

Supporting Information

Mechanistic Exploration of CO₂ Conversion to Dimethoxymethane (DMM) Using Transition Metal (Co, Ru) Catalysts: An Energy Span Model

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1. Gaussian full references

Gaussian 09, Revision D.01, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery, Jr., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, O. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, D.J. Fox, Gaussian, Inc., Wallingford CT, 2013.

2. Accuracy of basis sets and functional

The accuracy of the basis sets (ECP) has been tested for the whole catalytic cycle 1 i.e., the conversion of CO₂ to MF for both the Co and Ru-triphos catalysts using a larger triple-zeta + polarization quality basis set def2-TZVP for Co and Ru and 6-31++G(d,p) basis set for the main group elements (C, H, O and P). Likewise, the accuracy of the functional has also been tested using M06 functional for some those selected steps (TS1 for Co and Ru-triphos catalysts). The calculated free energy barriers with different functional (M06) and basis set [def2-TZVP for Co and Ru and 6-31++G(d,p) for light elements] are in quite agreement with a difference of 1-2.3 kcal/mol.

Table S1: Accuracy of basis sets (ECP): calculated reaction free energies of the transfer hydrogenation reaction for the conversion of CO₂ to MF using Ru and Co-triphos catalyst with B3LYP functional 6-31++G(d,p) Pople diffused basis set and def2TZVP ECP. $\Delta\Delta G^\ddagger$ is the total reaction free energy barrier for reaction. All the energy values are in kcal/mol.

Catalyst	1	2	TS1	3	4	5	6	7	8	TS2	9	1	$\Delta\Delta G^\ddagger$
Ru-triphos	0.0	6.2	8.8	-5.9	-15.1	-3.7	13.8	5.5	6.7	16.9	0.1	2.2	32.0
Co-triphos	0.0	7.6	9.2	-4.9	-13.2	-4.2	11.1	4.3	9.2	9.3	-0.3	2.2	24.6

Table S2: Evaluation of functional, basis sets (ECP) for Co and Ru-triphos catalysts.

Transition state	Functional	Basis set for non-metals	Basis set for Co and Ru atoms	Activation barrier (Kcal/mol)
TS1-Ru-triphos	B3LYP	6-31++G(d,p)	LANL2DZ	3.7
	B3LYP	6-31++G(d,p)	def2-TZVP	2.6
	M06	6-31++G(d,p)	def2-TZVP	4.6
TS1-Co-triphos	B3LYP	6-31++G(d,p)	LANL2DZ	2.0
	B3LYP	6-31++G(d,p)	def2-TZVP	1.6
	M06	6-31++G(d,p)	def2-TZVP	4.3

3. Imaginary frequencies of all the transition states

Table S3: All imaginary frequencies of the corresponding transition states.

<i>Co-triphos</i>		<i>Ru-triphos</i>	
<i>Transition states</i>	<i>Frequency</i>	<i>Transition states</i>	<i>Frequency</i>
<i>TS1</i>	-356.670 cm^{-1}	<i>TS1</i>	-261.081 cm^{-1}
<i>TS2</i>	-423.568 cm^{-1}	<i>TS2</i>	-1004.124 cm^{-1}
<i>TS3</i>	-530.072 cm^{-1}	<i>TS3</i>	-356.810 cm^{-1}
<i>TS4</i>	-442.617 cm^{-1}	<i>TS4</i>	-534.071 cm^{-1}
<i>TS5</i>	-294.549 cm^{-1}	<i>TS6</i>	-270.069 cm^{-1}
<i>TS6</i>	-1016.784 cm^{-1}		

4. Overall reaction free energy calculation of Co-triphos catalyst.

Table S4: Overall reaction free energy calculation of Co-triphos catalyst considering all the possible transition states and intermediates. All the reaction free energies are in kcal/mol, and Int. represents intermediate.

Figures	Energy (TDTS)	Energy (TDI)	Reaction free energy $\Delta\Delta G^{\ddagger R}$	Overall reaction free energy barrier (ΔG_{rxn})
Figure 1 (Co-triphos)	9.1 (TS1)	-14.1 (Int. 4)	2.2	$9.1 - (-14.1) + 2.2 = 25.4$ TDTS appears before TDI
	9.5 (TS2)	-14.1 (Int. 4)		$9.5 - (-14.1) = 23.6$ TDTS appears after TDI
	9.5 (TS2)	-0.1 (Int. 9)	2.2	$9.5 - (-0.1) + 2.2 = 11.8$ TDTS appears before TDI
Figure 3 (Co-triphos)	9.1 (TS1)	-14.1 (Int. 4)	2.2	$9.1 - (-14.1) + 2.2 = 25.4$ TDTS appears before TDI
	5.7 (TS3)	-14.1 (Int. 4)		$5.7 - (-14.1) = 19.8$ TDTS appears after TDI
Figure 5 (Co-triphos)	5.0 (TS4)	-0.4 (Int. 18)	5.6	$5.0 - (-0.4) + 5.6 = 11$ TDTS appears before TDI
	10.0 (TS5)	-0.4 (Int. 18)		$10.0 - (-0.4) = 10.4$ TDTS appears after TDI
	10.0 (TS5)	3.3 (Int. 9)	5.6	$10.0 - 3.3 + 5.6 = 12.3$ TDTS appears before TDI
	12.9 (TS2)	-0.4 (Int. 18)		$12.9 - (-0.4) = 13.3$ TDTS appears after TDI
	12.9 (TS2)	3.3 (Int. 9)	5.6	$12.9 - 3.3 + 5.6 = 15.2$ TDTS appears before TDI
Figure 6 (Co-triphos)	5.0 (TS4)	0.0 (Int. 1)		$5.0 - 0.0 = 5.0$ TDTS appears after TDI
	5.0 (TS4)	1.9 (Int. 17)	7.4	$5.0 - 1.9 + 7.4 = 10.5$ TDTS appears after TDI
	20.6 (TS6)	0.0 (Int. 1)		$20.6 - 0.0 = 20.6$ TDTS appears after TDI

5. Reaction free energy of the transfer hydrogenation reaction free energy in the presence of methanol for the conversion of CO₂ to MF via HCOOH using Ru-triphos catalyst.

Table S5: Transfer hydrogenation reaction free energy in the presence of methanol for the conversion of CO₂ to MF via HCOOH using Ru-triphos catalyst. $\Delta\Delta G^\ddagger$ is the total reaction free energy barrier for reaction. All the energy values are in kcal/mol.

Catalyst	1	2	TS1	3	4	5	6	7	8	TS2	9	1	$\Delta\Delta G^\ddagger$
Ru-triphos	0.0	6.6	10.3	-5.5	-13.3	-2.5	15.0	8.0	10.5	19.3	1.5	2.2	32.6

6. Optimized conformations of the transition states of CO₂ conversion to DMM catalyzed by Co and Ru-triphos catalyst

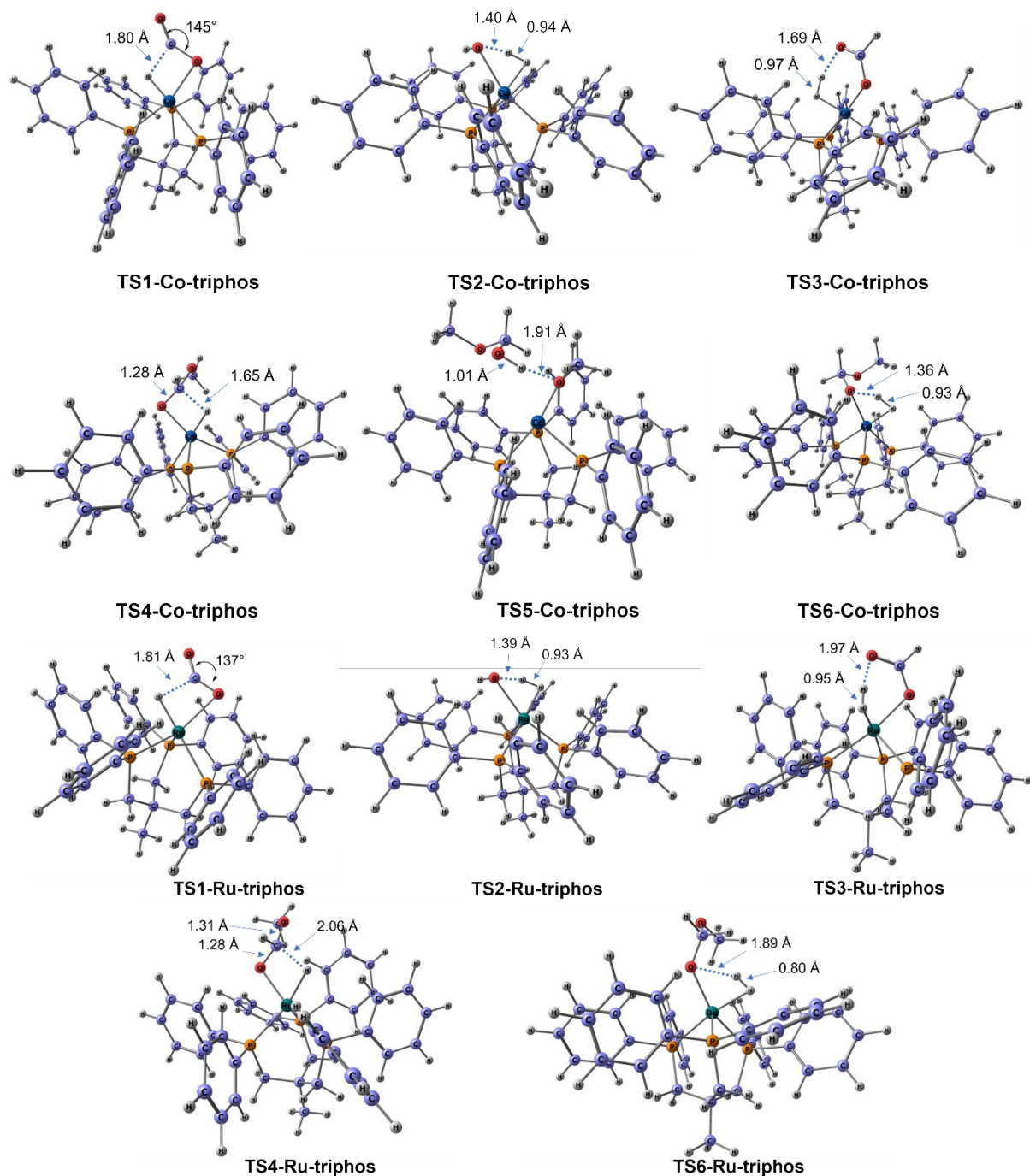


Figure S1: Optimized geometries of the transition states for the hydrogenation of CO₂ to DMM catalyzed by Ru-triphos catalyst. Bond lengths and bond angles are in Å and °, respectively

7. Reaction free energy of the molecular hydrogen-initiated conversion of CO₂ to MF via HCOOH using Ru-triphos catalyst.

Table S6: Molecular hydrogen-initiated conversion of CO₂ to MF via HCOOH using Ru-triphos catalyst. $\Delta\Delta G^{\ddagger R}$ and ΔG_{rxn} denote the total reaction free energy barrier and total reaction free energy of the catalytic cycle, respectively. All the energy values are in kcal/mol.

Catalyst	1	2	TS1	3	4	10	TS3	11	1	12	13	14	15	1	$\Delta\Delta G^{\ddagger R}$
Ru-triphos	0.0	6.6	10.3	-5.5	-13.3	1.0	0.2	1.3	5.6	6.6	7.6	13	9.0	2.2	25.8

8. Reaction free energy profile diagram for the formation of the intermediate **18** via first incorporation of methanol.

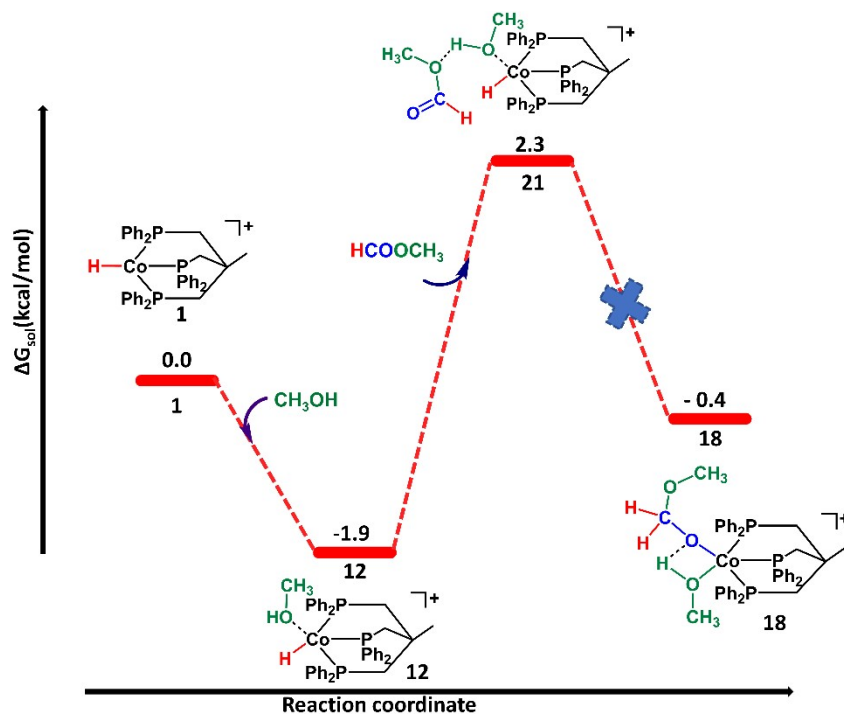


Figure S2. Reaction free energy profile diagram for the formation intermediate **18** via first incorporation of methanol

9. Reaction Free energy of the transfer hydrogenation mechanism to form DMM via MM from MF using Ru-triphos catalyst.

Table S7: Transfer hydrogenation mechanism to form DMM via MM from MF using Ru-triphos catalyst. $\Delta\Delta G^{\ddagger R}$ and ΔG_{rxn} denote the total reaction free energy barrier and total reaction free energy of the catalytic cycle, respectively. All the energy values are in kcal/mol.

Catalyst	1	16	TS4	17	18	TS5	19	20	8	TS2	9	1	$\Delta\Delta G^{\ddagger R}$
Ru-triphos	0.0	-0.1	12.7	4.6	3.1	-	14.1	10.8	14.0	22.8	5.0	5.6	23.4

10. Non-covalent interactions (NCI) of the intermediate 18-Co-triphos.

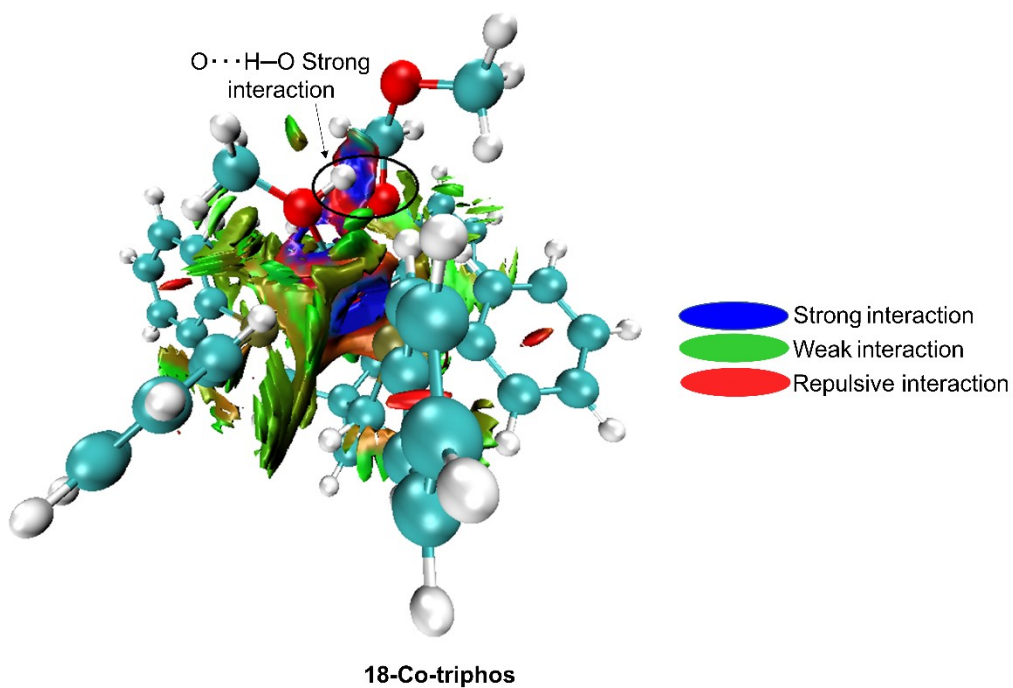


Figure S3. Non-covalent interactions of intermediate **18** of the complex Co-triphos. Different colors on the NCI map represent different types of interactions present in the intermediate (blue and green color denote strong and weak interactions respectively, and red color denotes repulsive interaction).

11. Figure of the intermediate 19-Co-triphos and 19-Ru-triphos with NBO charges showing on oxygen atoms and metal center

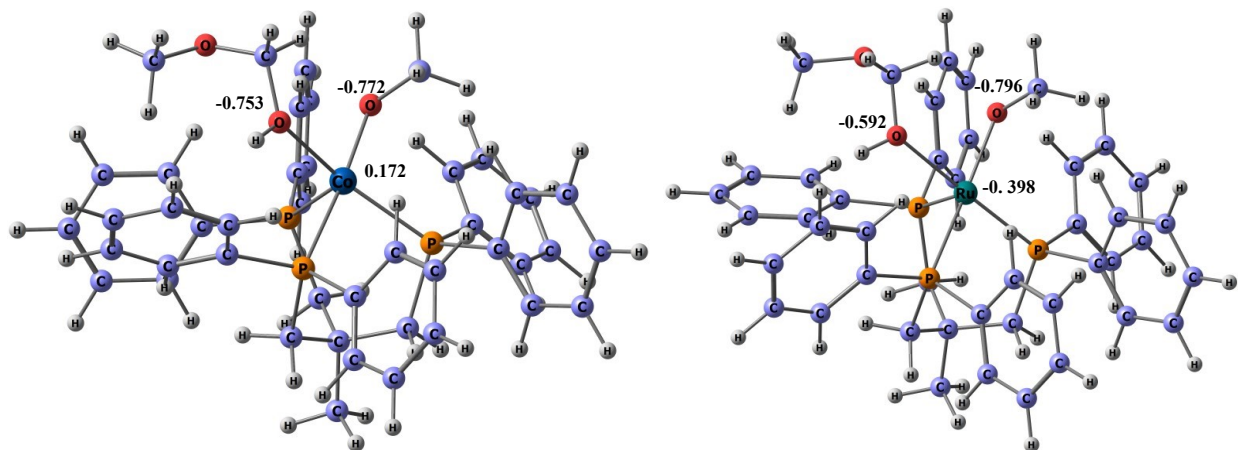


Figure S4. NBO analysis of the intermediate **19** for Co and Ru triphos complexes.

