251	159.105301	55.910392
1419.032708	103.989739	36.988010
1441.289081	108.546906	39.214494
1463.867593	220.622788	80.952494
1535.384550	32.483573	12.501411
1547.848268	50.929418	19.759464
1566.284105	67.561648	26.524600
1587.776510	135.319860	53.855366
1865.100303	223.724346	104.590806
1938.517385	3158.157077	1534.551602
2008.800097	2399.478295	1208.179929
3096.291109	0.566271	0.439485
3102.879339	62.161144	48.346157
3103.355240	2.440967	1.898766
3105.473857	8.160704	6.352338
3110.989927	6.390519	4.983251
3118.913446	17.622593	13.776891
3126.240711	4.949767	3.878692
3135.613062	0.644103	0.506239

Zero-Point Energy : 0.184162 a.u.
========== 5.011316 eV
(imaginary frequencies were excluded from the summation)

P4-{D,H}
Coordinates in Frequency Displacement 0

Atom	X	Y	Z (Angstrom)
1.O	1.591669	-3.518772	-1.041079
2.O	-2.317040	-1.685991	-1.437725
3.C	1.101070	-2.523376	-0.695949
4.C	-1.319899	-1.400556	-0.921942
5.H	-0.226437	2.124237	-0.596302
6.Ru	0.289950	-0.945164	-0.067445
7.C	-0.676114	2.006236	0.389033
8.H	-1.286615	4.055634	0.613868
9.N	-0.618167	0.760769	0.908083
10.H	0.195289	-3.862028	1.462622
11.C	-1.262885	3.067703	1.071336
12.C	-0.405292	-1.793534	1.712700
13.C	-0.282316	-3.132493	2.117371
14.C	-1.152597	0.508085	2.143260
15.C	-1.810655	2.829145	2.337457
16.C	-1.038270	-0.878312	2.595728
17.C	-1.753206	1.545648	2.873328

18.C	-0.765623	-3.555813	3.363801
19.H	-0.656133	-4.600918	3.657707
20.H	-2.279412	3.636311	2.900999
21.C	-1.522569	-1.310211	3.847128
22.H	-2.173315	1.341311	3.855480
23.C	-1.387474	-2.644503	4.230612
24.H	-2.004206	-0.605135	4.524035
25.H	-1.764013	-2.973930	5.199044
26.Cl	1.173138	0.481606	-1.948605
27.H.D	1.666814	-0.732607	1.166185
28.H	1.921719	-0.276448	0.549566

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
34.794241	261.002485	2.276303
48.856277	25.074943	0.307071
66.072627	120.855296	2.001545
77.543946	29.851701	0.580223
83.738148	13.041085	0.273725
92.762357	12.741719	0.296263
103.975191	3.577682	0.093242
124.998973	330.690469	10.361108
181.084062	103.792290	4.711112
196.446926	16.033309	0.789490
219.672648	416.162825	22.914867
247.744850	85.216744	5.291851
270.478611	313.023263	21.222064
277.630751	22.377569	1.557251
292.810309	289.588461	21.254245
323.260126	524.462461	42.495664
359.429911	99.338580	8.949736
368.465700	68.008545	6.281142
412.043589	131.690011	13.601101
433.270717	30.810976	3.346130
460.902614	209.948870	24.254972
465.580568	4.869864	0.568316
476.011281	161.131077	19.225366
495.456384	17.412213	2.162407
525.526363	93.846265	12.362024
549.275504	158.927910	21.881066
555.032556	304.122746	42.310234
589.540841	487.279037	72.006167
620.495495	71.086246	11.056108
630.995182	301.329553	47.659100
638.734895	57.318300	9.176816
654.729292	3.651022	0.599176
709.555830	96.778600	17.212501
720.382475	302.748761	54.666791
736.823341	761.723591	140.682103
745.280007	102.991284	19.239687
752.900546	86.266571	16.280143
780.342133	13.566865	2.653644
843.316334	2.703384	0.571448
864.266898	3.178725	0.688619
922.997515	3.345818	0.774071
959.654293	1.330241	0.319980
961.914014	4.909139	1.183640
977.929243	0.127566	0.031270
993.215527	15.604690	3.884872
999.574711	165.359525	41.430726
1011.060088	5.448248	1.380740
1039.270951	1.899522	0.494824
1045.391257	113.129598	29.643753
1086.691859	8.474109	2.308227
1096.029376	26.128838	7.178279
1120.331928	24.032427	6.748736
1137.402069	34.050934	9.707806
1231.944310	56.192477	17.351911
1260.882934	83.962965	26.536314
1263.955842	108.516802	34.380086
1278.158931	37.580952	12.040117