12. Figure of the frontier molecular orbital of the intermediate 19 for Co and Ru complexes

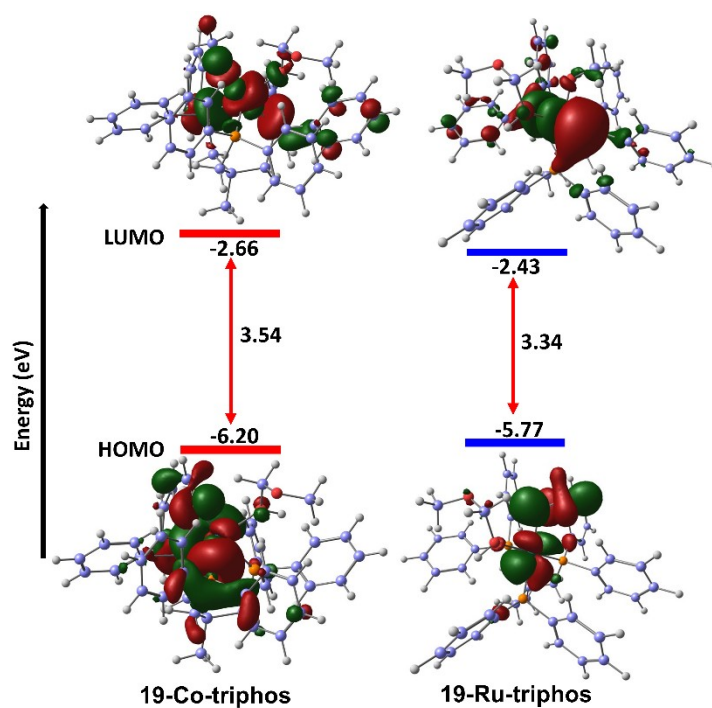
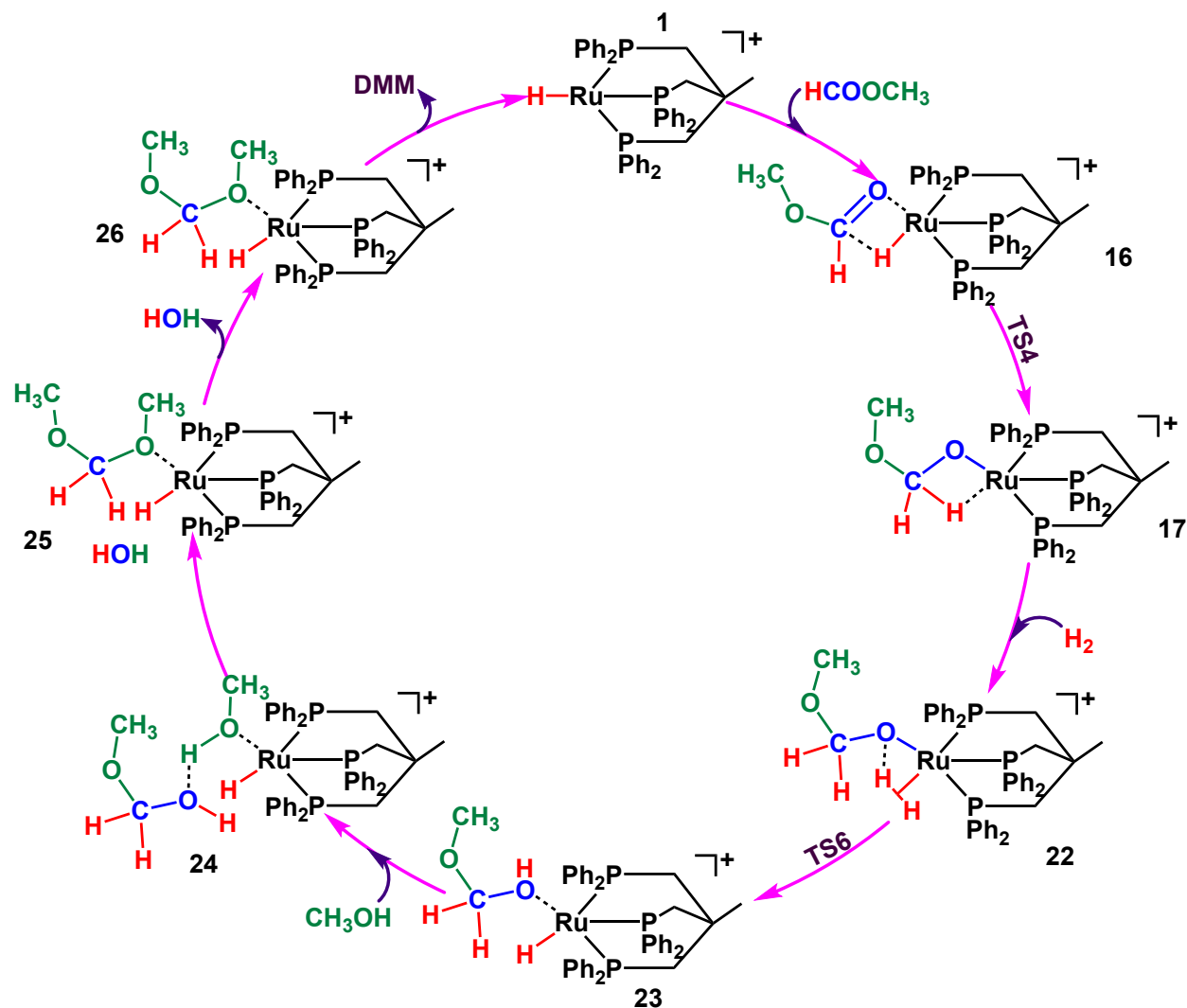


Figure S5. Frontier molecular orbitals on the intermediate **19** for Co and Ru triphos complexes.

13. Catalytic cycle for the molecular hydrogen-initiated conversion of MF to DMM via MM using Ru-triphos catalyst.



Scheme S1. Catalytic cycle for the molecular hydrogen-initiated conversion of MF to DMM via MM with Ru-triphos catalysts.

14. Reaction free energy of the molecular hydrogen-initiated conversion of MF to DMM via MM using Ru-triphos catalyst.

Table S8: Molecular hydrogen-initiated conversion of MF to DMM via MM using Ru-triphos catalyst. $\Delta\Delta G^{\ddagger R}$ and ΔG_{rxn} denote the total reaction free energy barrier and total reaction free energy of the catalytic cycle, respectively. All the energy values are in kcal/mol.

Catalyst	1	16	TS4	17	22	TS6	23	24	25	26	1	$\Delta\Delta G^{\ddagger R}$
Ru-triphos	0.0	-0.1	12.7	4.6	15.9	13.1	11.5	8.8	11.3	6.6	5.6	13.7

15. Microkinetic model

Text S1. The microkinetic modeling has been evaluated considering the Livermore Solver for Ordinary Differential Equations (LSODA) algorithm as employed in the Complex Pathway Simulator (COPASI) software (version 4.24).^{1,2} Here, in this microkinetic modeling, we have only considered the most favorable pathways for the conversion of CO₂ to DMM via HCOOH, methyl formate (MF) and methoxy methanol (MM) using the Co-triphos catalyst. To consider the dimerization steps which are going through barrier less, the rate constants have been calculated by the diffusion-controlled method using the rate constant equation given by $k=800k_B T/3\eta$ where k_B is the Boltzmann constant, T is the temperature, and η is the viscosity of the solvent considered.^{3,4} The diffusion-controlled rate constant value has been calculated at 298.15 K with the viscosity of THF at 298.15 while all other rate constants have been calculated at 373.15 K. Further to mimic the experimental environment we have considered all the experimental conditions. We have considered the catalyst concentration of 0.0125 mmol and varied the concentration of gaseous reactants (CO₂ and H₂) for the time course of 48 hours and evaluated the effect of concentration of the gaseous molecules on the product formation.⁵

16. Reaction free energies, reaction free energy barriers, and rate constants of the important steps for the formation of DMM from CO₂

Table S9: Gibbs free energies of the mechanisms elementary steps and rate constant. All free energies are in kcal/mol and rate constants are in M⁻¹S⁻¹.

Steps	Reaction free energy barrier at 298.15 K in kcal/mol	Rate constant (at 373.15 K) (k) in M ⁻¹ S ⁻¹
1 + CO ₂ = 4	9.1	3.59E+7
4 = 1 + CO ₂	23.2	1.94E-1
4 + CH ₃ OH → 7		1.38E+10
7 + H ₂ = 1 + H ₂ O + MF	5.2	6.94E+9
1 + H ₂ O + MF = 7 + H ₂	7.3	4.00E+8
1 + MF = 17	5.0	9.09E+9
17 = 1 + MF	3.1	1.18E+11
17 + CH ₃ OH = 19	8.1	1.30E+8
19 = 17 + CH ₃ OH	4.3	2.30E+10
19 → 20		1.38E + 10
20 + H ₂ = DMM + 9	6.3	1.50E+9
DMM + 9 = 20 + H ₂	9.6	1.80E+7
9 → 1		1.38E + 10

17. Cartesian coordinates and energies (in Hartree) in solvent phase for all the species

H₂

1	0.000000000	0.000000000	0.371975000
1	0.000000000	0.000000000	-0.371975000

-1.180462

CO₂

6	0.000000000	0.000000000	0.000000000
8	0.000000000	0.000000000	1.169170000
8	0.000000000	0.000000000	-1.169170000

-188.602354

H₂O

8	0.000000000	0.000000000	0.117627000
1	0.000000000	0.767285000	-0.470507000
1	0.000000000	-0.767285000	-0.470507000

-76.437760

HCOOH

1	-0.697225000	-1.344426000	0.000000000
8	-1.035930000	-0.429889000	0.000000000
8	1.168302000	0.098528000	0.000000000
6	0.000000000	0.422739000	0.000000000
1	-0.361756000	1.458882000	0.000000000

-189.773891

CH₃OH

8	-0.047176000	-0.761868000	0.000000000
6	-0.047176000	0.670788000	0.000000000
1	0.442675000	1.077807000	0.893988000
1	0.442675000	1.077807000	-0.893988000
1	-1.093103000	0.985975000	0.000000000
1	0.868209000	-1.071375000	0.000000000

-115.713075

MF

6	-0.938097000	-0.084952000	0.000000000
8	-0.731124000	-1.282045000	0.000000000
8	0.000000000	0.866235000	0.000000000
6	1.379391000	0.415931000	0.000000000

1	1.578588000	-0.179603000	0.893475000
1	1.578588000	-0.179603000	-0.893475000
1	1.979111000	1.324234000	0.000000000
1	-1.935058000	0.375585000	0.000000000

-229.054574

MM

6	-0.680010000	-0.549509000	0.262230000
8	-1.471280000	0.532334000	-0.198869000
8	0.593703000	-0.610098000	-0.335642000
6	1.489599000	0.420490000	0.085728000
1	1.169446000	1.405525000	-0.276574000
1	1.572499000	0.446213000	1.181908000
1	2.465717000	0.187200000	-0.342899000
1	-1.194320000	-1.462035000	-0.042606000
1	-1.268861000	1.328769000	0.310237000
1	-0.581401000	-0.509443000	1.358275000

-230.223230

DMM

8	0.863751000	0.261045000	-0.416093000
6	2.186179000	0.267267000	0.114668000
1	2.745811000	1.026727000	-0.434160000
1	2.186907000	0.520910000	1.184806000
1	2.677100000	-0.707662000	-0.019343000
6	0.025588000	-0.696295000	0.216582000
1	0.360109000	-1.715151000	-0.022266000
1	0.053567000	-0.539298000	1.311196000
8	-1.271377000	-0.575163000	-0.274904000
6	-1.941902000	0.622995000	0.135420000
1	-1.967964000	0.696661000	1.231516000
1	-1.452104000	1.511258000	-0.276546000
1	-2.961609000	0.555697000	-0.247246000

-269.501373

1-Co-triphos

1	6.326932000	-2.512420000	0.369286000
1	5.735218000	-1.099159000	2.330273000
6	5.464715000	-1.853659000	0.324640000
6	5.130276000	-1.061832000	1.429062000
1	4.924639000	-2.423674000	-1.687336000
6	4.681427000	-1.801426000	-0.831921000
6	4.016943000	-0.218358000	1.378565000

1	3.783496000	0.392165000	2.244828000
1	3.896297000	5.320964000	0.961096000
1	4.000410000	5.961750000	-1.441456000
1	3.574829000	-5.946070000	-1.458318000
1	3.220509000	-5.535480000	0.968697000
6	3.564013000	-0.965752000	-0.878562000
6	3.515850000	4.646356000	0.199702000
6	3.575423000	5.005477000	-1.151052000
6	3.220315000	-0.167886000	0.223979000
1	2.935137000	3.158154000	1.629915000
6	2.888505000	-5.170044000	-1.132683000
6	2.966181000	3.417800000	0.576578000
6	2.690249000	-4.938853000	0.232259000
1	2.942211000	-0.946227000	-1.768861000
6	3.083156000	4.131281000	-2.125858000
1	3.123366000	4.405281000	-3.176025000
1	2.361434000	-4.566200000	-3.138934000
6	2.206305000	-4.396119000	-2.077629000
6	2.458681000	2.542201000	-0.396537000
1	1.888348000	1.196074000	2.458675000
6	2.524064000	2.907275000	-1.749692000
6	1.811067000	-3.938471000	0.656879000
1	1.669066000	-3.775999000	1.720743000
1	1.450427000	-1.468408000	2.033440000
1	2.113203000	2.242774000	-2.504424000
1	0.972237000	-0.129388000	4.216630000
15	1.737437000	0.907205000	0.033219000
6	1.336259000	-3.389436000	-1.655645000
6	1.053103000	1.164348000	1.753893000
6	1.131815000	-3.153972000	-0.286223000
1	0.827733000	-2.772523000	-2.393005000
1	0.613917000	2.167110000	1.756891000
1	-0.127485000	1.261797000	4.148594000
6	0.373301000	-1.327425000	1.904469000
6	0.015855000	0.227269000	3.819088000
1	-0.117833000	-2.009772000	2.602420000
6	-0.001698000	0.137955000	2.275689000
1	-0.783465000	-0.383807000	4.251818000
15	-0.039801000	-1.816441000	0.160502000
27	-0.002789000	0.068105000	-1.177047000
1	-1.487745000	-3.521904000	2.221403000
1	-0.187345000	5.595466000	-1.160323000
1	-0.195030000	3.126996000	-1.347704000
6	-0.866031000	5.011896000	-0.545083000
6	-0.863498000	3.616701000	-0.650195000
6	-1.455559000	0.482782000	1.824320000

6	-2.106713000	-3.420496000	1.335617000
1	-1.844553000	1.284393000	2.457954000
6	-1.668569000	-2.673584000	0.230282000
1	-1.734648000	6.728388000	0.432511000
6	-1.732435000	5.645591000	0.348280000
1	-2.086760000	-0.394242000	1.997702000
15	-1.685282000	0.998567000	0.039836000
6	-1.717958000	2.842186000	0.144622000
1	-3.685767000	-4.617715000	2.175406000
6	-3.354309000	-4.049392000	1.311306000
6	-2.604358000	4.879591000	1.133480000
6	-2.597922000	3.487606000	1.032631000
6	-2.492985000	-2.585284000	-0.902800000
1	-3.288772000	5.366088000	1.822320000
1	-2.174905000	-2.004805000	-1.763629000
1	-3.288158000	2.911320000	1.642610000
6	-4.172050000	-3.949066000	0.179986000
6	-3.419120000	0.565144000	-0.373276000
6	-3.736667000	-3.219905000	-0.929752000
1	-2.980435000	0.699585000	-2.484986000
1	-4.182705000	0.326230000	1.643493000
1	-5.144137000	-4.433004000	0.166957000
6	-3.746641000	0.505397000	-1.738302000
6	-4.407946000	0.291052000	0.582661000
1	-4.369014000	-3.125163000	-1.806815000
6	-5.042270000	0.179032000	-2.141481000
6	-5.703096000	-0.044866000	0.176585000
1	-5.282356000	0.131153000	-3.199552000
1	-6.459401000	-0.264585000	0.924418000
6	-6.022779000	-0.101570000	-1.183147000
1	-7.028490000	-0.367641000	-1.494731000
1	0.010177000	1.286411000	-2.023497000

-2755.071359

2-Co-triphos

1	3.100206000	-6.047831000	-0.600629000
1	1.244648000	-5.936453000	-2.256696000
6	2.385913000	-5.230403000	-0.561678000
6	1.344608000	-5.166153000	-1.497122000
1	3.306824000	-4.282450000	1.148246000
6	2.500940000	-4.244653000	0.421468000
6	0.428626000	-4.113135000	-1.454712000
1	-0.380838000	-4.087717000	-2.178866000
1	-5.060304000	-3.943607000	-1.180197000
1	-5.462551000	-4.356731000	1.239486000

1	6.716280000	-2.391685000	1.011420000
1	6.030175000	-2.229334000	-1.374851000
6	1.582800000	-3.190807000	0.464163000
6	-4.327764000	-3.626252000	-0.443789000
6	-4.553134000	-3.858924000	0.916020000
6	0.549159000	-3.108303000	-0.479139000
1	-3.009183000	-2.812645000	-1.925722000
6	5.809216000	-1.859816000	0.740102000
6	-3.161023000	-2.980822000	-0.864599000
6	5.422961000	-1.769897000	-0.600345000
1	1.681177000	-2.428387000	1.227535000
6	-3.605926000	-3.444827000	1.859039000
1	-3.776025000	-3.618752000	2.917522000
1	5.315885000	-1.326364000	2.775536000
6	5.022366000	-1.262399000	1.731830000
6	-2.213135000	-2.554982000	0.076829000
1	-0.632923000	-1.936620000	-2.800297000
6	-2.444202000	-2.793305000	1.442187000
6	4.252024000	-1.091786000	-0.953501000
1	3.974724000	-1.037732000	-2.001067000
1	1.752804000	-1.078937000	-2.235599000
1	-1.721624000	-2.458097000	2.180557000
1	0.498723000	-0.633172000	-4.487797000
15	-0.644850000	-1.710658000	-0.367470000
6	3.851153000	-0.589567000	1.380684000
6	-0.870520000	-1.116962000	-2.116843000
6	3.452598000	-0.501139000	0.035966000
1	3.241104000	-0.133698000	2.156225000
1	-1.930019000	-0.883545000	-2.254601000
1	-1.064578000	0.204147000	-4.431190000
6	1.465432000	-0.034656000	-2.077851000
6	-0.037843000	0.215240000	-4.049793000
1	2.093607000	0.568970000	-2.738045000
6	-0.026203000	0.131185000	-2.505909000
1	0.444459000	1.137779000	-4.390447000
15	1.889667000	0.401392000	-0.309815000
27	0.006109000	0.060888000	0.960593000
1	3.862190000	1.763751000	-2.063494000
1	-5.387496000	-0.572074000	1.674287000
1	-3.018338000	0.127827000	1.652537000
6	-4.982004000	-0.075554000	0.798344000
6	-3.644121000	0.323331000	0.786442000
6	-0.663740000	1.454678000	-1.979924000
6	3.438399000	2.511128000	-1.398613000
1	-1.467500000	1.753098000	-2.657947000
6	2.475105000	2.151098000	-0.438331000

1	-6.820318000	-0.184334000	-0.325683000
6	-5.783215000	0.137953000	-0.326634000
1	0.083866000	2.252980000	-2.020078000
15	-1.324263000	1.450030000	-0.234771000
6	-3.093054000	0.947118000	-0.344373000
1	4.618413000	4.096850000	-2.248444000
6	3.875276000	3.832548000	-1.501686000
6	-5.243188000	0.758250000	-1.458703000
6	-3.906327000	1.166221000	-1.467451000
6	1.981744000	3.133749000	0.428910000
1	-5.860650000	0.925204000	-2.336444000
1	1.251704000	2.861620000	1.180944000
1	-3.515031000	1.651164000	-2.356003000
6	3.359744000	4.812652000	-0.643117000
6	-1.422172000	3.229982000	0.213841000
6	2.417250000	4.459205000	0.324625000
1	-1.282528000	2.792740000	2.322163000
1	-1.567977000	4.012087000	-1.806677000
1	3.696515000	5.841705000	-0.728490000
6	-1.397103000	3.572419000	1.574605000
6	-1.541506000	4.245852000	-0.747374000
1	2.011401000	5.209156000	0.997231000
6	-1.484167000	4.909171000	1.969728000
6	-1.617457000	5.584357000	-0.350711000
1	-1.457644000	5.161609000	3.025703000
1	-1.696469000	6.363370000	-1.103380000
6	-1.588563000	5.919004000	1.006761000
1	-1.643224000	6.959805000	1.312101000
1	0.398382000	1.233944000	1.783669000
8	0.295185000	-1.157570000	2.906991000
6	0.654784000	-0.515010000	3.826327000
8	1.014379000	0.096592000	4.746543000

-2943.662394

TS1-Co-triphos

Frequency = - 356.6703 cm⁻¹

1	4.171478000	-5.335531000	-0.324691000
1	2.526653000	-5.455130000	-2.189450000
6	3.306911000	-4.678425000	-0.330167000
6	2.384332000	-4.743546000	-1.381552000
1	3.828527000	-3.699087000	1.522563000
6	3.113559000	-3.765129000	0.708572000
6	1.277078000	-3.892672000	-1.398249000
1	0.571982000	-3.967998000	-2.220122000

1	-4.334152000	-4.781025000	-1.000975000
1	-4.693138000	-5.098246000	1.439126000
1	6.962356000	-1.472095000	1.066546000
1	6.297512000	-1.346345000	-1.327930000
6	2.007421000	-2.911801000	0.692338000
6	-3.670831000	-4.303417000	-0.285967000
6	-3.871853000	-4.481756000	1.086073000
6	1.085973000	-2.960412000	-0.364225000
1	-2.480716000	-3.382548000	-1.815626000
6	5.993320000	-1.067118000	0.790579000
6	-2.618255000	-3.507250000	-0.746471000
6	5.619006000	-0.998585000	-0.554487000
1	1.874381000	-2.197159000	1.494742000
6	-3.017500000	-3.859760000	2.003014000
1	-3.172820000	-3.988823000	3.069995000
1	5.394551000	-0.666732000	2.827799000
6	5.113578000	-0.614983000	1.780119000
6	-1.763860000	-2.876854000	0.169182000
1	-0.287895000	-2.103261000	-2.743940000
6	-1.971421000	-3.056699000	1.547053000
6	4.369494000	-0.484306000	-0.913723000
1	4.105205000	-0.442807000	-1.965093000
1	1.939554000	-0.851134000	-2.204572000
1	-1.324441000	-2.556893000	2.263090000
1	0.653958000	-0.683193000	-4.457538000
15	-0.354494000	-1.814854000	-0.321161000
6	3.863737000	-0.107535000	1.422688000
6	-0.655761000	-1.313922000	-2.084194000
6	3.477578000	-0.039230000	0.073644000
1	3.181751000	0.222294000	2.200276000
1	-1.737575000	-1.258798000	-2.232584000
1	-1.024949000	-0.108094000	-4.438565000
6	1.477654000	0.129769000	-2.057452000
6	-0.018344000	0.078983000	-4.049508000
1	2.002059000	0.828523000	-2.715026000
6	-0.013000000	0.040649000	-2.504175000
1	0.313248000	1.057451000	-4.412892000
15	1.810003000	0.642323000	-0.288465000
27	-0.070492000	0.039939000	0.985639000
1	3.626874000	2.266350000	-1.994263000
1	-5.315346000	-1.322488000	1.657919000
1	-3.094631000	-0.245532000	1.653820000
6	-4.951380000	-0.846591000	0.752952000
6	-3.697443000	-0.234307000	0.750438000
6	-0.855253000	1.260634000	-2.019314000
6	3.066969000	2.948514000	-1.360545000

1	-1.677455000	1.429003000	-2.719159000
6	2.135024000	2.455185000	-0.429485000
1	-6.688781000	-1.359426000	-0.419304000
6	-5.719411000	-0.870132000	-0.414806000
1	-0.236390000	2.162799000	-2.051699000
15	-1.546641000	1.168945000	-0.294432000
6	-3.200835000	0.371867000	-0.415046000
1	4.017397000	4.689008000	-2.195228000
6	3.295826000	4.320492000	-1.472001000
6	-5.231147000	-0.272104000	-1.581094000
6	-3.980361000	0.351892000	-1.581937000
6	1.459853000	3.359331000	0.400242000
1	-5.821748000	-0.289801000	-2.492251000
1	0.751785000	2.990675000	1.131708000
1	-3.628588000	0.813621000	-2.498510000
6	2.599974000	5.218544000	-0.651645000
6	-1.940804000	2.909458000	0.142029000
6	1.686353000	4.735176000	0.287330000
1	-1.750162000	2.540559000	2.262095000
1	-2.214479000	3.618690000	-1.893178000
1	2.775425000	6.286372000	-0.743346000
6	-1.987773000	3.272844000	1.496564000
6	-2.233919000	3.871124000	-0.837995000
1	1.142778000	5.421102000	0.930285000
6	-2.313877000	4.579146000	1.867417000
6	-2.551747000	5.180065000	-0.464769000
1	-2.340435000	4.848729000	2.919000000
1	-2.766384000	5.918820000	-1.231246000
6	-2.591539000	5.537259000	0.886699000
1	-2.834982000	6.555893000	1.173582000
1	0.045358000	1.288170000	1.833269000
8	0.641155000	-0.743089000	2.885620000
6	0.569989000	0.372873000	3.332663000
8	0.637421000	1.243825000	4.120037000

-2943.659158

3-Co-triphos

1	1.413833000	6.653154000	-0.931743000
1	3.163903000	5.345114000	-2.127191000
6	1.466989000	5.575625000	-0.806992000
6	2.450491000	4.840367000	-1.482472000
1	-0.202006000	5.483040000	0.559432000
6	0.561573000	4.921107000	0.030338000
6	2.517525000	3.455715000	-1.327216000
1	3.291443000	2.899031000	-1.849012000

1	6.489611000	-0.306958000	-0.907546000
1	6.970837000	-0.058783000	1.519119000
1	-4.358193000	5.595685000	1.075031000
1	-3.376262000	5.372151000	-1.200902000
6	0.628193000	3.532836000	0.192422000
6	5.702213000	-0.004226000	-0.223781000
6	5.971854000	0.135567000	1.140281000
6	1.598045000	2.791165000	-0.494618000
1	4.229715000	0.124230000	-1.779360000
6	-3.875963000	4.669369000	0.777800000
6	4.416749000	0.239824000	-0.717023000
6	-3.323668000	4.544710000	-0.499678000
1	-0.059939000	3.034387000	0.862310000
6	4.951729000	0.520451000	2.018421000
1	5.155006000	0.625891000	3.079922000
1	-4.233482000	3.681906000	2.666916000
6	-3.806110000	3.595602000	1.672604000
6	3.392204000	0.618803000	0.160493000
1	1.817317000	1.192735000	-2.761463000
6	3.665561000	0.756284000	1.533100000
6	-2.693744000	3.357203000	-0.884306000
1	-2.272981000	3.291927000	-1.881043000
1	-0.632981000	1.941838000	-2.092062000
1	2.867588000	1.036633000	2.216612000
1	0.125025000	0.942990000	-4.481945000
15	1.670305000	0.958020000	-0.347958000
6	-3.177527000	2.409775000	1.291678000
6	1.485009000	0.377122000	-2.113631000
6	-2.611579000	2.280656000	0.011747000
1	-3.133782000	1.585073000	1.995481000
1	2.172445000	-0.457694000	-2.275600000
1	0.864146000	-0.669897000	-4.487343000
6	-1.050742000	0.931405000	-2.079909000
6	0.034049000	-0.075753000	-4.091243000
1	-1.867884000	0.931261000	-2.805776000
6	0.054107000	-0.070307000	-2.546311000
1	-0.902506000	-0.504119000	-4.463743000
15	-1.788695000	0.688645000	-0.385623000
27	-0.011279000	0.008708000	0.955786000
1	-3.724404000	-0.029797000	-2.616384000
1	4.381264000	-2.919206000	2.024008000
1	2.117451000	-1.985181000	1.819791000
6	3.851223000	-3.005168000	1.081016000
6	2.565752000	-2.476886000	0.961966000
6	-0.243477000	-1.525068000	-2.082418000
6	-3.944760000	-0.625269000	-1.736318000

1	0.293230000	-2.230235000	-2.720766000
6	-3.185610000	-0.489474000	-0.562836000
1	5.466510000	-4.014980000	0.069187000
6	4.460463000	-3.616240000	-0.018394000
1	-1.308168000	-1.738396000	-2.209913000
15	0.174296000	-1.857577000	-0.314498000
6	1.871818000	-2.557675000	-0.257092000
1	-5.580868000	-1.639207000	-2.698044000
6	-5.004258000	-1.534739000	-1.783831000
6	3.775702000	-3.703715000	-1.234077000
6	2.485325000	-3.180743000	-1.354628000
6	-3.513163000	-1.264600000	0.560546000
1	4.243433000	-4.176812000	-2.092188000
1	-2.920566000	-1.182577000	1.465961000
1	1.975984000	-3.268651000	-2.307989000
6	-5.323977000	-2.304058000	-0.659083000
6	-0.904705000	-3.218771000	0.255630000
6	-4.580228000	-2.163760000	0.515601000
1	-0.592321000	-2.697544000	2.335691000
1	-1.416951000	-4.000452000	-1.703097000
1	-6.145642000	-3.012700000	-0.701705000
6	-1.076173000	-3.378593000	1.640478000
6	-1.540715000	-4.100771000	-0.629781000
1	-4.812558000	-2.765782000	1.388176000
6	-1.884819000	-4.403159000	2.134222000
6	-2.352913000	-5.122424000	-0.130980000
1	-2.019008000	-4.514724000	3.205818000
1	-2.850334000	-5.796759000	-0.821430000
6	-2.528002000	-5.273908000	1.248043000
1	-3.164939000	-6.065580000	1.630771000
1	-1.483575000	0.481944000	3.311278000
8	0.089978000	1.329292000	2.320220000
6	-0.692310000	1.259484000	3.358292000
8	-0.598254000	1.975587000	4.354447000

-2943.681758

4-Co-triphos

1	-2.132222000	-6.470558000	0.412180000
1	-0.216632000	-6.174969000	1.974950000
6	-1.543323000	-5.558588000	0.383250000
6	-0.468313000	-5.391609000	1.266320000
1	-2.683292000	-4.672798000	-1.223370000
6	-1.851902000	-4.553348000	-0.535350000
6	0.283358000	-4.216409000	1.239960000
1	1.118358000	-4.107830000	1.926370000

1	5.734219000	-2.900992000	0.976510000
1	6.130699000	-3.202962000	-1.459450000
1	-6.442921000	-3.231056000	-1.142640000
1	-5.889721000	-2.909317000	1.261910000
6	-1.097031000	-3.376628000	-0.568990000
6	4.926219000	-2.741982000	0.268800000
6	5.148159000	-2.911171000	-1.100720000
6	-0.036651000	-3.194019000	0.328400000
1	3.515449000	-2.229691000	1.802930000
6	-5.600601000	-2.608397000	-0.856190000
6	3.665399000	-2.359961000	0.736460000
6	-5.288721000	-2.429167000	0.495170000
1	-1.332491000	-2.607948000	-1.291780000
6	4.105219000	-2.698592000	-2.009780000
1	4.274589000	-2.824002000	-3.075040000
1	-5.055631000	-2.122756000	-2.889750000
6	-4.822061000	-1.985686000	-1.838050000
6	2.621449000	-2.140851000	-0.172190000
1	0.887749000	-1.990890000	2.713910000
6	2.846739000	-2.311011000	-1.549750000
6	-4.201680000	-1.632707000	0.867920000
1	-3.981540000	-1.508307000	1.923230000
1	-1.615780000	-1.515948000	2.093910000
1	2.040739000	-2.128290000	-2.256490000
1	-0.499270000	-0.975979000	4.435370000
15	0.934980000	-1.633930000	0.315510000
6	-3.731660000	-1.196237000	-1.467720000
6	0.998680000	-1.099570000	2.091110000
6	-3.411280000	-1.013177000	-0.112190000
1	-3.118050000	-0.735867000	-2.236150000
1	1.994510000	-0.693470000	2.287830000
1	0.898971000	0.116930000	4.464000000
6	-1.499320000	-0.429968000	2.019060000
6	-0.104679000	-0.029559000	4.050860000
1	-2.230419000	0.005372000	2.704830000
6	-0.066539000	-0.043899000	2.506570000
1	-0.746109000	0.781021000	4.412560000
15	-1.954659000	0.039112000	0.270230000
27	0.088381000	-0.042869000	-1.044740000
1	-3.687699000	1.468913000	2.307220000
1	5.421271000	0.575749000	-1.676090000
1	2.971071000	0.812949000	-1.668140000
6	4.914621000	0.862828000	-0.760230000
6	3.526271000	0.999359000	-0.753530000
6	0.348771000	1.384371000	2.046040000
6	-3.465618000	2.146023000	1.488170000

1	1.085852000	1.790190000	2.743000000
6	-2.675428000	1.730482000	0.402990000
1	6.722521000	0.947848000	0.414230000
6	5.643491000	1.069009000	0.414680000
1	-0.520268000	2.045601000	2.098440000
15	1.022401000	1.527900000	0.322810000
6	2.850211000	1.353319000	0.426430000
1	-4.587697000	3.755104000	2.373170000
6	-3.983537000	3.442323000	1.526510000
6	4.978721000	1.423358000	1.592430000
6	3.588711000	1.571149000	1.599250000
6	-2.431578000	2.626432000	-0.649630000
1	5.538791000	1.585919000	2.508450000
1	-1.820468000	2.316362000	-1.489430000
1	3.099982000	1.856409000	2.524630000
6	-3.727317000	4.333813000	0.477070000
6	0.771232000	3.279100000	-0.158010000
6	-2.956717000	3.921523000	-0.612360000
1	1.011582000	2.839280000	-2.261850000
1	0.483783000	4.058861000	1.848960000
1	-4.126317000	5.343323000	0.512460000
6	0.851523000	3.612950000	-1.519540000
6	0.539243000	4.287441000	0.790220000
1	-2.745728000	4.608663000	-1.426050000
6	0.688092000	4.938470000	-1.926500000
6	0.371053000	5.611211000	0.376820000
1	0.742783000	5.186350000	-2.982380000
1	0.183053000	6.383611000	1.116570000
6	0.442093000	5.939091000	-0.980540000
1	0.305464000	6.968171000	-1.299310000
1	-0.807740000	-0.109099000	-4.401140000
8	-0.415619000	1.013751000	-2.721020000
6	-0.533340000	-0.090749000	-3.338080000
8	-0.336920000	-1.174559000	-2.702680000

-2943.696166

5-Co-triphos

1	0.975531000	-6.923448000	-0.568262000
1	-1.411609000	-6.482488000	-1.120214000
6	0.585652000	-5.910887000	-0.530297000
6	-0.756847000	-5.662650000	-0.840349000
1	2.462881000	-5.021737000	0.072528000
6	1.418643000	-4.849711000	-0.170055000
6	-1.267279000	-4.363976000	-0.786863000
1	-2.313448000	-4.195930000	-1.020119000

1	-6.008350000	-2.231511000	-1.118776000
1	-6.465119000	-2.479929000	1.312689000
1	6.312523000	-3.648202000	0.764746000
1	5.796782000	-3.100266000	-1.607183000
6	0.909016000	-3.548558000	-0.121823000
6	-5.196480000	-2.160208000	-0.401451000
6	-5.452294000	-2.300059000	0.965134000
6	-0.434121000	-3.289118000	-0.429007000
1	-3.721730000	-1.824504000	-1.921533000
6	5.500435000	-2.967508000	0.527454000
6	-3.895847000	-1.924094000	-0.855733000
6	5.210365000	-2.660079000	-0.806073000
1	1.583133000	-2.744635000	0.139381000
6	-4.402808000	-2.198506000	1.884650000
1	-4.594841000	-2.296588000	2.948801000
1	4.947823000	-2.642819000	2.590383000
6	4.735742000	-2.402289000	1.552869000
6	-2.842065000	-1.817592000	0.062072000
1	-0.966321000	-1.953093000	-2.801086000
6	-3.105844000	-1.953875000	1.435123000
6	4.163990000	-1.787276000	-1.116017000
1	3.955536000	-1.571357000	-2.158813000
1	1.521450000	-1.580206000	-2.243766000
1	-2.297815000	-1.856486000	2.152242000
1	0.397747000	-0.939741000	-4.556990000
15	-1.092461000	-1.565977000	-0.415888000
6	3.685666000	-1.533865000	1.244796000
6	-1.068016000	-1.043907000	-2.201453000
6	3.392653000	-1.212660000	-0.091890000
1	3.076201000	-1.127589000	2.045667000
1	-2.042353000	-0.608503000	-2.438312000
1	-0.943387000	0.222290000	-4.542848000
6	1.458525000	-0.491337000	-2.148239000
6	0.056723000	0.016507000	-4.146680000
1	2.194797000	-0.074826000	-2.840722000
6	0.038900000	-0.028273000	-2.600870000
1	0.733147000	0.801729000	-4.500241000
15	1.993671000	-0.056430000	-0.407228000
27	-0.048302000	-0.062236000	0.967155000
1	4.158639000	0.917952000	-2.229447000
1	-5.390481000	1.109527000	1.684924000
1	-2.922410000	1.107998000	1.634131000
6	-4.872588000	1.295849000	0.749543000
6	-3.478489000	1.298545000	0.720663000
6	-0.297659000	1.410706000	-2.111621000
6	3.857935000	1.740387000	-1.587358000

1	-1.011472000	1.869074000	-2.800227000
6	2.852854000	1.564380000	-0.618641000
1	-6.682269000	1.489860000	-0.409384000
6	-5.596740000	1.505494000	-0.428241000
1	0.607689000	2.021560000	-2.162393000
15	-0.958045000	1.591491000	-0.384465000
6	-2.792218000	1.520414000	-0.484242000
1	5.265483000	3.098117000	-2.483417000
6	4.492226000	2.974742000	-1.730802000
6	-4.920320000	1.721686000	-1.632100000
6	-3.522628000	1.735162000	-1.661650000
6	2.511559000	2.641943000	0.209463000
1	-5.476872000	1.880877000	-2.550871000
1	1.737393000	2.528905000	0.955801000
1	-3.023125000	1.917422000	-2.607194000
6	4.135408000	4.049592000	-0.905108000
6	-0.683810000	3.356267000	0.046860000
6	3.147438000	3.879630000	0.065892000
1	-1.061837000	3.011232000	2.146310000
1	-0.259096000	4.052983000	-1.968317000
1	4.628482000	5.010324000	-1.020403000
6	-0.847128000	3.751026000	1.385062000
6	-0.380273000	4.322467000	-0.925271000
1	2.857190000	4.705824000	0.707528000
6	-0.691165000	5.091179000	1.745116000
6	-0.225174000	5.661980000	-0.558782000
1	-0.808687000	5.382901000	2.784535000
1	0.016776000	6.399387000	-1.318363000
6	-0.375605000	6.049192000	0.775926000
1	-0.247845000	7.089863000	1.058798000
1	2.266696000	0.767165000	2.683827000
8	0.292986000	1.167104000	2.407554000
6	1.372957000	1.252728000	3.118736000
8	1.454038000	1.832079000	4.204249000
8	0.441498000	-1.560270000	2.327116000
6	0.841318000	-2.888315000	2.753812000
1	0.728594000	-3.599507000	1.931768000
1	1.879903000	-2.861624000	3.092594000
1	0.187645000	-3.160284000	3.580057000
1	0.429883000	-0.897704000	3.076029000

-3059.394990

6-Co-triphos

1	1.730697000	6.677257000	-0.294566000
1	3.377387000	5.429935000	-1.685876000

6	1.753910000	5.591701000	-0.266648000
6	2.678419000	4.890784000	-1.053145000
1	0.151831000	5.424346000	1.171450000
6	0.870033000	4.890356000	0.555832000
6	2.704563000	3.496087000	-1.025993000
1	3.435448000	2.970502000	-1.634150000
1	6.586849000	-0.088951000	-1.253659000
1	7.215269000	-0.380739000	1.137408000
1	-3.869867000	6.057181000	1.004122000
1	-3.563878000	5.514550000	-1.405541000
6	0.895315000	3.491398000	0.589861000
6	5.841111000	0.034910000	-0.473949000
6	6.194149000	-0.127213000	0.868645000
6	1.802391000	2.786517000	-0.212172000
1	4.286258000	0.476426000	-1.874713000
6	-3.444344000	5.101684000	0.711453000
6	4.526253000	0.355484000	-0.824148000
6	-3.270468000	4.798271000	-0.643576000
1	0.223207000	2.939054000	1.238373000
6	5.224555000	0.035581000	1.863102000
1	5.486217000	-0.092698000	2.909271000
1	-3.192670000	4.406540000	2.739852000
6	-3.066075000	4.173204000	1.686513000
6	3.545292000	0.511586000	0.168243000
1	2.077680000	1.364066000	-2.592851000
6	3.910177000	0.349522000	1.514610000
6	-2.721530000	3.570628000	-1.023001000
1	-2.604327000	3.351868000	-2.079685000
1	-0.349485000	2.262221000	-2.070190000
1	3.166772000	0.450732000	2.295399000
1	0.524873000	1.386883000	-4.435857000
15	1.796448000	0.942352000	-0.217888000
6	-2.509254000	2.947038000	1.311931000
6	1.644222000	0.528334000	-2.037248000
6	-2.330900000	2.640414000	-0.046256000
1	-2.165162000	2.246496000	2.065131000
1	2.277766000	-0.342851000	-2.227238000
1	1.147926000	-0.272535000	-4.523808000
6	-0.828621000	1.280264000	-2.136067000
6	0.332115000	0.349986000	-4.141062000
1	-1.601286000	1.377593000	-2.902824000
6	0.227159000	0.232173000	-2.602719000
1	-0.598291000	0.025538000	-4.618940000
15	-1.633801000	0.996796000	-0.480317000
27	0.018956000	-0.032918000	0.946518000
1	-3.251852000	0.219117000	-2.978480000

1	4.398286000	-3.103325000	1.536088000
1	2.214420000	-1.962415000	1.430082000
6	3.789717000	-3.193024000	0.642157000
6	2.553014000	-2.546691000	0.580710000
6	-0.201727000	-1.231530000	-2.292325000
6	-3.717588000	-0.190923000	-2.088960000
1	0.314503000	-1.912167000	-2.973403000
6	-3.165466000	0.023014000	-0.816536000
1	5.212904000	-4.420194000	-0.415306000
6	4.246605000	-3.926431000	-0.454765000
1	-1.267791000	-1.347743000	-2.494709000
15	0.125090000	-1.793024000	-0.555734000
6	1.759617000	-2.629861000	-0.573195000
1	-5.291658000	-1.116686000	-3.228569000
6	-4.883800000	-0.949585000	-2.236017000
6	3.458088000	-4.021826000	-1.608022000
6	2.217820000	-3.383554000	-1.666745000
6	-3.816010000	-0.521604000	0.303598000
1	3.807331000	-4.595281000	-2.461403000
1	-3.397075000	-0.372803000	1.292454000
1	1.617856000	-3.485217000	-2.565439000
6	-5.521350000	-1.487856000	-1.114342000
6	-1.037561000	-3.179055000	-0.211917000
6	-4.988052000	-1.264268000	0.159001000
1	0.266948000	-3.995344000	1.321244000
1	-2.590397000	-2.646887000	-1.634574000
1	-6.423995000	-2.079750000	-1.232043000
6	-0.695231000	-4.074197000	0.823431000
6	-2.278044000	-3.324861000	-0.850351000
1	-5.471537000	-1.682970000	1.036422000
6	-1.577181000	-5.087185000	1.207554000
6	-3.150376000	-4.349539000	-0.471463000
1	-1.297582000	-5.764870000	2.008320000
1	-4.105506000	-4.444681000	-0.978186000
6	-2.808720000	-5.228259000	0.558870000
1	-3.494570000	-6.015702000	0.855665000
1	-1.532916000	0.044880000	3.715034000
8	-1.219587000	-1.339252000	2.297173000
6	-1.751797000	-1.006069000	3.503720000
8	-2.371507000	-1.784966000	4.187920000
8	-0.156545000	1.225576000	2.324778000
6	0.866712000	1.273444000	3.283793000
1	1.693128000	1.939574000	2.981377000
1	0.460778000	1.666644000	4.229733000
1	1.297260000	0.280998000	3.511718000
1	-1.411355000	-2.275654000	2.082574000