1299.298469	56.825255	18.506675
1309.529544	83.371216	27.365885
1400.395227	142.890975	50.157224
1415.711314	78.700752	27.927474
1435.816642	14.869002	5.351295
1461.400148	452.946171	165.918117
1532.821151	59.829134	22.986999
1545.290945	114.422831	44.320129
1563.027859	157.651895	61.765219
1587.074651	251.551902	100.069800
1937.372096	3089.225314	1500.170757
2010.305190	2271.626994	1144.661524
3014.351551	49.805963	37.631654
3083.540325	3.176766	2.455347
3097.773261	3.357464	2.606988
3101.274566	19.072228	14.825854
3104.729903	68.446246	53.266177
3108.575055	2.584117	2.013500
3111.252059	29.766193	23.213283
3129.737818	2.966358	2.327071
3137.636190	0.539731	0.424480

Zero-Point Energy : 0.186362 a.u.
========== 5.071173 eV

P3-{H,D}

Coordinates in Frequency Displacement 0

Atom	X	Y	Z (Angstrom)
1.O	-2.592196	-0.204867	4.871256
2.O	0.163139	-3.823322	4.542926
3.C	-1.448302	-0.423383	4.827113
4.C	0.282948	-2.675597	4.604106
5.H	3.032232	-0.238810	6.365638
6.Ru	0.399978	-0.689996	4.713009
7.C	3.452464	-0.391199	5.372722
8.H	5.505344	-0.140215	5.958227
9.N	2.553609	-0.637043	4.395025
10.H	-1.423026	-0.671414	1.737946
11.C	4.823493	-0.344157	5.133833
12.C	0.629374	-0.731833	2.410130
13.C	-0.405687	-0.976214	1.495649
14.C	2.999805	-0.839638	3.117498
15.C	5.290962	-0.555483	3.832060
16.C	1.967862	-1.082224	2.104676
17.C	4.369171	-0.803104	2.818588
18.C	-0.117039	-1.591557	0.275121
19.H	-0.917520	-1.787149	-0.438495
20.H	6.357249	-0.519048	3.608615
21.C	2.239696	-1.697060	0.872468
22.H	4.697387	-0.955737	1.792705
23.C	1.204895	-1.948563	-0.032904
24.H	3.256528	-2.001179	0.627332
25.H	1.429651	-2.431677	-0.983731
26.Cl	0.630789	-0.779423	7.127182
27.H	0.456440	0.179489	3.123062
28.H.D	0.531776	0.937598	4.904968

Intensities
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Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
40.309279	110.143715	1.112866
50.140061	22.689675	0.285162
65.241448	153.903385	2.516807
71.438902	48.100115	0.861309
73.479598	9.438252	0.173835
90.143906	39.259017	0.887062
101.059903	71.956328	1.822745
130.569913	123.976130	4.057507