-3059.371009

7-Co-triphos

1	4.253807000	5.799506000	0.148245000
1	5.591417000	4.007860000	-0.947740000
6	3.875993000	4.781814000	0.116788000
6	4.628436000	3.774616000	-0.503021000
1	2.054649000	5.245972000	1.179348000
6	2.644134000	4.472108000	0.696773000
6	4.142925000	2.467564000	-0.550102000
1	4.740722000	1.695624000	-1.027391000
1	6.327632000	-2.469292000	-0.136733000
1	6.340552000	-2.722989000	2.337065000
1	-2.087175000	6.620285000	1.453600000
1	-0.630805000	6.431948000	-0.554709000
6	2.157944000	3.160627000	0.656368000
6	5.567628000	-1.979942000	0.465518000
6	5.575200000	-2.121248000	1.856353000
6	2.897256000	2.153803000	0.023821000
1	4.594359000	-1.117128000	-1.240381000
6	-1.887404000	5.647607000	1.014281000
6	4.580879000	-1.211481000	-0.159384000
6	-1.068898000	5.541891000	-0.113431000
1	1.215762000	2.909009000	1.125716000
6	4.590960000	-1.491527000	2.626961000
1	4.588354000	-1.602661000	3.707378000
1	-3.088206000	4.567899000	2.451202000
6	-2.448979000	4.494769000	1.576368000
6	3.588830000	-0.586019000	0.608183000
1	2.942203000	0.788259000	-2.389842000
6	3.599171000	-0.731657000	2.006321000
6	-0.802088000	4.290411000	-0.679326000
1	-0.159789000	4.236364000	-1.551345000
1	0.832644000	2.346780000	-1.958596000
1	2.821604000	-0.260414000	2.602907000
1	1.648382000	1.339150000	-4.362816000
15	2.239415000	0.437266000	-0.086272000
6	-2.184303000	3.244477000	1.015908000
6	2.218676000	0.112291000	-1.926078000
6	-1.355578000	3.132630000	-0.116698000
1	-2.628739000	2.355558000	1.457150000
1	2.578380000	-0.906691000	-2.097894000
1	1.745127000	-0.427113000	-4.499125000
6	0.091695000	1.578622000	-2.197330000
6	1.122751000	0.402804000	-4.148255000

1	-0.487672000	1.968553000	-3.037664000
6	0.838626000	0.272179000	-2.635399000
1	0.187935000	0.395150000	-4.718748000
15	-1.028932000	1.431874000	-0.721447000
27	0.104845000	0.100991000	0.776931000
1	-2.491541000	1.673400000	-3.377111000
1	2.894664000	-4.391281000	2.023194000
1	1.255105000	-2.596265000	1.630741000
6	2.520911000	-4.218574000	1.019114000
6	1.591593000	-3.201416000	0.794154000
6	-0.029978000	-1.007456000	-2.445000000
6	-3.117035000	1.149463000	-2.662283000
1	0.365796000	-1.802641000	-3.079883000
6	-2.669134000	0.895418000	-1.356194000
1	3.717200000	-5.773899000	0.121698000
6	2.984748000	-4.990694000	-0.049858000
1	-1.048518000	-0.814324000	-2.791267000
15	-0.140849000	-1.615847000	-0.694706000
6	1.113291000	-2.946911000	-0.501482000
1	-4.721047000	0.920536000	-4.078912000
6	-4.387209000	0.726235000	-3.064038000
6	2.509036000	-4.748067000	-1.342625000
6	1.573764000	-3.734175000	-1.568325000
6	-3.513582000	0.223896000	-0.458634000
1	2.863173000	-5.346281000	-2.177049000
1	-3.169478000	0.005723000	0.546110000
1	1.211438000	-3.576051000	-2.578754000
6	-5.223642000	0.057274000	-2.163839000
6	-1.736822000	-2.498405000	-0.534679000
6	-4.786429000	-0.188244000	-0.859561000
1	-1.734047000	-2.222719000	1.609969000
1	-2.046168000	-2.931968000	-2.637227000
1	-6.207593000	-0.275638000	-2.480748000
6	-2.259124000	-2.648155000	0.759958000
6	-2.433002000	-3.032287000	-1.628045000
1	-5.424734000	-0.722160000	-0.162936000
6	-3.468476000	-3.315350000	0.959893000
6	-3.646926000	-3.694746000	-1.425156000
1	-3.868532000	-3.417910000	1.964003000
1	-4.187328000	-4.096731000	-2.276770000
6	-4.166959000	-3.835353000	-0.134533000
1	-5.113854000	-4.344852000	0.017873000
1	-3.379787954	-0.239802897	2.635786002
8	-1.493230259	-0.719086307	3.084520955
6	-2.798571407	-0.865936472	3.326927912
8	-3.284422859	-1.585241208	4.176299907

8	0.193812000	1.170487000	2.263079000
6	-0.577559176	-1.484329554	3.916790526
1	0.410520660	-1.287339918	3.501170396
1	-0.648823574	-1.140992159	4.951298665
1	-0.828205474	-2.546576891	3.867387395
1	-0.433580000	1.905258000	2.312892000

-3059.379884

8-Co-triphos

1	6.639429000	1.366529000	0.409339000
1	5.395843000	2.056250000	2.452222000
6	5.554689000	1.413755000	0.396138000
6	4.856278000	1.798194000	1.545953000
1	5.385416000	0.776210000	-1.659928000
6	4.853031000	1.085328000	-0.766274000
6	3.460661000	1.855218000	1.535171000
1	2.945522000	2.170244000	2.436463000
1	-1.595049000	5.918761000	0.410574000
1	-0.075867000	7.055433000	-1.205039000
1	6.322105000	-2.906520000	-1.520448000
1	5.788907000	-2.777735000	0.906279000
6	3.457759000	1.130890000	-0.776248000
6	-0.739598000	5.392434000	-0.001051000
6	0.109884000	6.026937000	-0.910617000
6	2.748323000	1.513973000	0.373830000
1	-1.202525000	3.601151000	1.064377000
6	5.315892000	-2.658384000	-1.196356000
6	-0.507938000	4.067753000	0.377404000
6	5.017179000	-2.585110000	0.167047000
1	2.924682000	0.856267000	-1.680658000
6	1.198966000	5.328963000	-1.442917000
1	1.864220000	5.810711000	-2.153033000
1	4.541008000	-2.457762000	-3.203362000
6	4.316166000	-2.406874000	-2.142288000
6	0.591754000	3.364642000	-0.140071000
1	0.966812000	1.762361000	2.684219000
6	1.440086000	4.007821000	-1.061807000
6	3.725327000	-2.258375000	0.589264000
1	3.520336000	-2.208080000	1.653268000
1	2.020717000	-0.640639000	2.096295000
1	2.294547000	3.485903000	-1.479176000
1	0.929604000	0.008374000	4.324354000
15	0.916601000	1.600216000	0.265271000
6	3.027640000	-2.074517000	-1.723166000
6	0.249625000	1.336758000	1.978496000

6	2.722193000	-1.994741000	-0.354617000
1	2.264587000	-1.861497000	-2.466761000
1	-0.656761000	1.937074000	2.073975000
1	-0.753905000	0.569186000	4.334733000
6	1.049094000	-1.102204000	1.901233000
6	-0.072197000	-0.184288000	3.926208000
1	1.006970000	-2.020386000	2.492534000
6	-0.067354000	-0.133567000	2.381731000
1	-0.398363000	-1.168347000	4.278874000
15	0.994080000	-1.581084000	0.102004000
27	0.019371000	0.078928000	-1.174848000
1	1.514303000	-4.062674000	1.608081000
1	-3.803048000	3.961872000	-1.840665000
1	-2.555120000	1.819835000	-1.810556000
6	-3.703911000	3.408647000	-0.911530000
6	-3.014822000	2.194248000	-0.901023000
6	-1.481179000	-0.597632000	1.909593000
6	0.654527000	-4.242858000	0.969224000
1	-2.232537000	-0.234465000	2.615041000
6	0.174185000	-3.233711000	0.114345000
1	-0.035488000	-1.157051000	-2.515211000
1	-4.756402000	4.878082000	0.268848000
6	-4.236306000	3.924841000	0.273692000
1	-1.520397000	-1.690334000	1.963725000
15	-1.981652000	-0.139074000	0.176883000
6	-2.866450000	1.472346000	0.295457000
1	0.422358000	-6.265159000	1.662004000
6	0.042254000	-5.495857000	0.996515000
6	-4.087923000	3.214007000	1.469203000
6	-3.416019000	1.987661000	1.480063000
6	-0.910298000	-3.514751000	-0.725678000
1	-4.496998000	3.609198000	2.394348000
1	-1.294706000	-2.762831000	-1.399324000
1	-3.326951000	1.451936000	2.419153000
6	-1.055331000	-5.760656000	0.167002000
6	-3.347778000	-1.297734000	-0.238958000
6	-1.526348000	-4.770155000	-0.696292000
1	-3.192682000	-0.805762000	-2.341767000
1	-3.779872000	-2.006317000	1.766315000
1	-1.534387000	-6.734787000	0.193568000
6	-3.708656000	-1.401520000	-1.592870000
6	-4.028622000	-2.071579000	0.712438000
1	-2.376444000	-4.961724000	-1.343781000
6	-4.725162000	-2.271869000	-1.991276000
6	-5.042457000	-2.946954000	0.310909000
1	-4.990515000	-2.345406000	-3.041706000

1	-5.558272000	-3.546688000	1.055109000
6	-5.390536000	-3.052082000	-1.039081000
1	-6.174800000	-3.736778000	-1.347693000
8	-0.333071000	1.346769000	-2.485924000
1	-0.770777000	-0.934759000	-2.454333000
1	-0.279146000	2.270266000	-2.207119000

-2831.495956

TS2-Co-triphos

Frequency = - 423.5681 cm⁻¹

1	-6.585827000	1.751083000	0.501015000
1	-5.668702000	0.733494000	2.578279000
6	-5.648672000	1.203414000	0.470802000
6	-5.132094000	0.634795000	1.639464000
1	-5.340049000	1.521373000	-1.642894000
6	-4.952111000	1.072611000	-0.734164000
6	-3.923764000	-0.066319000	1.605768000
1	-3.552305000	-0.508870000	2.523496000
1	-0.748625000	-5.890255000	-0.689777000
1	-3.131652000	-6.461740000	-1.160110000
1	-4.420440000	5.310379000	-1.386107000
1	-3.787825000	5.156631000	1.014300000
6	-3.739430000	0.383438000	-0.766783000
6	-1.519659000	-5.128627000	-0.624538000
6	-2.855915000	-5.447152000	-0.888621000
6	-3.213772000	-0.191827000	0.401373000
1	-0.123090000	-3.596791000	-0.089200000
6	-3.630838000	4.633222000	-1.074538000
6	-1.164805000	-3.823115000	-0.280251000
6	-3.276574000	4.546111000	0.276008000
1	-3.190611000	0.302642000	-1.700414000
6	-3.834057000	-4.452271000	-0.803615000
1	-4.874020000	-4.690286000	-1.006571000
1	-3.247956000	3.898788000	-3.069444000
6	-2.971884000	3.843049000	-2.020834000
6	-2.144549000	-2.818482000	-0.186177000
1	-1.727233000	-1.379599000	2.649616000
6	-3.483897000	-3.143908000	-0.455639000
6	-2.260457000	3.677543000	0.682680000
1	-1.988690000	3.635678000	1.732857000
1	-1.547480000	1.355847000	2.156912000
1	-4.257937000	-2.387388000	-0.391405000
1	-0.967507000	0.158878000	4.339660000
15	-1.633147000	-1.103173000	0.235435000

6	-1.968352000	2.961722000	-1.614876000
6	-0.904398000	-1.254153000	1.940988000
6	-1.604083000	2.874905000	-0.262358000
1	-1.485340000	2.326794000	-2.351720000
1	-0.357390000	-2.201617000	1.952661000
1	0.267690000	-1.113660000	4.342079000
6	-0.470845000	1.300514000	1.973158000
6	0.022107000	-0.116985000	3.960849000
1	-0.015292000	2.070929000	2.600775000
6	0.039115000	-0.105941000	2.414787000
1	0.752911000	0.592420000	4.363324000
15	-0.222927000	1.757403000	0.188848000
27	-0.046260000	-0.119567000	-1.104799000
1	1.967731000	2.608890000	2.137115000
1	2.610276000	-4.791937000	-2.461721000
1	2.201281000	-2.379473000	-2.099980000
6	2.510022000	-4.408361000	-1.450764000
6	2.299935000	-3.044116000	-1.248023000
6	1.510668000	-0.360951000	1.982251000
6	2.131232000	3.074586000	1.172778000
1	1.918904000	-1.173990000	2.586654000
6	1.237288000	2.881970000	0.110104000
1	0.818286000	0.624455000	-2.983840000
1	2.717088000	-6.345458000	-0.517148000
6	2.568859000	-5.281595000	-0.358017000
1	2.115056000	0.512989000	2.232489000
15	1.845323000	-0.720988000	0.177415000
6	2.156437000	-2.530730000	0.054824000
1	3.941738000	4.018353000	1.847916000
6	3.257856000	3.887869000	1.014759000
6	2.428511000	-4.779575000	0.938048000
6	2.228234000	-3.410133000	1.145697000
6	1.484195000	3.540039000	-1.108269000
1	2.469887000	-5.449190000	1.791841000
1	0.794183000	3.436560000	-1.939908000
1	2.117698000	-3.056139000	2.164481000
6	3.503104000	4.522661000	-0.203869000
6	3.520261000	-0.004107000	-0.067997000
6	2.606100000	4.353273000	-1.263951000
1	3.003766000	0.990103000	-1.913848000
1	4.364473000	-0.873936000	1.731202000
1	4.382800000	5.146737000	-0.327383000
6	3.784880000	0.790456000	-1.190495000
6	4.546187000	-0.248125000	0.861859000
1	2.780199000	4.850411000	-2.213417000
6	5.055032000	1.344091000	-1.379392000

6	5.811964000	0.309137000	0.674446000
1	5.245250000	1.966616000	-2.248373000
1	6.597539000	0.118299000	1.399721000
6	6.068188000	1.107583000	-0.447475000
1	7.052914000	1.542358000	-0.591330000
8	-0.076052000	-1.383650000	-2.442478000
1	0.881865000	1.282871000	-2.628130000
1	-0.384976000	-2.273461000	-2.229715000

-2831.497589

9-Co-triphos

1	5.643033000	3.911835000	0.433107000
1	4.088806000	4.386994000	2.318730000
6	4.631549000	3.516814000	0.416913000
6	3.759242000	3.780319000	1.480382000
1	4.866946000	2.529460000	-1.489800000
6	4.197093000	2.745212000	-0.663249000
6	2.460665000	3.267080000	1.467065000
1	1.796199000	3.498074000	2.294176000
1	-3.451386000	5.088181000	0.620520000
1	-2.766322000	6.296538000	-1.446255000
1	6.984959000	-0.662875000	-1.537657000
1	6.455668000	-0.781104000	0.890120000
6	2.898813000	2.227939000	-0.673993000
6	-2.565456000	4.778839000	0.074623000
6	-2.183116000	5.454256000	-1.086566000
6	2.022311000	2.474017000	0.393073000
1	-2.163486000	3.174548000	1.428431000
6	5.955527000	-0.772911000	-1.209731000
6	-1.823504000	3.688438000	0.538235000
6	5.658283000	-0.837835000	0.154902000
1	2.577803000	1.619325000	-1.511979000
6	-1.043219000	5.038463000	-1.784144000
1	-0.731938000	5.558482000	-2.685251000
1	5.146220000	-0.791887000	-3.213065000
6	4.922788000	-0.845613000	-2.151593000
6	-0.678631000	3.265711000	-0.150745000
1	0.467052000	1.920974000	2.727928000
6	-0.295122000	3.954370000	-1.319203000
6	4.333713000	-0.973615000	0.581798000
1	4.127680000	-1.022478000	1.646102000
1	2.175109000	0.060647000	2.068536000
1	0.601389000	3.656872000	-1.857081000
1	0.941140000	0.203404000	4.349137000
15	0.317070000	1.782881000	0.297575000

6	3.599382000	-0.973569000	-1.726877000
6	-0.135614000	1.321663000	2.041349000
6	3.294159000	-1.036623000	-0.357203000
1	2.794646000	-1.007284000	-2.457379000
1	-1.175624000	1.603286000	2.218021000
1	-0.833174000	0.184588000	4.359895000
6	1.423923000	-0.715954000	1.893202000
6	0.056631000	-0.290238000	3.932327000
1	1.712835000	-1.577734000	2.500200000
6	0.044692000	-0.186490000	2.390055000
1	0.069555000	-1.339062000	4.247679000
15	1.521721000	-1.209686000	0.092505000
27	0.068400000	-0.022699000	-1.123067000
1	2.779798000	-3.358200000	1.709387000
1	-5.026398000	2.439098000	-1.739463000
1	-3.165518000	0.817563000	-1.786127000
6	-4.685936000	1.983936000	-0.814169000
6	-3.633659000	1.068387000	-0.838911000
6	-1.147971000	-1.060989000	1.888908000
6	2.047844000	-3.821144000	1.053626000
1	-1.971436000	-0.982072000	2.603328000
6	1.297848000	-3.042928000	0.152897000
1	0.030786000	-1.206824000	-2.032521000
1	-6.091399000	3.055121000	0.426853000
6	-5.282993000	2.330606000	0.402367000
1	-0.842637000	-2.112475000	1.897946000
15	-1.773314000	-0.725610000	0.162874000
6	-3.168364000	0.471918000	0.346093000
1	2.459619000	-5.793744000	1.807134000
6	1.873864000	-5.204751000	1.107447000
6	-4.828797000	1.744859000	1.587069000
6	-3.782799000	0.815891000	1.559387000
6	0.393580000	-3.679843000	-0.704761000
1	-5.286462000	2.007367000	2.536475000
1	-0.170398000	-3.086024000	-1.412266000
1	-3.458893000	0.372282000	2.494755000
6	0.949249000	-5.830531000	0.261003000
6	-2.676711000	-2.266138000	-0.285379000
6	0.214011000	-5.066018000	-0.647523000
1	-2.308610000	-1.948396000	-2.385867000
1	-3.207169000	-2.883850000	1.726051000
1	0.809861000	-6.906575000	0.308915000
6	-2.789048000	-2.584122000	-1.647435000
6	-3.270621000	-3.109999000	0.666150000
1	-0.504606000	-5.539492000	-1.310084000
6	-3.479803000	-3.728255000	-2.054516000

6	-3.951164000	-4.261325000	0.259170000
1	-3.554527000	-3.965973000	-3.111722000
1	-4.398260000	-4.912990000	1.004330000
6	-4.058262000	-4.572407000	-1.100745000
1	-4.586040000	-5.468295000	-1.414275000
8	-0.606341000	1.108545000	-2.723373000
1	-1.079267000	0.635167000	-3.420715000
1	-1.060033000	1.953732000	-2.578538000

-2831.512765

10-Co-triphos

1	6.131001000	2.819563000	0.461095000
1	4.747605000	3.460434000	2.427269000
6	5.061118000	2.633840000	0.455911000
6	4.284576000	2.990904000	1.564626000
1	5.057329000	1.745839000	-1.512032000
6	4.459977000	2.034733000	-0.653173000
6	2.909006000	2.750543000	1.565664000
1	2.324108000	3.053100000	2.428217000
1	-2.938189000	5.444708000	0.142362000
1	-1.671984000	6.774423000	-1.542501000
1	6.890296000	-1.660059000	-0.942822000
1	6.204258000	-1.169487000	1.398416000
6	3.086945000	1.779022000	-0.652202000
6	-1.971634000	5.101583000	-0.213204000
6	-1.262328000	5.844400000	-1.160033000
6	2.303965000	2.132889000	0.458969000
1	-2.034858000	3.342122000	0.997580000
6	5.837581000	-1.582326000	-0.688089000
6	-1.449972000	3.902066000	0.279264000
6	5.452991000	-1.306152000	0.626359000
1	2.629841000	1.291190000	-1.507226000
6	-0.021569000	5.383365000	-1.614369000
1	0.538283000	5.953107000	-2.349857000
1	5.150233000	-1.973564000	-2.699168000
6	4.861086000	-1.757903000	-1.674976000
6	-0.202299000	3.439610000	-0.165577000
1	0.522491000	2.061029000	2.773308000
6	0.506095000	4.188634000	-1.122796000
6	4.099624000	-1.196167000	0.957525000
1	3.834772000	-0.976673000	1.985288000
1	2.015319000	-0.038920000	2.290698000
1	1.472135000	3.849444000	-1.482369000
1	0.755594000	0.382031000	4.473071000
15	0.499319000	1.826775000	0.364489000

6	3.509656000	-1.647605000	-1.348331000
6	-0.110585000	1.498988000	2.082066000
6	3.117573000	-1.360561000	-0.030241000
1	2.762857000	-1.772354000	-2.123431000
1	-1.110668000	1.926002000	2.175350000
1	-1.007181000	0.575602000	4.431397000
6	1.178955000	-0.710769000	2.082102000
6	-0.171633000	-0.023497000	4.054744000
1	1.322460000	-1.597284000	2.704139000
6	-0.134528000	0.002121000	2.509565000
1	-0.293145000	-1.048531000	4.420160000
15	1.316567000	-1.254377000	0.302925000
27	0.001309000	0.106567000	-1.041950000
1	2.152559000	-3.520403000	1.986859000
1	-5.002216000	2.885772000	-1.769408000
1	-3.335977000	1.079109000	-1.762448000
6	-4.663412000	2.474673000	-0.823350000
6	-3.713798000	1.452815000	-0.814816000
6	-1.404256000	-0.757724000	2.013140000
6	1.388547000	-3.883402000	1.305322000
1	-2.228931000	-0.576569000	2.706594000
6	0.807181000	-3.024983000	0.352893000
1	-5.887725000	3.785138000	0.379272000
6	-5.161090000	2.978454000	0.382982000
1	-1.207227000	-1.833303000	2.058391000
15	-1.976160000	-0.418339000	0.275249000
6	-3.252404000	0.908759000	0.396863000
1	1.455120000	-5.874031000	2.115093000
6	1.001430000	-5.221485000	1.375056000
6	-4.717019000	2.438598000	1.592884000
6	-3.774589000	1.404376000	1.601304000
6	-0.138528000	-3.536439000	-0.544364000
1	-5.101118000	2.818873000	2.534741000
1	-0.560774000	-2.897817000	-1.305778000
1	-3.457155000	1.004899000	2.557748000
6	0.032849000	-5.720005000	0.493444000
6	-2.986783000	-1.882799000	-0.179501000
6	-0.528869000	-4.877840000	-0.467253000
1	-2.623545000	-1.579581000	-2.289014000
1	-3.525850000	-2.481356000	1.836865000
1	-0.273178000	-6.760206000	0.554773000
6	-3.140194000	-2.176292000	-1.544181000
6	-3.621792000	-2.691265000	0.776300000
1	-1.277693000	-5.253102000	-1.158193000
6	-3.916409000	-3.266078000	-1.946103000
6	-4.389517000	-3.786038000	0.370458000

1	-4.022258000	-3.489675000	-3.003595000
1	-4.870710000	-4.410672000	1.117331000
6	-4.538806000	-4.075301000	-0.990144000
1	-5.133536000	-4.928547000	-1.302598000
1	0.684957000	-1.274808000	-4.339719000
8	-0.214731000	-1.186480000	-2.523136000
6	0.637042000	-0.743351000	-3.375953000
8	1.375632000	0.237022000	-3.141548000
1	-0.458797000	1.396371000	-2.300319000
1	-1.132069000	1.201310000	-1.988061000

-2944.852786

TS3-Co-triphos

Frequency = - 530.0722 cm⁻¹

1	-2.529834000	-6.471378000	-0.639308000
1	-4.007675000	-4.950464000	-1.944445000
6	-2.400261000	-5.395357000	-0.568212000
6	-3.230874000	-4.540182000	-1.305778000
1	-0.764377000	-5.517889000	0.834378000
6	-1.411181000	-4.861249000	0.260105000
6	-3.062786000	-3.158039000	-1.219277000
1	-3.719126000	-2.505062000	-1.788383000
1	-5.189090000	0.494293000	3.023118000
1	-6.909749000	1.185761000	1.359518000
1	3.476390000	-6.181531000	1.230938000
1	2.436936000	-5.915518000	-1.015312000
6	-1.242180000	-3.474605000	0.352911000
6	-4.980813000	0.423895000	1.959652000
6	-5.946831000	0.811452000	1.024856000
6	-2.059526000	-2.615977000	-0.395686000
1	-2.992596000	-0.337993000	2.259946000
6	3.115661000	-5.209346000	0.908504000
6	-3.738850000	-0.044859000	1.526894000
6	2.531553000	-5.061213000	-0.351780000
1	-0.483791000	-3.063772000	1.009061000
6	-5.668202000	0.717938000	-0.341940000
1	-6.413800000	1.017380000	-1.072653000
1	3.685200000	-4.207538000	2.736600000
6	3.233899000	-4.100407000	1.754784000
6	-3.450465000	-0.139784000	0.154368000
1	-1.973198000	-1.096773000	-2.713174000
6	-4.427945000	0.242256000	-0.777305000
6	2.061764000	-3.811725000	-0.768696000
1	1.614134000	-3.728608000	-1.752156000

1	0.308097000	-2.128921000	-2.085483000
1	-4.238029000	0.176591000	-1.843568000
1	-0.330459000	-1.071799000	-4.466097000
15	-1.796379000	-0.796828000	-0.296121000
6	2.763551000	-2.853469000	1.344172000
6	-1.548109000	-0.305567000	-2.089340000
6	2.171855000	-2.699434000	0.078792000
1	2.843963000	-2.005288000	2.014582000
1	-2.138675000	0.592256000	-2.279563000
1	-0.831104000	0.629176000	-4.493124000
6	0.867879000	-1.189751000	-2.082511000
6	-0.087643000	-0.070129000	-4.096657000
1	1.682003000	-1.315812000	-2.800614000
6	-0.082849000	-0.047251000	-2.551520000
1	0.893930000	0.211935000	-4.491917000
15	1.605615000	-1.021029000	-0.392566000
27	0.096152000	-0.010694000	0.994956000
1	3.579275000	-0.538234000	-2.643681000
1	-3.275779000	4.477866000	2.004390000
1	-1.221680000	3.154326000	1.826857000
6	-2.963907000	4.106575000	1.033065000
6	-1.800177000	3.345359000	0.928935000
6	0.446924000	1.354361000	-2.124537000
6	3.917238000	-0.025085000	-1.749682000
1	0.023639000	2.126694000	-2.770759000
6	3.174227000	-0.078574000	-0.559737000
1	-4.638761000	4.966499000	-0.024547000
6	-3.726584000	4.383610000	-0.106639000
1	1.527916000	1.387216000	-2.285449000
15	0.161847000	1.830736000	-0.358688000
6	-1.378032000	2.846262000	-0.316155000
1	5.675532000	0.738250000	-2.726336000
6	5.112997000	0.695900000	-1.798545000
6	-3.306343000	3.907651000	-1.349642000
6	-2.138163000	3.146611000	-1.456096000
6	3.654601000	0.586700000	0.579780000
1	-3.886127000	4.120395000	-2.242595000
1	3.085376000	0.569614000	1.504148000
1	-1.842465000	2.802058000	-2.439512000
6	5.583644000	1.357826000	-0.659518000
6	1.480345000	3.016300000	0.096151000
6	4.854159000	1.298386000	0.530920000
1	1.259101000	2.591175000	2.209258000
1	1.960998000	3.662687000	-1.919159000
1	6.510476000	1.921855000	-0.702469000
6	1.776257000	3.182261000	1.458914000

6	2.177879000	3.767725000	-0.860976000
1	5.204399000	1.820263000	1.415639000
6	2.757916000	4.089369000	1.860167000
6	3.168665000	4.665747000	-0.455679000
1	2.983353000	4.206076000	2.915795000
1	3.712351000	5.236782000	-1.202223000
6	3.459576000	4.828430000	0.902533000
1	4.232571000	5.525029000	1.212705000
1	0.327873000	-2.148001000	4.166754000
8	-0.181752000	-0.182433000	4.100114000
6	0.145139000	-1.249160000	3.552745000
8	0.305164000	-1.452425000	2.290003000
1	-0.558527477	0.625359033	2.663493044
1	-0.978996000	0.994372000	1.883342000

-2944.846852

11-Co-triphos

1	4.657879000	4.928378000	-0.809994000
1	5.120683000	3.110656000	-2.447271000
6	4.153837000	3.970888000	-0.716206000
6	4.411606000	2.949637000	-1.640362000
1	3.035101000	4.540783000	1.040442000
6	3.247960000	3.753151000	0.323909000
6	3.760495000	1.720030000	-1.526030000
1	3.985356000	0.937031000	-2.244639000
1	5.622270000	-3.374352000	-1.239653000
1	6.168599000	-3.695645000	1.166596000
1	0.004576000	7.097838000	0.985341000
1	0.301705000	6.348714000	-1.369864000
6	2.592068000	2.522791000	0.436266000
6	5.067210000	-2.834664000	-0.477818000
6	5.375059000	-3.014320000	0.874333000
6	2.834928000	1.498897000	-0.491212000
1	3.822786000	-1.841934000	-1.913360000
6	-0.165652000	6.059177000	0.717724000
6	4.042335000	-1.962472000	-0.857521000
6	0.002561000	5.638600000	-0.604516000
1	1.881122000	2.366755000	1.238995000
6	4.654880000	-2.315189000	1.849386000
1	4.885865000	-2.450260000	2.902001000
1	-0.690632000	5.455099000	2.724140000
6	-0.555527000	5.136352000	1.694637000
6	3.308975000	-1.265386000	0.114867000
1	2.180974000	-0.198177000	-2.717843000
6	3.626647000	-1.449361000	1.470821000

6	-0.209996000	4.301104000	-0.951082000
1	-0.073359000	4.003837000	-1.984888000
1	0.642792000	1.936811000	-2.161862000
1	3.060164000	-0.925077000	2.234947000
1	0.728179000	0.603965000	-4.434177000
15	1.939642000	-0.102004000	-0.278909000
6	-0.764377000	3.798979000	1.352370000
6	1.434581000	-0.581506000	-2.016759000
6	-0.587269000	3.368316000	0.026955000
1	-1.047666000	3.088607000	2.120739000
1	1.484632000	-1.673518000	-2.075183000
1	0.361184000	-1.132067000	-4.401587000
6	-0.277555000	1.352390000	-2.075660000
6	0.038903000	-0.150074000	-4.039121000
1	-0.987660000	1.792327000	-2.779810000
6	0.022640000	-0.116796000	-2.494161000
1	-0.958979000	0.053632000	-4.442323000
15	-0.906666000	1.595525000	-0.345149000
27	-0.049191000	-0.074410000	1.028704000
1	-2.965119000	2.218405000	-2.502295000
1	2.348945000	-5.086651000	0.932411000
1	1.272589000	-2.870164000	1.119283000
6	1.475048000	-4.861855000	0.328179000
6	0.872577000	-3.603662000	0.432166000
6	-1.109266000	-1.083554000	-2.036219000
6	-3.472819000	1.911250000	-1.593778000
1	-1.085535000	-1.982253000	-2.657996000
6	-2.748054000	1.552865000	-0.446145000
1	1.425921000	-6.792212000	-0.634679000
6	0.958501000	-5.815476000	-0.551277000
1	-2.074733000	-0.599760000	-2.209597000
15	-1.040883000	-1.618627000	-0.250555000
6	-0.244275000	-3.282664000	-0.348169000
1	-5.418339000	2.150448000	-2.482069000
6	-4.869942000	1.879225000	-1.584717000
6	-0.170217000	-5.509838000	-1.322953000
6	-0.767743000	-4.252905000	-1.222595000
6	-3.448448000	1.176702000	0.711315000
1	-0.585694000	-6.250081000	-2.000337000
1	-2.906573000	0.882016000	1.604731000
1	-1.649686000	-4.040716000	-1.820472000
6	-5.558607000	1.501846000	-0.426761000
6	-2.764715000	-2.010541000	0.233270000
6	-4.844452000	1.154292000	0.722975000
1	-2.246642000	-1.872834000	2.325208000
1	-3.609447000	-2.204906000	-1.755793000

1	-6.644158000	1.472702000	-0.424064000
6	-3.038919000	-2.077639000	1.609377000
6	-3.793741000	-2.252964000	-0.687522000
1	-5.369191000	0.846653000	1.621966000
6	-4.324060000	-2.383857000	2.058489000
6	-5.082377000	-2.551534000	-0.234794000
1	-4.527046000	-2.427712000	3.124453000
1	-5.875944000	-2.728180000	-0.954788000
6	-5.349895000	-2.617528000	1.135760000
1	-6.353289000	-2.844910000	1.483329000
1	0.980631000	1.479295000	4.516199000
8	0.924273000	-0.476161000	4.023020000
6	0.761210000	0.781629000	3.703504000
8	0.399310000	1.184671000	2.591634000
1	0.682696000	-1.007430000	3.192432000
1	0.308437000	-1.303551000	1.852748000

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12-Co-triphos

1	6.729156000	0.988040000	0.339073000
1	5.543475000	1.789170000	2.375872000
6	5.650320000	1.111958000	0.328001000
6	4.983920000	1.558862000	1.473912000
1	5.427611000	0.449798000	-1.715670000
6	4.921721000	0.814724000	-0.827374000
6	3.594307000	1.711561000	1.465647000
1	3.104778000	2.067542000	2.366122000
1	0.716877000	6.524585000	1.011503000
1	0.669209000	7.110578000	-1.407419000
1	6.094810000	-3.258703000	-1.281007000
1	5.565625000	-3.062128000	1.141515000
6	3.533630000	0.959790000	-0.832767000
6	0.760114000	5.742187000	0.259410000
6	0.734600000	6.071199000	-1.099414000
6	2.855807000	1.409336000	0.311318000
1	0.864593000	4.177285000	1.719027000
6	5.104685000	-2.944753000	-0.964019000
6	0.840436000	4.404646000	0.658300000
6	4.807638000	-2.834505000	0.397789000
1	2.969008000	0.700588000	-1.723683000
6	0.790280000	5.055743000	-2.060333000
1	0.768825000	5.302538000	-3.117871000
1	4.355548000	-2.705555000	-2.975904000
6	4.127332000	-2.637426000	-1.916258000
6	0.881170000	3.380947000	-0.301050000

1	1.091085000	1.944928000	2.589508000
6	0.859821000	3.718765000	-1.662683000
6	3.535439000	-2.427915000	0.810614000
1	3.328162000	-2.349786000	1.873263000
1	1.941651000	-0.572663000	2.202809000
1	0.872766000	2.931607000	-2.410616000
1	0.868378000	0.347598000	4.363485000
15	1.026978000	1.604260000	0.162880000
6	2.860558000	-2.219445000	-1.505788000
6	0.349478000	1.535759000	1.899143000
6	2.550459000	-2.119060000	-0.139072000
1	2.119486000	-1.940776000	-2.249097000
1	-0.503278000	2.221039000	1.925047000
1	-0.759108000	1.051599000	4.285808000
6	0.934247000	-0.967879000	2.041951000
6	-0.139205000	0.210872000	3.955902000
1	0.811763000	-1.820565000	2.715803000
6	-0.100981000	0.134073000	2.412906000
1	-0.557043000	-0.709301000	4.378586000
15	0.840133000	-1.602846000	0.287754000
27	-0.027814000	0.037305000	-1.092860000
1	1.475163000	-4.096753000	1.781896000
1	-2.717717000	4.884485000	-1.268751000
1	-1.700956000	2.630757000	-1.403526000
6	-2.999006000	4.123628000	-0.546612000
6	-2.420581000	2.852431000	-0.624600000
6	-1.544731000	-0.238172000	1.943192000
6	0.514554000	-4.236614000	1.295103000
1	-2.265056000	0.245442000	2.607963000
6	-0.029702000	-3.219623000	0.490220000
1	-4.365860000	5.401066000	0.529254000
6	-3.920167000	4.412859000	0.462342000
1	-1.684112000	-1.317729000	2.063041000
15	-1.972574000	0.183404000	0.173961000
6	-2.749436000	1.858999000	0.306851000
1	0.261688000	-6.217024000	2.096783000
6	-0.169111000	-5.440188000	1.471845000
6	-4.271170000	3.420755000	1.387141000
6	-3.692955000	2.152621000	1.308146000
6	-1.259857000	-3.440455000	-0.140489000
1	-4.995601000	3.633968000	2.167874000
1	-1.692525000	-2.673843000	-0.768484000
1	-3.992256000	1.395961000	2.027605000
6	-1.405484000	-5.646322000	0.844818000
6	-3.433055000	-0.863897000	-0.216801000
6	-1.948412000	-4.645144000	0.037078000

1	-3.138052000	-0.529500000	-2.330545000
1	-3.999242000	-1.410336000	1.804713000
1	-1.936973000	-6.582870000	0.985649000
6	-3.747925000	-1.022328000	-1.577445000
6	-4.220186000	-1.511229000	0.747000000
1	-2.906105000	-4.790583000	-0.453594000
6	-4.829006000	-1.815099000	-1.968267000
6	-5.299049000	-2.309671000	0.354324000
1	-5.059312000	-1.932148000	-3.023201000
1	-5.896955000	-2.812531000	1.108884000
6	-5.604689000	-2.465191000	-1.001330000
1	-6.439662000	-3.090583000	-1.302971000
1	-0.480046000	1.186966000	-1.908532000
8	-0.164325000	-1.005719000	-2.912531000
6	-0.503905000	-2.361133000	-3.282011000
1	-1.583086000	-2.521913000	-3.204386000
1	-0.162175000	-2.562939000	-4.300557000
1	0.011227000	-3.020904000	-2.585858000
1	-0.519679000	-0.394136000	-3.570711000

-2870.788151

13-Co-triphos

1	5.917672000	-3.649514000	-0.039731000
1	4.879756000	-3.442313000	-2.292598000
6	4.890005000	-3.312649000	-0.137400000
6	4.308309000	-3.193897000	-1.403131000
1	4.594537000	-3.064099000	1.987384000
6	4.146394000	-2.988014000	1.001512000
6	2.987223000	-2.754852000	-1.532644000
1	2.559277000	-2.681727000	-2.526451000
1	-1.642983000	-6.147665000	-1.811704000
1	-2.286012000	-6.779043000	0.509048000
1	7.039413000	0.458073000	1.615649000
1	6.634971000	1.007785000	-0.777702000
6	2.832946000	-2.535524000	0.871923000
6	-1.399986000	-5.492384000	-0.980436000
6	-1.759100000	-5.847754000	0.323721000
6	2.239735000	-2.416348000	-0.395008000
1	-0.454511000	-4.043246000	-2.243188000
6	6.024280000	0.575257000	1.248182000
6	-0.727978000	-4.291197000	-1.222870000
6	5.797513000	0.885077000	-0.097273000
1	2.271613000	-2.256741000	1.759779000
6	-1.440769000	-4.997323000	1.387300000
1	-1.720636000	-5.261673000	2.402612000

1	5.105808000	0.137585000	3.153144000
6	4.940207000	0.401163000	2.112805000
6	-0.421180000	-3.425621000	-0.160344000
1	0.669174000	-2.059402000	-2.855108000
6	-0.777032000	-3.792418000	1.145863000
6	4.492982000	1.036942000	-0.574157000
1	4.343488000	1.272495000	-1.622876000
1	2.464494000	-0.100945000	-2.176656000
1	-0.560704000	-3.123028000	1.972277000
1	1.390144000	-0.455506000	-4.470480000
15	0.488074000	-1.847563000	-0.429879000
6	3.636721000	0.542691000	1.633151000
6	0.101502000	-1.399317000	-2.194477000
6	3.398804000	0.876132000	0.291975000
1	2.800206000	0.363641000	2.298525000
1	-0.951760000	-1.652866000	-2.348839000
1	-0.376683000	-0.403323000	-4.629847000
6	1.673634000	0.642824000	-2.047113000
6	0.486781000	0.082082000	-4.162468000
1	1.965725000	1.521881000	-2.628503000
6	0.344433000	0.080659000	-2.622966000
1	0.551555000	1.106540000	-4.544248000
15	1.657019000	1.126690000	-0.242287000
27	0.023868000	-0.067807000	0.885437000
1	3.099493000	3.328588000	-1.671191000
1	-4.453879000	-3.280158000	0.010137000
1	-2.543388000	-1.809066000	0.499641000
6	-4.340400000	-2.351429000	-0.541140000
6	-3.254007000	-1.515279000	-0.261023000
6	-0.857907000	1.012001000	-2.281643000
6	2.311974000	3.769571000	-1.068193000
1	-1.637670000	0.883904000	-3.037829000
6	1.474391000	2.962874000	-0.276649000
1	-6.110035000	-2.637731000	-1.741848000
6	-5.266015000	-1.990550000	-1.521976000
1	-0.512122000	2.047953000	-2.352998000
15	-1.636663000	0.787921000	-0.596045000
6	-3.077045000	-0.314908000	-0.960267000
1	2.800054000	5.766296000	-1.701921000
6	2.148137000	5.155137000	-1.084660000
6	-5.105837000	-0.784916000	-2.218660000
6	-4.021591000	0.047335000	-1.938377000
6	0.483059000	3.572813000	0.504577000
1	-5.827552000	-0.492430000	-2.975880000
1	-0.171815000	2.968590000	1.117981000
1	-3.922007000	0.986031000	-2.476566000