155.066987	13.477254	0.523840
170.377851	141.992901	6.063981
205.448738	66.906660	3.445489
229.975998	40.784886	2.351039
268.250158	4.949977	0.332829
302.382281	649.970202	49.263794
340.126817	70.129803	5.978904
353.649899	7.682298	0.680993
379.485819	124.342499	11.827507
392.555780	55.062949	5.417999
399.939121	101.411701	10.166232
426.874056	79.580030	8.514947
446.229987	7.928923	0.886852
476.429999	21.063349	2.515386
506.992500	97.887246	12.439580
544.547213	24.930589	3.402876
556.775819	38.819291	5.417589
569.143156	289.579541	41.311167
611.365205	131.281487	20.117883
616.694064	56.077865	8.668407
621.602712	590.001095	91.927148
634.852843	438.550850	69.786448
648.806126	142.841281	23.229868
707.682843	71.658680	12.711170
724.814828	560.254851	101.786637
739.346620	656.492658	121.662304
745.150958	6.482429	1.210766
778.949693	13.787921	2.692069
853.562745	11.780530	2.520452
872.587555	2.271163	0.496747
936.729904	16.282428	3.823064
950.236832	62.549006	14.898081
959.698813	9.487746	2.282317
969.937536	40.207023	9.775157
973.200060	60.535972	14.767049
979.908456	0.093982	0.023084
994.839174	20.484102	5.107965
1009.757248	3.951483	1.000127
1032.919771	21.784161	5.640083
1043.672277	59.923763	15.676218
1085.566622	16.686933	4.540577
1099.386847	15.429148	4.251778
1119.797379	15.367668	4.313457
1135.007451	12.660738	3.601935
1235.995121	16.932190	5.245755
1264.856428	29.126420	9.234352
1279.433759	60.871664	19.521404
1299.924229	30.466764	9.927101
1322.075491	214.101627	70.950309
1339.124236	263.597848	88.479121
1365.039423	408.106733	139.635879
1404.946636	274.822326	96.780956
1423.757091	101.543539	36.238171
1446.217388	331.435974	120.146547
1473.876809	44.587171	16.472108
1538.090095	24.031150	9.264765
1554.146745	44.306024	17.259685
1572.655220	40.871043	16.111178
1587.737910	77.432454	30.816259
1921.929565	3500.746846	1686.460774
1997.169618	2067.159032	1034.824995
2241.885596	290.834949	163.432382
3101.242115	0.199549	0.155118
3109.009243	1.932368	1.505878
3110.744063	8.927300	6.960853
3115.908467	29.477583	23.022614
3116.896283	13.096387	10.231797
3121.943150	13.190196	10.321773
3129.593697	6.517337	5.112534
3136.878532	0.079262	0.062322

Zero-Point Energy : **0.187730 a.u.**

========== 5.108384 eV

TS2-{H,D}

Coordinates in Frequency Displacement 0

Atom	X	Y	Z (Angstrom)
1.O	1.735844	-3.418345	-1.135031
2.O	-2.391373	-1.744990	-1.379085
3.C	1.187183	-2.468216	-0.747788
4.C	-1.378689	-1.412143	-0.933413
5.H	-0.132287	2.135186	-0.559323
6.Ru	0.324606	-0.943757	-0.071908
7.C	-0.597827	2.019065	0.418898
8.H	-1.185182	4.075144	0.641888
9.N	-0.566120	0.769392	0.928882
10.H	0.441855	-3.799315	1.662843
11.C	-1.182509	3.085408	1.096550
12.C	-0.286138	-1.768571	1.834659
13.C	-0.167808	-3.107096	2.243703
14.C	-1.125327	0.525480	2.154559
15.C	-1.750050	2.853562	2.354567
16.C	-1.046676	-0.861387	2.619401
17.C	-1.717867	1.566711	2.884655
18.C	-0.829326	-3.554920	3.392299
19.H	-0.742230	-4.599004	3.694852
20.H	-2.210003	3.666518	2.916920
21.C	-1.705023	-1.323728	3.772868
22.H	-2.145995	1.363407	3.863642
23.C	-1.599544	-2.662806	4.153841
24.H	-2.310413	-0.643435	4.370372
25.H	-2.116396	-3.012164	5.047624
26.Cl	1.063422	0.434494	-1.995219
27.H	0.982596	-1.207588	1.452714
28.H.D	1.742113	-0.531030	0.743129