6	1.147624000	5.754973000	-0.308184000
6	-2.484215000	2.387360000	-0.262646000
6	0.318756000	4.961736000	0.486757000
1	-2.891837000	1.791259000	1.777719000
1	-2.257610000	3.297610000	-2.218744000
1	1.018794000	6.833196000	-0.326436000
6	-2.995817000	2.574660000	1.033574000
6	-2.636928000	3.410955000	-1.209114000
1	-0.466290000	5.413147000	1.085689000
6	-3.638807000	3.765119000	1.376811000
6	-3.278004000	4.604579000	-0.862377000
1	-4.025724000	3.896780000	2.383203000
1	-3.382718000	5.391200000	-1.603970000
6	-3.776423000	4.787186000	0.430289000
1	-4.268282000	5.717327000	0.699142000
1	-0.948446000	-1.014168000	1.519992000
8	-0.206254000	1.190452000	2.579842000
6	0.793996000	1.778197000	3.439597000
1	0.327468000	2.524964000	4.087570000
1	1.284981000	1.009861000	4.044566000
1	1.523816000	2.268767000	2.797400000
1	-0.956106000	0.907195000	3.125710000
1	-2.030271000	-0.698683000	2.435655000
8	-2.594737000	-0.263341000	3.140706000
8	-3.537496000	-2.308854000	3.351200000
6	-3.445779000	-1.145950000	3.682335000
1	-4.053899000	-0.670311000	4.463832000

-3060.555116

14-Co-triphos

1	-6.745289000	0.889680000	-0.784240000
1	-5.530018000	1.879870000	-2.717831000
6	-5.670349000	1.035592000	-0.734725000
6	-4.986904000	1.588840000	-1.823495000
1	-5.480864000	0.218053000	1.255713000
6	-4.963809000	0.663801000	0.411930000
6	-3.602569000	1.770757000	-1.766836000
1	-3.099962000	2.209871000	-2.622435000
1	-0.900968000	6.521844000	-1.383546000
1	-0.706643000	7.155407000	1.015595000
1	-6.084647000	-3.507976000	0.789731000
1	-5.463882000	-3.179381000	-1.597843000
6	-3.579625000	0.838965000	0.464042000
6	-0.881440000	5.753355000	-0.616401000
6	-0.772874000	6.109255000	0.731963000

6	-2.883795000	1.391597000	-0.621622000
1	-1.051140000	4.158925000	-2.037589000
6	-5.093324000	-3.149847000	0.528523000
6	-0.964388000	4.407634000	-0.984872000
6	-4.745305000	-2.964287000	-0.812511000
1	-3.036735000	0.521195000	1.347135000
6	-0.744757000	5.112652000	1.712916000
1	-0.655482000	5.379066000	2.761948000
1	-4.423336000	-3.003566000	2.577117000
6	-4.160981000	-2.867745000	1.532069000
6	-0.927935000	3.401743000	-0.005892000
1	-1.081158000	1.932692000	-2.857491000
6	-0.818435000	3.767539000	1.343853000
6	-3.472680000	-2.496872000	-1.152382000
1	-3.230728000	-2.362891000	-2.201252000
1	-1.937052000	-0.595327000	-2.423831000
1	-0.762893000	2.998362000	2.107086000
1	-0.896482000	0.314569000	-4.601319000
15	-1.063006000	1.615734000	-0.430440000
6	-2.891755000	-2.395622000	1.194156000
6	-0.351357000	1.523822000	-2.154579000
6	-2.535167000	-2.202845000	-0.150265000
1	-2.186618000	-2.157791000	1.981445000
1	0.503780000	2.206667000	-2.170412000
1	0.730303000	1.022616000	-4.547983000
6	-0.927080000	-0.985500000	-2.270122000
6	0.116234000	0.182842000	-4.205375000
1	-0.808003000	-1.839221000	-2.942741000
6	0.095968000	0.117701000	-2.660937000
1	0.531049000	-0.739211000	-4.626659000
15	-0.829730000	-1.615904000	-0.514743000
27	0.082039000	0.056924000	0.819272000
1	-1.149968000	-4.043469000	-2.218216000
1	2.745057000	4.927448000	0.733785000
1	1.638824000	2.730092000	0.942145000
6	3.071863000	4.101310000	0.109136000
6	2.441133000	2.858414000	0.227889000
6	1.540385000	-0.256772000	-2.209904000
6	-0.285835000	-4.192435000	-1.577080000
1	2.258727000	0.245165000	-2.863686000
6	0.101258000	-3.200780000	-0.658123000
1	4.597348000	5.239763000	-0.907486000
6	4.107061000	4.275484000	-0.811489000
1	1.679109000	-1.333458000	-2.352221000
15	1.989992000	0.136378000	-0.441277000
6	2.828329000	1.780326000	-0.577204000

1	0.122313000	-6.145218000	-2.381910000
6	0.428639000	-5.387566000	-1.666657000
6	4.515325000	3.198144000	-1.608764000
6	3.882721000	1.959815000	-1.491624000
6	1.200079000	-3.439419000	0.176541000
1	5.327802000	3.321578000	-2.318798000
1	1.518782000	-2.685717000	0.885054000
1	4.225821000	1.135034000	-2.109533000
6	1.534797000	-5.611123000	-0.835501000
6	3.393317000	-0.985807000	-0.054439000
6	1.917328000	-4.637000000	0.088552000
1	3.125010000	-0.697969000	2.077446000
1	3.931613000	-1.503749000	-2.093297000
1	2.091041000	-6.540804000	-0.910342000
6	3.705309000	-1.189567000	1.300983000
6	4.150447000	-1.638414000	-1.039187000
1	2.775529000	-4.795106000	0.734415000
6	4.754602000	-2.037596000	1.662039000
6	5.198769000	-2.487967000	-0.673388000
1	4.982042000	-2.192665000	2.712724000
1	5.773279000	-2.992926000	-1.444402000
6	5.501432000	-2.692077000	0.676056000
1	6.311546000	-3.358178000	0.957705000
1	0.640341000	1.210211000	1.562451000
8	-0.535995000	-0.682523000	2.920244000
6	0.114459000	-1.861677000	3.494417000
1	1.061080000	-1.547954000	3.935275000
1	-0.537937000	-2.312097000	4.241875000
1	0.273009000	-2.537800000	2.659022000
1	2.739521000	1.484894000	3.735633000
1	1.574679000	0.960473000	2.869103000
8	2.074182000	0.785429000	3.690883000
8	-1.161463000	-0.005917000	4.995815000
6	-1.101463000	0.176002000	3.805369000
1	-1.501269000	1.044961000	3.271339000

-3060.549348

15-Co-triphos

1	-6.434910000	2.099019000	-0.645318000
1	-5.066222000	2.897334000	-2.565046000
6	-5.351146000	2.046216000	-0.600372000
6	-4.582099000	2.491493000	-1.681577000
1	-5.308421000	1.163102000	1.369987000
6	-4.720511000	1.526135000	0.532925000
6	-3.187645000	2.417823000	-1.630236000

1	-2.615160000	2.780394000	-2.478015000
1	0.309268000	6.584502000	-1.211069000
1	0.634271000	7.139795000	1.193357000
1	-6.595554000	-2.362053000	0.790236000
1	-5.910129000	-2.132112000	-1.591044000
6	-3.327250000	1.445105000	0.579526000
6	0.197087000	5.814419000	-0.453458000
6	0.378335000	6.126580000	0.897994000
6	-2.546378000	1.887061000	-0.499420000
1	-0.268355000	4.294519000	-1.891206000
6	-5.553863000	-2.188598000	0.537137000
6	-0.128483000	4.510304000	-0.836842000
6	-5.169197000	-2.058535000	-0.800430000
1	-2.846192000	1.014296000	1.451686000
6	0.232501000	5.128314000	1.866826000
1	0.375542000	5.360842000	2.918007000
1	-4.882320000	-2.178315000	2.590279000
6	-4.592334000	-2.087232000	1.547608000
6	-0.263830000	3.500779000	0.129461000
1	-0.695543000	2.106245000	-2.740818000
6	-0.083838000	3.823263000	1.482512000
6	-3.830222000	-1.829469000	-1.129987000
1	-3.561332000	-1.732524000	-2.176488000
1	-1.958308000	-0.221058000	-2.371178000
1	-0.163380000	3.044889000	2.234615000
1	-0.738003000	0.520585000	-4.518886000
15	-0.714641000	1.771514000	-0.312519000
6	-3.256270000	-1.851137000	1.219936000
6	-0.037409000	1.579478000	-2.045421000
6	-2.860571000	-1.720625000	-0.121282000
1	-2.525462000	-1.742145000	2.012718000
1	0.917855000	2.113065000	-2.064652000
1	0.986232000	0.931993000	-4.430464000
6	-1.035996000	-0.786905000	-2.211916000
6	0.229184000	0.207832000	-4.110800000
1	-1.058745000	-1.639342000	-2.896805000
6	0.171501000	0.124734000	-2.568077000
1	0.483510000	-0.766494000	-4.541788000
15	-1.073049000	-1.449833000	-0.466504000
27	0.109874000	0.007102000	0.910484000
1	-1.915325000	-3.774841000	-2.130843000
1	3.587067000	4.347278000	1.059980000
1	2.164840000	2.331617000	1.220819000
6	3.733623000	3.529811000	0.360209000
6	2.923824000	2.393089000	0.451421000
6	1.523204000	-0.501102000	-2.100563000

6	-1.053837000	-4.078513000	-1.542924000
1	2.323702000	-0.144979000	-2.753637000
6	-0.447050000	-3.177103000	-0.649980000
1	5.340725000	4.497217000	-0.706834000
6	4.713804000	3.613660000	-0.630708000
1	1.471161000	-1.587151000	-2.229411000
15	2.003031000	-0.170258000	-0.328819000
6	3.075315000	1.333020000	-0.450881000
1	-1.039244000	-6.064335000	-2.370548000
6	-0.563414000	-5.378033000	-1.676216000
6	4.889723000	2.549050000	-1.524061000
6	4.078809000	1.416735000	-1.433657000
6	0.644709000	-3.609607000	0.113107000
1	5.658712000	2.599667000	-2.289356000
1	1.130110000	-2.930970000	0.802201000
1	4.244960000	0.598631000	-2.128188000
6	0.536431000	-5.797505000	-0.915364000
6	3.224483000	-1.473198000	0.097304000
6	1.137878000	-4.912155000	-0.018970000
1	2.928891000	-1.109615000	2.206050000
1	3.743054000	-2.090214000	-1.916913000
1	0.917318000	-6.808811000	-1.022547000
6	3.464535000	-1.696292000	1.463654000
6	3.910430000	-2.240467000	-0.855234000
1	1.992996000	-5.222777000	0.573668000
6	4.373059000	-2.674553000	1.872062000
6	4.817165000	-3.222515000	-0.444424000
1	4.546579000	-2.841729000	2.931000000
1	5.338072000	-3.817061000	-1.189182000
6	5.048470000	-3.443191000	0.916870000
1	5.748808000	-4.210824000	1.232245000
1	0.879691000	0.986243000	1.702902000
8	-0.563244000	-0.765050000	2.948440000
6	-0.112157000	-2.076620000	3.408255000
1	0.953847000	-2.031330000	3.635232000
1	-0.680550000	-2.367669000	4.291395000
1	-0.303404000	-2.752202000	2.579106000
8	-0.328398000	0.053437000	5.053388000
6	-0.629134000	0.207437000	3.895896000
1	-1.002823000	1.133232000	3.445278000

-2984.118170

16-Co-triphos

1	-6.520053000	-1.714136000	-0.980207000
1	-5.779961000	-0.179167000	-2.794713000

6	-5.585928000	-1.168651000	-0.884206000
6	-5.168178000	-0.308447000	-1.906680000
1	-5.100291000	-2.004596000	1.047755000
6	-4.794326000	-1.328022000	0.255998000
6	-3.963054000	0.388925000	-1.790860000
1	-3.667231000	1.056950000	-2.593673000
1	-3.178433000	5.769806000	-1.260377000
1	-3.401555000	6.319812000	1.156581000
1	-4.153379000	-5.622885000	0.789397000
1	-3.689267000	-5.114424000	-1.600575000
6	-3.586220000	-0.636179000	0.366183000
6	-2.926527000	5.029299000	-0.506885000
6	-3.052653000	5.337716000	0.851363000
6	-3.155884000	0.225171000	-0.653337000
1	-2.387800000	3.550502000	-1.962313000
6	-3.384603000	-4.902536000	0.525719000
6	-2.473602000	3.767207000	-0.902498000
6	-3.124686000	-4.616059000	-0.817947000
1	-2.960317000	-0.788355000	1.238402000
6	-2.723872000	4.378366000	1.815338000
1	-2.816165000	4.611621000	2.872095000
1	-2.853491000	-4.470384000	2.574927000
6	-2.654415000	-4.255528000	1.528931000
6	-2.130510000	2.805054000	0.060127000
1	-1.635707000	1.457103000	-2.818019000
6	-2.262168000	3.120453000	1.421129000
6	-2.141206000	-3.683777000	-1.162588000
1	-1.958742000	-3.476197000	-2.212060000
1	-1.495583000	-1.230399000	-2.416105000
1	-1.980501000	2.387130000	2.170985000
1	-0.804269000	0.049835000	-4.568986000
15	-1.560836000	1.115680000	-0.394872000
6	-1.676731000	-3.319480000	1.188039000
6	-0.824860000	1.332946000	-2.095565000
6	-1.415476000	-3.024081000	-0.160519000
1	-1.126062000	-2.800020000	1.966478000
1	-0.280158000	2.282253000	-2.076751000
1	0.430107000	1.320360000	-4.453381000
6	-0.414493000	-1.213457000	-2.249745000
6	0.170196000	0.304124000	-4.137983000
1	0.019431000	-1.940210000	-2.940767000
6	0.128827000	0.204178000	-2.595743000
1	0.916466000	-0.383389000	-4.550693000
15	-0.114764000	-1.772327000	-0.500941000
27	-0.026621000	0.067839000	0.887553000
1	1.103470000	-3.695156000	-2.499781000

1	0.751853000	5.566212000	0.946212000
1	0.492567000	3.107847000	1.077172000
6	1.387977000	4.925529000	0.342315000
6	1.234580000	3.536559000	0.414777000
6	1.592105000	0.394239000	-2.093949000
6	1.755926000	-3.617897000	-1.635620000
1	2.079606000	1.161060000	-2.702209000
6	1.426460000	-2.783279000	-0.554947000
1	2.470065000	6.558461000	-0.562978000
6	2.350033000	5.480595000	-0.504264000
1	2.135668000	-0.540451000	-2.262220000
15	1.803919000	0.855747000	-0.290944000
6	2.031513000	2.690091000	-0.366212000
1	3.181976000	-5.005645000	-2.455965000
6	2.933466000	-4.368867000	-1.611914000
6	3.165706000	4.641063000	-1.274776000
6	3.008400000	3.256096000	-1.205574000
6	2.283020000	-2.730425000	0.555187000
1	3.924012000	5.065190000	-1.926583000
1	2.035990000	-2.087791000	1.391898000
1	3.658008000	2.620023000	-1.800631000
6	3.788603000	-4.301763000	-0.505118000
6	3.495903000	0.275578000	0.135902000
6	3.458070000	-3.486129000	0.579738000
1	3.067519000	0.466422000	2.243078000
1	4.254072000	-0.035656000	-1.873021000
1	4.707189000	-4.881083000	-0.492356000
6	3.813893000	0.197236000	1.501742000
6	4.466068000	-0.086001000	-0.810277000
1	4.120170000	-3.419004000	1.437411000
6	5.073005000	-0.237927000	1.916697000
6	5.725558000	-0.529261000	-0.394754000
1	5.301050000	-0.298474000	2.976820000
1	6.464846000	-0.815163000	-1.137306000
6	6.031600000	-0.608470000	0.966803000
1	7.008543000	-0.959037000	1.286228000
1	-0.004079000	1.317176000	1.693065000
6	0.430353000	-0.203704000	3.599284000
8	0.363843000	-1.026293000	2.678530000
8	-0.535605000	0.048711000	4.453034000
6	-1.814627000	-0.603988000	4.216760000
1	-2.219734000	-0.251868000	3.266095000
1	-1.685296000	-1.686848000	4.196144000
1	-2.449202000	-0.299313000	5.045760000
1	1.329290000	0.375418000	3.829637000

-2984.125669

TS4-Co-triphos

Frequency = - 442.617 cm⁻¹

1	-6.484640000	-1.957489000	-1.004374000
1	-5.798105000	-0.377764000	-2.801721000
6	-5.562602000	-1.391854000	-0.908740000
6	-5.175032000	-0.506360000	-1.921606000
1	-5.040733000	-2.240567000	1.008536000
6	-4.757692000	-1.547785000	0.222271000
6	-3.986053000	0.217565000	-1.806217000
1	-3.714670000	0.904967000	-2.601182000
1	-3.248152000	5.615742000	-1.353595000
1	-3.508783000	6.183966000	1.055536000
1	-3.868875000	-5.815968000	1.047333000
1	-3.438769000	-5.396573000	-1.365701000
6	-3.566020000	-0.827958000	0.333492000
6	-2.999032000	4.884517000	-0.590335000
6	-3.146308000	5.202978000	0.763186000
6	-3.164410000	0.056083000	-0.678163000
1	-2.423803000	3.400655000	-2.025857000
6	-3.137442000	-5.071598000	0.746913000
6	-2.527238000	3.624396000	-0.969212000
6	-2.896627000	-4.835550000	-0.610227000
1	-2.936452000	-0.977268000	1.202515000
6	-2.821490000	4.255063000	1.739564000
1	-2.930152000	4.495371000	2.793018000
1	-2.623328000	-4.521558000	2.772309000
6	-2.437614000	-4.344908000	1.716917000
6	-2.188234000	2.673877000	0.006066000
1	-1.675734000	1.255429000	-2.864118000
6	-2.343507000	2.998336000	1.362775000
6	-1.961435000	-3.873237000	-1.002647000
1	-1.790961000	-3.703090000	-2.061001000
1	-1.441384000	-1.404241000	-2.357691000
1	-2.071737000	2.278505000	2.128950000
1	-0.773430000	-0.183054000	-4.563649000
15	-1.593680000	0.991831000	-0.438006000
6	-1.507569000	-3.379077000	1.329308000
6	-0.861688000	1.188872000	-2.137932000
6	-1.266975000	-3.135875000	-0.033514000
1	-0.980352000	-2.796021000	2.079888000
1	-0.352832000	2.157690000	-2.151184000
1	0.409466000	1.137743000	-4.485450000
6	-0.360885000	-1.343881000	-2.196763000

6	0.186528000	0.124350000	-4.134964000
1	0.094372000	-2.078674000	-2.864890000
6	0.135371000	0.079934000	-2.590825000
1	0.962791000	-0.548004000	-4.515845000
15	-0.036335000	-1.839775000	-0.437002000
27	-0.077762000	-0.011052000	0.914854000
1	1.347997000	-3.668008000	-2.406348000
1	0.498531000	5.478738000	1.077495000
1	0.419807000	3.011532000	1.176388000
6	1.125313000	4.894370000	0.410360000
6	1.078107000	3.497613000	0.466573000
6	1.583245000	0.352160000	-2.083454000
6	1.972703000	-3.551152000	-1.526596000
1	2.037722000	1.118723000	-2.716510000
6	1.568195000	-2.741366000	-0.452040000
1	2.002155000	6.612206000	-0.556731000
6	1.966306000	5.527907000	-0.506902000
1	2.173104000	-0.559657000	-2.215946000
15	1.765762000	0.878544000	-0.295623000
6	1.862186000	2.720214000	-0.396002000
1	3.501455000	-4.842534000	-2.316691000
6	3.194872000	-4.225216000	-1.477394000
6	2.768638000	4.759763000	-1.361394000
6	2.719424000	3.366020000	-1.304802000
6	2.395698000	-2.633921000	0.676541000
1	3.433275000	5.246596000	-2.069148000
1	2.093108000	-2.007552000	1.507647000
1	3.359866000	2.788735000	-1.965711000
6	4.020053000	-4.105550000	-0.352749000
6	3.492808000	0.412638000	0.130932000
6	3.615402000	-3.314025000	0.724628000
1	3.064587000	0.517754000	2.247602000
1	4.261352000	0.193553000	-1.886634000
1	4.973155000	-4.625177000	-0.320530000
6	3.823020000	0.333196000	1.493736000
6	4.482434000	0.140789000	-0.825886000
1	4.254016000	-3.205865000	1.595692000
6	5.115178000	-0.010178000	1.894210000
6	5.774343000	-0.212003000	-0.424509000
1	5.352333000	-0.073522000	2.952120000
1	6.528643000	-0.428079000	-1.175526000
6	6.094004000	-0.288766000	0.934295000
1	7.097082000	-0.567632000	1.243164000
1	-0.156710000	1.209505000	1.840760000
6	0.299706000	0.335438000	3.168287000
8	0.482304000	-0.824309000	2.661012000

8	-0.700103000	0.606444000	4.031672000
6	-1.855646000	-0.256345000	3.991200000
1	-2.409818000	-0.081997000	3.063980000
1	-1.561269000	-1.305128000	4.056973000
1	-2.465277000	0.029768000	4.846731000
1	1.136672000	1.013710000	3.356064000

-2984.118038

17-Co-triphos

1	-6.700103031	1.399148790	-0.938112886
1	-5.379320031	2.726889790	-2.577609886
6	-5.617996031	1.440778790	-0.857495886
6	-4.875051031	2.184649790	-1.783334886
1	-5.529773031	0.172215790	0.889449114
6	-4.964602031	0.755488790	0.169210114
6	-3.483355031	2.235691790	-1.687723886
1	-2.928169031	2.831626790	-2.405880886
1	0.089918969	6.411411790	-1.212194886
1	-0.032791031	6.975228790	1.208359114
1	-6.016036031	-3.661465210	1.032920114
1	-5.537350031	-3.282079210	-1.377543886
6	-3.571176031	0.804049790	0.263209114
6	-0.144710031	5.641299790	-0.483533886
6	-0.214858031	5.957709790	0.875923114
6	-2.818645031	1.532870790	-0.668198886
1	-0.308315031	4.112536790	-1.975208886
6	-5.043435031	-3.290410210	0.723771114
6	-0.369647031	4.330984790	-0.914593886
6	-4.775386031	-3.076525210	-0.631662886
1	-3.074369031	0.258598790	1.056532114
6	-0.517959031	4.958832790	1.807444114
1	-0.574308031	5.195412790	2.865674114
1	-4.262391031	-3.186724210	2.736334114
6	-4.058251031	-3.023506210	1.682288114
6	-0.659848031	3.322457790	0.016276114
1	-1.054930031	1.801933790	-2.906940886
6	-0.737920031	3.648982790	1.379736114
6	-3.527773031	-2.590806210	-1.034977886
1	-3.340324031	-2.428370210	-2.091227886
1	-1.945461031	-0.632565210	-2.399014886
1	-0.961850031	2.883003790	2.116051114
1	-0.787433031	0.123636790	-4.618700886
15	-0.988974031	1.585917790	-0.482772886
6	-2.812850031	-2.535640210	1.285090114
6	-0.304691031	1.427569790	-2.205775886

6	-2.543813031	-2.313944210	-0.076275886
1	-2.049388031	-2.309168210	2.025068114
1	0.559813969	2.092524790	-2.281329886
1	0.850808969	0.800474790	-4.531793886
6	-0.951384031	-1.060548210	-2.235216886
6	0.205586969	-0.009969210	-4.176440886
1	-0.868573031	-1.925084210	-2.898028886
6	0.124482969	-0.005075210	-2.633258886
1	0.617669969	-0.958350210	-4.537226886
15	-0.884589031	-1.659426210	-0.481089886
27	-0.134121031	-0.026577210	0.883917114
1	-0.578104031	-3.951412210	-2.380271886
1	2.917957969	4.596425790	1.474796114
1	1.929536969	2.341628790	1.485058114
6	3.083998969	3.935037790	0.630226114
6	2.523862969	2.655702790	0.634173114
6	1.546095969	-0.368510210	-2.102410886
6	0.117453969	-4.085942210	-1.557733886
1	2.289490969	0.077040790	-2.767535886
6	0.192294969	-3.150968210	-0.510026886
1	4.258628969	5.363633790	-0.481049886
6	3.831708969	4.365190790	-0.468689886
1	1.686208969	-1.451646210	-2.168538886
15	1.942445969	0.111410790	-0.341034886
6	2.704849969	1.787913790	-0.454068886
1	0.877737969	-5.928037210	-2.367164886
6	0.939044969	-5.214364210	-1.550922886
6	4.025305969	3.506073790	-1.556618886
6	3.470597969	2.223756790	-1.548039886
6	1.079579969	-3.375899210	0.552717114
1	4.609697969	3.832166790	-2.412041886
1	1.129404969	-2.667483210	1.370476114
1	3.646488969	1.574957790	-2.400141886
6	1.838218969	-5.423517210	-0.497698886
6	3.363352969	-0.967871210	0.097615114
6	1.901572969	-4.506941210	0.553966114
1	2.870932969	-0.892086210	2.198550114
1	4.119045969	-1.279235210	-1.913803886
1	2.482493969	-6.297799210	-0.499564886
6	3.566762969	-1.263597210	1.454632114
6	4.249050969	-1.491703210	-0.857502886
1	2.599242969	-4.657486210	1.372114114
6	4.637199969	-2.067205210	1.852622114
6	5.314818969	-2.303293210	-0.458778886
1	4.778236969	-2.293253210	2.905449114
1	5.989853969	-2.708935210	-1.206691886

6	5.511934969	-2.591882210	0.895874114
1	6.339107969	-3.225110210	1.202744114
1	0.319463766	0.949034213	2.650049024
6	0.403360149	0.022735630	3.274014032
8	0.203860969	-1.034482210	2.470240114
8	-0.467146716	0.214932338	4.353521535
6	-1.860553553	0.071113750	4.062676992
1	-2.185309650	0.829097075	3.337659326
1	-2.085351129	-0.923698903	3.670398280
1	-2.387173040	0.230013027	5.004148860
1	1.416251941	0.121729821	3.688504378

-2984.122958

18-Co-triphos

1	-6.685920000	1.871898000	-0.253451000
1	-5.558875000	2.244582000	-2.441925000
6	-5.603357000	1.824397000	-0.323805000
6	-4.970789000	2.030628000	-1.554366000
1	-5.320952000	1.369855000	1.768033000
6	-4.838084000	1.547094000	0.812243000
6	-3.578240000	1.964461000	-1.649227000
1	-3.112480000	2.141514000	-2.612746000
1	0.633890000	6.224379000	-1.692748000
1	0.181589000	7.134252000	0.580335000
1	-6.646488000	-2.360406000	1.536941000
1	-6.148023000	-2.557194000	-0.893175000
6	-3.447640000	1.469774000	0.716070000
6	0.227963000	5.581806000	-0.917065000
6	-0.026125000	6.091618000	0.358271000
6	-2.804427000	1.677222000	-0.514028000
1	0.176350000	3.873086000	-2.202638000
6	-5.635249000	-2.203027000	1.173913000
6	-0.033862000	4.238216000	-1.204164000
6	-5.355653000	-2.313993000	-0.191571000
1	-2.865205000	1.228633000	1.600611000
6	-0.551329000	5.252722000	1.348646000
1	-0.753144000	5.640679000	2.342860000
1	-4.822114000	-1.769000000	3.127485000
6	-4.611180000	-1.875348000	2.067600000
6	-0.550157000	3.391175000	-0.213193000
1	-1.146067000	1.796002000	-2.938488000
6	-0.810589000	3.911594000	1.065833000
6	-4.056271000	-2.109030000	-0.663772000
1	-3.868528000	-2.197812000	-1.728829000
1	-2.366956000	-0.549385000	-2.245555000

1	-1.198176000	3.263848000	1.842574000
1	-1.422709000	0.023045000	-4.538605000
15	-0.963506000	1.627508000	-0.518687000
6	-3.315812000	-1.661267000	1.595063000
6	-0.437312000	1.303269000	-2.268684000
6	-3.021743000	-1.785514000	0.228575000
1	-2.538481000	-1.365854000	2.289768000
1	0.519426000	1.812128000	-2.409825000
1	0.291013000	0.457774000	-4.695269000
6	-1.415186000	-1.069779000	-2.108192000
6	-0.407445000	-0.242306000	-4.224503000
1	-1.472666000	-1.999707000	-2.680663000
6	-0.275377000	-0.187877000	-2.684788000
1	-0.185927000	-1.248387000	-4.596332000
15	-1.280604000	-1.537807000	-0.305131000
27	-0.083592000	0.039713000	0.906971000
1	-2.252001000	-4.050377000	-1.542939000
1	3.274902000	4.381783000	0.260321000
1	1.984217000	2.302070000	0.675550000
6	3.402659000	3.529794000	-0.401104000
6	2.669863000	2.360408000	-0.165066000
6	1.135103000	-0.747727000	-2.331487000
6	-1.289811000	-4.257545000	-1.084686000
1	1.839507000	-0.434892000	-3.107098000
6	-0.597877000	-3.252381000	-0.384370000
1	4.841506000	4.516387000	-1.670694000
6	4.277407000	3.606564000	-1.486174000
1	1.095002000	-1.841250000	-2.365763000
15	1.838178000	-0.272325000	-0.663447000
6	2.809500000	1.258241000	-1.021041000
1	-1.296012000	-6.306550000	-1.738301000
6	-0.751670000	-5.540189000	-1.194426000
6	4.428609000	2.503664000	-2.338619000
6	3.702666000	1.335091000	-2.105038000
6	0.630004000	-3.562638000	0.215139000
1	5.113455000	2.554317000	-3.180302000
1	1.165231000	-2.810815000	0.777625000
1	3.845124000	0.484179000	-2.765327000
6	0.485338000	-5.836925000	-0.606966000
6	3.178784000	-1.507419000	-0.400969000
6	1.171419000	-4.847200000	0.098918000
1	3.235175000	-1.076722000	1.715046000
1	3.385561000	-2.195279000	-2.449752000
1	0.905547000	-6.834155000	-0.698665000
6	3.665215000	-1.660070000	0.908558000
6	3.735852000	-2.286577000	-1.427045000

1	2.130960000	-5.063000000	0.559404000
6	4.685666000	-2.571256000	1.188036000
6	4.754583000	-3.202223000	-1.146022000
1	5.047021000	-2.679122000	2.206631000
1	5.173539000	-3.801228000	-1.949447000
6	5.231077000	-3.348542000	0.160365000
1	6.019411000	-4.063531000	0.376422000
1	-0.019313000	0.954414000	3.904386000
8	2.021505000	0.741042000	4.358872000
6	3.321242000	1.230212000	4.000857000
1	3.542273000	1.020980000	2.948998000
1	3.378296000	2.312554000	4.173254000
1	4.044553000	0.721526000	4.641408000
8	0.709839000	1.251324000	2.169918000
6	0.951948000	1.286488000	3.503259000
1	0.921505000	2.386036000	3.588048000
8	0.727887000	-1.114400000	2.421141000
6	0.048331000	-1.976929000	3.352006000
1	0.784585000	-2.450153000	4.008174000
1	-0.671810000	-1.414182000	3.955774000
1	-0.467769000	-2.749423000	2.783206000
1	1.193817000	-0.346179000	2.859122000

-3099.839628

TS5-Co-triphos

Frequency = – 294.5495 cm⁻¹

1	3.714873000	-5.694397000	-0.022639000
1	2.716810000	-5.361968000	-2.278357000
6	2.954224000	-4.934525000	-0.174624000
6	2.396839000	-4.745136000	-1.443823000
1	2.972139000	-4.269901000	1.879687000
6	2.535815000	-4.138255000	0.894659000
6	1.425983000	-3.760712000	-1.645982000
1	1.003680000	-3.640191000	-2.638220000
1	-4.207833000	-4.210270000	-2.431221000
1	-5.166727000	-4.535671000	-0.157899000
1	6.673076000	-2.670370000	1.666403000
1	6.284492000	-2.447624000	-0.781662000
6	1.571477000	-3.149689000	0.691988000
6	-3.701181000	-3.802278000	-1.561560000
6	-4.238862000	-3.985268000	-0.283249000
6	1.010379000	-2.948609000	-0.579334000
1	-2.108549000	-2.963389000	-2.726623000
6	5.831923000	-2.090777000	1.297985000

6	-2.509956000	-3.091235000	-1.726497000
6	5.612899000	-1.967368000	-0.076150000
1	1.269801000	-2.522194000	1.525649000
6	-3.583878000	-3.451480000	0.830607000
1	-4.004184000	-3.580796000	1.822557000
1	5.121591000	-1.554615000	3.266894000
6	4.960878000	-1.465135000	2.196570000
6	-1.854324000	-2.551873000	-0.608847000
1	0.166944000	-1.824823000	-3.138186000
6	-2.397644000	-2.731829000	0.672487000
6	4.527412000	-1.227246000	-0.555029000
1	4.387391000	-1.148915000	-1.627013000
1	2.411768000	-0.932782000	-2.229031000
1	-1.920667000	-2.288868000	1.542220000
1	1.548214000	-0.474712000	-4.582573000
15	-0.272252000	-1.639315000	-0.741204000
6	3.873719000	-0.731982000	1.720588000
6	-0.198623000	-1.023740000	-2.491209000
6	3.642431000	-0.607497000	0.340061000
1	3.200672000	-0.262591000	2.428613000
1	-1.225985000	-0.816144000	-2.802014000
1	-0.012334000	0.345361000	-4.782922000
6	2.063663000	0.084769000	-2.030550000
6	0.932421000	0.359140000	-4.229077000
1	2.776814000	0.765428000	-2.504431000
6	0.673089000	0.245231000	-2.709129000
1	1.453656000	1.293369000	-4.463334000
15	2.176453000	0.371930000	-0.184415000
27	0.062243000	0.064258000	0.754006000
1	4.584192000	1.762678000	-1.193134000
1	-5.389671000	-0.652972000	0.300697000
1	-3.113066000	0.116258000	0.789543000
6	-4.819166000	-0.155193000	-0.477138000
6	-3.523283000	0.285166000	-0.200835000
6	-0.064066000	1.549708000	-2.277302000
6	3.966880000	2.498865000	-0.685007000
1	-0.707267000	1.883417000	-3.095641000
6	2.760880000	2.116412000	-0.069891000
1	-6.364358000	-0.335860000	-1.972900000
6	-5.361947000	0.019507000	-1.752910000
1	0.674076000	2.343115000	-2.123815000
15	-1.074919000	1.475891000	-0.716065000
6	-2.759074000	0.913769000	-1.196647000
1	5.319252000	4.116056000	-1.116840000
6	4.387209000	3.828635000	-0.639039000
6	-4.606697000	0.647181000	-2.750369000

6	-3.313056000	1.097527000	-2.473826000
6	1.994866000	3.076335000	0.605732000
1	-5.022653000	0.786479000	-3.743915000
1	1.077562000	2.777287000	1.102147000
1	-2.750392000	1.587403000	-3.262068000
6	3.609614000	4.788687000	0.022982000
6	-1.332298000	3.231771000	-0.250365000
6	2.418801000	4.409452000	0.646288000
1	-1.794282000	2.698004000	1.788692000
1	-0.897313000	4.104647000	-2.190982000
1	3.936415000	5.824052000	0.053646000
6	-1.717168000	3.507688000	1.072247000
6	-1.187131000	4.289373000	-1.161982000
1	1.811469000	5.146254000	1.163994000
6	-1.950786000	4.824531000	1.475212000
6	-1.415731000	5.606209000	-0.752335000
1	-2.242068000	5.028598000	2.501566000
1	-1.295725000	6.417967000	-1.463851000
6	-1.797463000	5.876622000	0.565744000
1	-1.972321000	6.900746000	0.882309000
1	-1.929075000	0.633261000	3.183057000
8	-3.604459000	-0.470924000	3.080749000
6	-4.443894000	-1.392298000	3.784020000
1	-3.953283000	-2.363940000	3.904990000
1	-4.710162000	-0.995642000	4.773427000
1	-5.348426000	-1.512191000	3.185259000
8	-1.554517000	-1.365269000	3.601391000
6	-2.390985000	-0.204512000	3.712551000
1	-2.546935000	0.035450000	4.777442000
8	0.028988000	1.229357000	2.174340000
6	0.945534000	1.020561000	3.218216000
1	0.498925000	1.359125000	4.165975000
1	1.223674000	-0.041091000	3.350760000
1	1.876873000	1.591363000	3.068286000
1	-0.661422148	-0.996959761	3.075339776

-3099.823040

19-Co-triphos

1	4.667339000	-5.069078000	-0.402218000
1	3.389429000	-4.924901000	-2.533573000
6	3.779127000	-4.447376000	-0.463081000
6	3.063545000	-4.363310000	-1.663213000
1	3.905882000	-3.774847000	1.584748000
6	3.351164000	-3.726008000	0.653369000
6	1.925545000	-3.558626000	-1.747645000

1	1.380591000	-3.521780000	-2.685198000
1	-4.614330000	-3.635126000	-1.195168000
1	-4.264356000	-5.429635000	0.497442000
1	7.050003000	-1.473747000	1.495579000
1	6.644880000	-1.027278000	-0.919778000
6	2.218201000	-2.913832000	0.566817000
6	-3.652030000	-3.745596000	-0.705357000
6	-3.456057000	-4.750000000	0.245719000
6	1.498036000	-2.816814000	-0.633807000
1	-2.818536000	-2.076995000	-1.746713000
6	6.099550000	-1.062641000	1.168607000
6	-2.620253000	-2.858400000	-1.024066000
6	5.871784000	-0.813144000	-0.187686000
1	1.909260000	-2.341735000	1.435396000
6	-2.212284000	-4.873011000	0.873162000
1	-2.044894000	-5.651389000	1.611369000
1	5.257986000	-0.982053000	3.156350000
6	5.094912000	-0.785155000	2.100824000
6	-1.366039000	-2.976702000	-0.405403000
1	0.261087000	-1.857372000	-3.070742000
6	-1.172751000	-3.997404000	0.548201000
6	4.648002000	-0.287960000	-0.612809000
1	4.504663000	-0.104281000	-1.671892000
1	2.415042000	-0.610326000	-2.177846000
1	-0.206399000	-4.124891000	1.026917000
1	1.430853000	-0.346946000	-4.531136000
15	-0.005862000	-1.757541000	-0.658900000
6	3.869676000	-0.268878000	1.676510000
6	-0.169662000	-1.118365000	-2.391521000
6	3.631925000	-0.012701000	0.316417000
1	3.091593000	-0.084293000	2.406818000
1	-1.231850000	-1.065729000	-2.637057000
1	-0.242802000	0.214728000	-4.708264000
6	1.904266000	0.340262000	-2.000031000
6	0.699286000	0.387166000	-4.176874000
1	2.486225000	1.113758000	-2.508056000
6	0.493918000	0.267815000	-2.649346000
1	1.061995000	1.386562000	-4.439334000
15	1.999433000	0.696089000	-0.163368000
27	0.044396000	-0.038203000	0.885865000
1	4.027291000	2.459157000	-1.431073000
1	-5.655148000	-0.736576000	0.605751000
1	-3.403322000	0.179261000	1.021548000
6	-5.054090000	-0.390445000	-0.229453000
6	-3.783019000	0.136062000	0.005737000
6	-0.410152000	1.462569000	-2.215989000

6	3.353367000	3.084789000	-0.852414000
1	-1.112740000	1.693932000	-3.020430000
6	2.299562000	2.515867000	-0.113690000
1	-6.522747000	-0.924482000	-1.720196000
6	-5.541311000	-0.497781000	-1.535913000
1	0.216593000	2.352371000	-2.099865000
15	-1.337496000	1.275490000	-0.612267000
6	-2.987967000	0.584390000	-1.062529000
1	4.368752000	4.896186000	-1.415153000
6	3.553356000	4.465564000	-0.841192000
6	-4.755006000	-0.057845000	-2.605082000
6	-3.489490000	0.490470000	-2.370017000
6	1.467016000	3.343080000	0.651668000
1	-5.123844000	-0.136717000	-3.623572000
1	0.676793000	2.891583000	1.243694000
1	-2.909187000	0.832859000	-3.219775000
6	2.704792000	5.292169000	-0.091919000
6	-1.784300000	2.997957000	-0.150253000
6	1.668809000	4.728180000	0.655349000
1	-1.934705000	2.473014000	1.934791000
1	-1.690546000	3.854481000	-2.143437000
1	2.858294000	6.367509000	-0.089959000
6	-2.062631000	3.261363000	1.200825000
6	-1.890979000	4.033788000	-1.091928000
1	1.007871000	5.360498000	1.241307000
6	-2.438814000	4.546118000	1.602056000
6	-2.259867000	5.318915000	-0.684987000
1	-2.644349000	4.743020000	2.650446000
1	-2.333379000	6.115168000	-1.420171000
6	-2.534745000	5.577759000	0.662250000
1	-2.818925000	6.577755000	0.976989000
1	-1.476495000	0.145232000	3.617628000
8	-3.270714000	-0.656376000	3.196522000
6	-3.993552000	-1.870377000	2.959558000
1	-3.795909000	-2.261842000	1.954302000
1	-3.735890000	-2.632521000	3.707238000
1	-5.053870000	-1.626956000	3.041782000
8	-1.234645000	-1.201042000	2.143557000
6	-1.894707000	-0.824301000	3.362755000
1	-1.677653000	-1.588519000	4.121508000
8	-0.011443000	1.249186000	2.258757000
6	0.935714000	1.146610000	3.285914000
1	0.542554000	1.629077000	4.195852000
1	1.171596000	0.100980000	3.558355000
1	1.886224000	1.651393000	3.036769000
1	-1.417395000	-2.127050000	1.919802000