Intensities

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Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
-953.771384	3500.366071	-836.827269
40.000229	188.271312	1.887664
53.041043	91.093808	1.211097
67.529414	39.745970	0.672766
76.006408	8.109159	0.154491
83.243888	56.258911	1.173875
88.240402	98.167697	2.171272
103.097343	5.462525	0.141162
130.038991	300.166365	9.783938
170.228923	2.446707	0.104398
192.107658	11.215031	0.540037
220.083284	251.250898	13.860304
240.262140	127.721511	7.691791
275.521431	104.202889	7.196366
300.306566	605.306973	45.563657
352.651530	68.056438	6.015795
364.829924	82.008969	7.499458
386.193351	772.400908	74.769700
407.749179	44.797843	4.578553
435.800869	36.221495	3.956695
447.449563	2.840989	0.318634
464.716434	17.592772	2.049276
477.281653	38.752847	4.636139
505.185654	53.124454	6.727033
540.892622	124.879709	16.930937
549.326966	18.782140	2.586152
586.159291	418.325650	61.462216
598.319139	719.465656	107.899898
604.740842	723.133691	109.613985
618.673900	87.816251	13.618045
641.672980	50.351416	8.098480

660.465333	140.049656	23.185162
708.004451	87.740286	15.570878
721.655851	387.077626	70.017448
738.267069	831.843134	153.933450
748.950396	12.661652	2.376958
780.535083	10.743968	2.102012
850.171140	6.448304	1.374137
868.245686	2.299443	0.500430
928.478271	235.939379	54.909849
932.084736	10.043314	2.346446
962.607271	3.302110	0.796744
967.176273	1.809866	0.438763
979.715643	0.172258	0.042302
989.876990	12.286147	3.048421
995.080247	12.268128	3.059951
1009.880955	13.888983	3.515756
1035.708085	4.944640	1.283660
1042.884807	79.950819	20.899569
1084.961609	26.890127	7.312827
1097.664007	19.852069	5.462020
1118.516114	21.218532	5.948886
1135.442532	25.850461	7.357182
1230.576584	13.621866	4.201683
1263.873876	45.005541	14.257645
1277.726394	58.631739	18.777973
1302.194114	36.216946	11.821311
1314.510206	34.330316	11.311491
1324.358001	92.705047	30.774205
1398.586020	76.415538	26.788533
1419.393394	111.126009	39.536350
1438.603043	72.404193	26.108551
1462.771344	248.668036	91.174728
1535.297570	33.112272	12.742646
1547.052214	37.669535	14.607413
1564.241171	35.930246	14.087761
1587.694494	135.427481	53.895413
1855.220661	1351.718520	628.579056
1933.667415	3190.975330	1546.618838
2014.072658	1800.045063	908.733590
3096.330812	0.529252	0.410760
3102.630698	38.043888	29.586463
3103.219308	28.960838	22.526912
3105.367821	5.792753	4.508957
3110.711246	5.758629	4.490109
3119.163524	16.816668	13.147893
3125.099908	5.230645	4.097295
3135.770471	0.549058	0.431560

Zero-Point Energy : 0.183953 a.u.
========== 5.005605 eV
(imaginary frequencies were excluded from the summation)

P4-{H,D}
Coordinates in Frequency Displacement 0

Atom	X	Y	Z (Angstrom)
1.O	1.591669	-3.518772	-1.041079
2.O	-2.317040	-1.685991	-1.437725
3.C	1.101070	-2.523376	-0.695949
4.C	-1.319899	-1.400556	-0.921942
5.H	-0.226437	2.124237	-0.596302
6.Ru	0.289950	-0.945164	-0.067445
7.C	-0.676114	2.006236	0.389033
8.H	-1.286615	4.055634	0.613868
9.N	-0.618167	0.760769	0.908083
10.H	0.195289	-3.862028	1.462622
11.C	-1.262885	3.067703	1.071336
12.C	-0.405292	-1.793534	1.712700
13.C	-0.282316	-3.132493	2.117371
14.C	-1.152597	0.508085	2.143260
15.C	-1.810655	2.829145	2.337457

16.C	-1.038270	-0.878312	2.595728
17.C	-1.753206	1.545648	2.873328
18.C	-0.765623	-3.555813	3.363801
19.H	-0.656133	-4.600918	3.657707
20.H	-2.279412	3.636311	2.900999
21.C	-1.522569	-1.310211	3.847128
22.H	-2.173315	1.341311	3.855480
23.C	-1.387474	-2.644503	4.230612
24.H	-2.004206	-0.605135	4.524035
25.H	-1.764013	-2.973930	5.199044
26.Cl	1.173138	0.481606	-1.948605
27.H	1.666814	-0.732607	1.166185
28.H.D	1.921719	-0.276448	0.549566

Intensities

Frequency cm-1	Dipole Strength 1e-40 esu2 cm2	Absorption Intensity (degeneracy not counted) km/mole
35.751922	261.928958	2.347259
48.519361	31.408640	0.381981
66.285362	120.127299	1.995894
77.679815	29.396822	0.572383
83.824451	11.501976	0.241669
92.743388	11.211877	0.260639
105.689151	4.440286	0.117630
125.408888	328.770712	10.334739
180.374904	106.159737	4.799699
195.977969	15.100520	0.741784
220.197361	434.893207	24.003402
244.415596	92.029936	5.638143
257.921015	21.625937	1.398105
272.902015	335.820937	22.971671
293.342113	267.375565	19.659578
326.980239	516.980353	42.371478
367.461023	78.782813	7.256394
380.305086	71.797306	6.844132
413.775437	105.271222	10.918235
438.206377	38.027754	4.176932
461.812096	254.771144	29.491279
465.333886	6.177238	0.720505
474.228645	130.521356	15.514845
496.298017	13.392047	1.665971
524.017850	92.547331	12.155926
549.648536	74.733047	10.296173
561.720384	416.791289	58.683619
589.085715	462.686924	68.319360
620.442434	69.544843	10.815447
630.865767	301.828285	47.728190
638.943184	55.461690	8.882463
654.444811	6.961526	1.141972
709.698843	101.728452	18.096501
720.108724	300.294831	54.203084
737.199248	802.664541	148.319083
742.209313	89.607982	16.670597
751.695633	28.260515	5.324762
780.326378	11.630026	2.274757
843.014406	2.801587	0.591994
865.191162	2.934264	0.636340
922.846502	3.228640	0.746839
959.899042	1.810263	0.435557
962.088081	3.283853	0.791911
978.175126	0.338836	0.083078
993.173630	14.675002	3.653267
999.876201	152.691222	38.268230
1010.556089	5.567138	1.410167
1039.175070	2.791989	0.727244
1045.116315	112.980128	29.596800
1086.258490	10.080528	2.744698
1096.342593	22.853172	6.280162
1120.532876	23.352985	6.559112
1137.455275	32.961979	9.397789
1232.341285	46.334716	14.312503
1260.968459	83.205789	26.298794

1268.805561	152.596380	48.530792
1278.184637	40.385763	12.938977
1299.040579	60.664736	19.753183
1309.390160	80.472017	26.411437
1400.061017	134.863629	47.328188
1415.761044	80.995355	28.742739
1435.872910	16.396949	5.901428
1461.360595	467.266533	171.159157
1532.748426	58.272273	22.387774
1545.289890	114.488283	44.345451
1562.949417	159.396800	62.445708
1587.022787	253.612055	100.886052
1937.352680	3085.566923	1498.379175
2010.418303	2265.701667	1141.740019
3008.330115	2.812505	2.120786
3083.905385	3.241633	2.505780
3097.768396	5.796189	4.500591
3100.812120	14.993374	11.653406
3105.033241	66.584942	51.822737
3108.397471	3.416965	2.662288
3111.409588	30.526956	23.807772
3129.280359	2.491723	1.954440
3136.695439	0.875185	0.688098

Zero-Point Energy : **0.186388 a.u.**
========== **5.071867 eV**