-3099.829938

20-Co-triphos

1	-5.515554000	-4.575783000	-0.280167000
1	-4.639187000	-4.338557000	2.036733000
6	-4.568508000	-4.074022000	-0.105188000
6	-4.078103000	-3.937832000	1.197583000
1	-4.222596000	-3.638185000	-2.192426000
6	-3.841635000	-3.552469000	-1.179698000
6	-2.863979000	-3.284186000	1.428409000
1	-2.507049000	-3.194537000	2.448979000
1	2.012623000	-5.829172000	2.234032000
1	3.287834000	-6.133055000	0.118730000
1	-6.694511000	-0.887465000	-2.921837000
1	-6.892342000	-0.545595000	-0.466249000
6	-2.633748000	-2.892788000	-0.949105000
6	1.847588000	-5.157405000	1.396721000
6	2.563312000	-5.328531000	0.205598000
6	-2.132407000	-2.752351000	0.355233000
1	0.365283000	-4.009262000	2.441164000
6	-5.834171000	-0.556215000	-2.347998000
6	0.916411000	-4.122557000	1.512452000
6	-5.945873000	-0.365270000	-0.967182000
1	-2.087257000	-2.464696000	-1.784481000
6	2.348040000	-4.459478000	-0.868223000
1	2.908901000	-4.581125000	-1.789777000
1	-4.518367000	-0.475997000	-4.059198000
6	-4.612178000	-0.324637000	-2.988026000
6	0.704012000	-3.243922000	0.437180000
1	-0.889217000	-2.023263000	2.939052000
6	1.423319000	-3.417165000	-0.755565000
6	-4.840426000	0.056117000	-0.223442000
1	-4.948312000	0.203714000	0.846478000
1	-2.973123000	-0.519842000	1.842817000
1	1.291539000	-2.704428000	-1.564905000
1	-2.191551000	-0.569800000	4.316464000
15	-0.520685000	-1.880827000	0.523162000
6	-3.503302000	0.086956000	-2.246919000
6	-0.421930000	-1.280568000	2.287351000
6	-3.610360000	0.277835000	-0.859464000
1	-2.551854000	0.244070000	-2.749344000
1	0.642332000	-1.283785000	2.543249000
1	-0.514887000	-0.139226000	4.707202000
6	-2.353318000	0.380019000	1.817836000
6	-1.384874000	0.139730000	4.103406000

1	-2.921052000	1.164185000	2.323249000
6	-1.031016000	0.125140000	2.599323000
1	-1.713534000	1.136295000	4.416944000
15	-2.116476000	0.843111000	0.037549000
27	-0.177259000	0.006803000	-0.802249000
1	-3.460871000	3.012033000	1.688805000
1	4.583322000	-2.160893000	0.746567000
1	2.479206000	-1.158548000	-0.037721000
6	4.236143000	-1.235535000	1.194693000
6	3.034875000	-0.673495000	0.751878000
6	-0.017858000	1.287679000	2.364845000
6	-2.929966000	3.464651000	0.857705000
1	0.703682000	1.308738000	3.186362000
6	-2.213764000	2.678237000	-0.058188000
1	5.923170000	-1.027386000	2.522603000
6	4.987416000	-0.594582000	2.180903000
1	-0.568730000	2.232670000	2.395565000
15	0.956079000	1.235160000	0.771259000
6	2.569650000	0.525517000	1.302591000
1	-3.525139000	5.452627000	1.427435000
6	-2.973883000	4.853566000	0.708732000
6	4.539805000	0.620118000	2.720052000
6	3.337520000	1.177686000	2.284873000
6	-1.556191000	3.303864000	-1.129736000
1	5.128146000	1.131546000	3.476280000
1	-0.985365000	2.712352000	-1.838966000
1	3.007161000	2.124187000	2.703991000
6	-2.311758000	5.468648000	-0.359104000
6	1.363899000	2.971215000	0.351893000
6	-1.606067000	4.690396000	-1.280766000
1	1.907646000	2.385908000	-1.659278000
1	0.888865000	3.888385000	2.260045000
1	-2.341390000	6.548671000	-0.467900000
6	1.826066000	3.209007000	-0.954297000
6	1.246010000	4.043487000	1.247268000
1	-1.077813000	5.159825000	-2.104487000
6	2.169530000	4.500050000	-1.355664000
6	1.582962000	5.337684000	0.838499000
1	2.523144000	4.672594000	-2.367892000
1	1.480917000	6.163646000	1.536184000
6	2.044769000	5.568527000	-0.460509000
1	2.301357000	6.575633000	-0.775465000
1	-2.100339753	-1.733280254	-5.003001917
8	-0.210415333	-2.573263010	-5.114292880
6	-0.642178866	-3.771188639	-5.750494674
1	0.213072753	-4.159875051	-6.306249909

1	-0.963959587	-4.522185933	-5.013836936
1	-1.470450861	-3.581005235	-6.448604342
8	1.392371529	0.045980024	-1.708192044
6	-1.235252931	-1.958215438	-4.353343041
1	-1.546681086	-2.610983640	-3.526509974
8	-0.733665972	-0.790553591	-3.770446326
6	-0.457711210	0.262660517	-4.707334536
1	-1.373913648	0.539201844	-5.244870557
1	-0.105130670	1.112821421	-4.123450262
1	0.316532976	-0.040160937	-5.416337834
1	2.205499361	0.379106859	-1.293954728

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21-Co-triphos

1	-3.568330000	6.101212000	-0.128912000
1	-1.942232000	6.061154000	-2.015644000
6	-2.839200000	5.299577000	-0.202101000
6	-1.928292000	5.274949000	-1.266433000
1	-3.500057000	4.300711000	1.595632000
6	-2.799700000	4.293891000	0.765646000
6	-0.996140000	4.241293000	-1.367355000
1	-0.289468000	4.251755000	-2.192108000
1	4.403359000	4.201497000	-2.158942000
1	5.248556000	4.608477000	0.144992000
1	-6.852703000	2.140434000	2.037607000
1	-6.733682000	1.689523000	-0.407463000
6	-1.861972000	3.260923000	0.666025000
6	3.826887000	3.869489000	-1.300433000
6	4.300757000	4.100174000	-0.005473000
6	-0.963224000	3.214208000	-0.405896000
1	2.274677000	3.029183000	-2.516170000
6	-5.974002000	1.663536000	1.613469000
6	2.614464000	3.202360000	-1.500653000
6	-5.906735000	1.411069000	0.239424000
1	-1.827419000	2.484133000	1.418729000
6	3.551636000	3.670967000	1.095866000
1	3.912619000	3.835852000	2.106257000
1	-4.940029000	1.507538000	3.503628000
6	-4.901255000	1.306395000	2.436952000
6	1.866083000	2.757882000	-0.401157000
1	-0.175954000	2.207532000	-2.913151000
6	2.341317000	3.007062000	0.896006000
6	-4.774672000	0.801946000	-0.309996000
1	-4.748659000	0.621229000	-1.379733000
1	-2.468449000	1.233911000	-1.927756000

1	1.761192000	2.670317000	1.749292000
1	-1.671851000	1.049089000	-4.406667000
15	0.274757000	1.848071000	-0.540501000
6	-3.767586000	0.704666000	1.885959000
6	0.167258000	1.346441000	-2.334576000
6	-3.691367000	0.443625000	0.508726000
1	-2.923052000	0.466843000	2.524606000
1	1.180804000	1.118205000	-2.677353000
1	-0.121974000	0.253356000	-4.747041000
6	-2.117340000	0.197018000	-1.916730000
6	-1.048917000	0.180367000	-4.167852000
1	-2.844907000	-0.388337000	-2.486045000
6	-0.744922000	0.126342000	-2.653034000
1	-1.582152000	-0.721568000	-4.487331000
15	-2.165052000	-0.369760000	-0.130371000
27	-0.016832000	0.077010000	0.809049000
1	-4.340646000	-1.848315000	-1.622676000
1	5.264551000	0.848861000	0.250381000
1	2.921737000	0.193357000	0.660370000
6	4.729050000	0.273074000	-0.498153000
6	3.403180000	-0.099606000	-0.265289000
6	-0.010940000	-1.220570000	-2.388905000
6	-3.766632000	-2.563828000	-1.041340000
1	0.658429000	-1.440304000	-3.224917000
6	-2.686601000	-2.139668000	-0.246907000
1	6.372619000	0.224782000	-1.894561000
6	5.345366000	-0.071061000	-1.703394000
1	-0.756454000	-2.020373000	-2.365603000
15	0.952455000	-1.319267000	-0.803197000
6	2.678634000	-0.820291000	-1.225310000
1	-4.959065000	-4.226829000	-1.707867000
6	-4.125094000	-3.911982000	-1.087139000
6	4.632940000	-0.794342000	-2.668356000
6	3.309616000	-1.172776000	-2.429732000
6	-1.985787000	-3.090629000	0.509288000
1	5.108671000	-1.066430000	-3.605996000
1	-1.141765000	-2.782323000	1.114729000
1	2.782673000	-1.746072000	-3.186618000
6	-3.414450000	-4.855312000	-0.332499000
6	1.168455000	-3.122096000	-0.498863000
6	-2.347856000	-4.441355000	0.467366000
1	2.133512000	-2.737881000	1.395197000
1	0.273384000	-3.873089000	-2.327995000
1	-3.693256000	-5.904311000	-0.371996000
6	1.795754000	-3.498329000	0.700626000
6	0.756678000	-4.123394000	-1.390346000

1	-1.783398000	-5.164989000	1.047757000
6	1.997131000	-4.843587000	1.010466000
6	0.957577000	-5.472098000	-1.079896000
1	2.481047000	-5.114889000	1.944215000
1	0.627503000	-6.235810000	-1.777987000
6	1.571975000	-5.836988000	0.120835000
1	1.720816000	-6.885379000	0.361538000
1	-0.473413000	1.100245000	1.795409000
8	2.676145000	-0.640906000	3.260940000
6	3.978545000	-1.292377000	3.275164000
1	4.566322000	-0.944099000	2.424092000
1	4.492188000	-1.068632000	4.210778000
1	3.770233000	-2.357081000	3.191406000
8	3.614701000	1.364226000	3.757846000
6	2.645590000	0.682218000	3.519370000
1	1.608285000	1.040493000	3.468393000
8	0.124856000	-1.289022000	2.361728000
6	-0.805683000	-1.240746000	3.462743000
1	-0.530446000	-1.990458000	4.209624000
1	-0.825485000	-0.241602000	3.906954000
1	-1.788122000	-1.478875000	3.056398000
1	1.033069000	-1.251977000	2.718460000

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22-Co-triphos

1	-0.521651000	6.993887000	-0.075677000
1	1.455721000	6.345761000	-1.445190000
6	-0.184249000	5.961900000	-0.090152000
6	0.925577000	5.597441000	-0.863734000
1	-1.712293000	5.263576000	1.267833000
6	-0.850547000	4.995101000	0.664541000
6	1.357875000	4.271555000	-0.887608000
1	2.229789000	4.012129000	-1.481429000
1	6.221420000	2.078107000	-0.723814000
1	6.638971000	2.036647000	1.728225000
1	-5.662028000	4.507975000	1.025571000
1	-4.966701000	4.316856000	-1.355948000
6	-0.415179000	3.666013000	0.642386000
6	5.392783000	1.966656000	-0.031019000
6	5.626683000	1.943644000	1.346583000
6	0.682305000	3.288832000	-0.140355000
1	3.937250000	1.861389000	-1.600682000
6	-4.952379000	3.743189000	0.724601000
6	4.092303000	1.840917000	-0.527444000
6	-4.560348000	3.636793000	-0.613051000

1	-0.949470000	2.935040000	1.231134000
6	4.554167000	1.792894000	2.232198000
1	4.728453000	1.767060000	3.303626000
1	-4.722923000	2.934998000	2.715962000
6	-4.424769000	2.861447000	1.674356000
6	3.014490000	1.683237000	0.355476000
1	1.420383000	2.115057000	-2.554142000
6	3.256261000	1.658253000	1.739022000
6	-3.640562000	2.658626000	-1.004109000
1	-3.354298000	2.601083000	-2.048734000
1	-1.150420000	2.052985000	-2.153205000
1	2.434728000	1.519203000	2.436131000
1	0.015638000	1.529230000	-4.438469000
15	1.272227000	1.542860000	-0.200144000
6	-3.503837000	1.887337000	1.285156000
6	1.337799000	1.164660000	-2.020738000
6	-3.099114000	1.777171000	-0.055842000
1	-3.096922000	1.213634000	2.033110000
1	2.256643000	0.606317000	-2.216434000
1	1.190652000	0.200864000	-4.502292000
6	-1.232271000	0.961367000	-2.145369000
6	0.203414000	0.495257000	-4.130416000
1	-1.991078000	0.697533000	-2.887377000
6	0.135629000	0.363011000	-2.591752000
1	-0.546800000	-0.145595000	-4.605484000
15	-1.870583000	0.468266000	-0.458508000
27	0.045858000	-0.036600000	0.962481000
1	-4.033422000	-0.156166000	-2.437943000
1	5.172661000	-1.529934000	1.722015000
1	2.715217000	-1.350197000	1.580964000
6	4.680374000	-1.647832000	0.762056000
6	3.290970000	-1.549171000	0.682211000
6	0.248566000	-1.153338000	-2.261584000
6	-3.892338000	-1.021011000	-1.795748000
1	0.917896000	-1.639139000	-2.975887000
6	-2.929417000	-1.005145000	-0.770603000
1	6.515655000	-1.925895000	-0.336931000
6	5.433090000	-1.865533000	-0.395215000
1	-0.733068000	-1.613772000	-2.398695000
15	0.803124000	-1.589319000	-0.549013000
6	2.638298000	-1.679426000	-0.554056000
1	-5.428978000	-2.155831000	-2.786831000
6	-4.689610000	-2.149200000	-1.991213000
6	4.790134000	-1.994225000	-1.630594000
6	3.397757000	-1.909059000	-1.711337000
6	-2.788189000	-2.122832000	0.064879000

1	5.369772000	-2.161473000	-2.533482000
1	-2.043350000	-2.113042000	0.855837000
1	2.922298000	-2.022575000	-2.679786000
6	-4.540254000	-3.267461000	-1.158847000
6	0.316079000	-3.338374000	-0.299529000
6	-3.594537000	-3.249655000	-0.132230000
1	1.105408000	-3.358871000	1.712519000
1	-0.565961000	-3.673240000	-2.257770000
1	-5.161421000	-4.144951000	-1.313692000
6	0.629966000	-3.939380000	0.931918000
6	-0.312048000	-4.101233000	-1.295276000
1	-3.469415000	-4.114934000	0.511880000
6	0.311131000	-5.277557000	1.163214000
6	-0.629664000	-5.441989000	-1.058957000
1	0.553177000	-5.728324000	2.121068000
1	-1.120087000	-6.019152000	-1.837099000
6	-0.323529000	-6.032102000	0.169588000
1	-0.575998000	-7.072383000	0.352543000
1	-0.166104000	-0.452585000	3.867126000
6	-0.401810000	-1.453601000	3.457776000
8	-0.436440000	-1.474782000	2.078293000
8	-1.628777000	-1.899025000	4.037038000
6	-2.723680000	-1.030431000	3.769023000
1	-2.507079000	-0.005051000	4.109277000
1	-2.964617000	-1.011436000	2.700094000
1	-3.584402000	-1.411980000	4.322742000
1	0.343194000	-2.171052000	3.835319000
1	0.043913000	1.125790000	2.261357000
1	-0.712272000	0.993536000	2.108755000

-2985.282141

TS5-Co-triphos

Frequency = - 1016.784 cm⁻¹

1	-4.755025000	-5.119776000	-0.489747000
1	-5.391466000	-3.319360000	-2.088316000
6	-4.250977000	-4.158430000	-0.455202000
6	-4.606300000	-3.147331000	-1.357864000
1	-2.965918000	-4.699377000	1.194253000
6	-3.250724000	-3.923348000	0.490177000
6	-3.955553000	-1.913251000	-1.319894000
1	-4.257376000	-1.138141000	-2.018351000
1	-5.840504000	3.112462000	-1.183680000
1	-6.242510000	3.540384000	1.234523000
1	0.229850000	-7.082560000	1.315461000

1	0.011890000	-6.531602000	-1.101606000
6	-2.599301000	-2.686097000	0.526843000
6	-5.227531000	2.621272000	-0.433517000
6	-5.454324000	2.859999000	0.925686000
6	-2.934409000	-1.673854000	-0.382869000
1	-4.055030000	1.580171000	-1.895061000
6	0.358623000	-6.059206000	0.976002000
6	-4.210553000	1.749795000	-0.834530000
6	0.234857000	-5.750006000	-0.381509000
1	-1.823087000	-2.516264000	1.262360000
6	-4.658932000	2.224466000	1.885479000
1	-4.824429000	2.412053000	2.942486000
1	0.748690000	-5.277517000	2.952333000
6	0.648487000	-5.045726000	1.896234000
6	-3.405824000	1.114842000	0.124022000
1	-2.425046000	-0.137264000	-2.719544000
6	-3.637598000	1.358846000	1.488257000
6	0.392137000	-4.432508000	-0.821456000
1	0.292635000	-4.220262000	-1.880417000
1	-0.758470000	-2.176632000	-2.083677000
1	-2.993806000	0.902171000	2.233712000
1	-1.001005000	-0.988264000	-4.455376000
15	-2.053187000	-0.051098000	-0.301066000
6	0.800441000	-3.728447000	1.460306000
6	-1.661503000	0.323447000	-2.087288000
6	0.665067000	-3.410070000	0.099798000
1	1.011701000	-2.947777000	2.184577000
1	-1.753487000	1.406149000	-2.219813000
1	-0.718374000	0.761055000	-4.541539000
6	0.134718000	-1.545626000	-2.102869000
6	-0.333526000	-0.180766000	-4.136214000
1	0.816023000	-2.000382000	-2.825994000
6	-0.255728000	-0.118339000	-2.593558000
1	0.655973000	-0.361835000	-4.569439000
15	0.903999000	-1.663554000	-0.417758000
27	0.041060000	-0.065980000	0.947051000
1	2.847586000	-2.202665000	-2.692978000
1	-2.459663000	4.661193000	1.382615000
1	-1.124853000	2.577975000	1.337848000
6	-1.738894000	4.503551000	0.586060000
6	-0.990019000	3.322626000	0.561884000
6	0.836279000	0.927173000	-2.240647000
6	3.393581000	-1.864003000	-1.818795000
1	0.707648000	1.799930000	-2.885956000
6	2.724716000	-1.532081000	-0.630071000
1	-2.159821000	6.374547000	-0.401695000

6	-1.573653000	5.460385000	-0.417103000
1	1.819556000	0.505997000	-2.469636000
15	0.895937000	1.526708000	-0.476000000
6	-0.075260000	3.089452000	-0.474496000
1	5.292333000	-2.010923000	-2.820078000
6	4.784907000	-1.761046000	-1.893141000
6	-0.647481000	5.240286000	-1.445456000
6	0.100788000	4.062798000	-1.474046000
6	3.468701000	-1.108339000	0.482756000
1	-0.508525000	5.984691000	-2.223866000
1	2.964134000	-0.826220000	1.402437000
1	0.821684000	3.918180000	-2.273148000
6	5.520201000	-1.338581000	-0.780113000
6	2.631736000	2.090485000	-0.264747000
6	4.859849000	-1.017366000	0.408970000
1	2.627628000	1.721396000	1.866827000
1	3.002154000	2.537884000	-2.359964000
1	6.601021000	-1.254834000	-0.842570000
6	3.185147000	2.112363000	1.024106000
6	3.399278000	2.544591000	-1.350442000
1	5.421362000	-0.673962000	1.272057000
6	4.481676000	2.590755000	1.226199000
6	4.699019000	3.014579000	-1.145073000
1	4.900371000	2.594118000	2.228329000
1	5.284514000	3.358352000	-1.992628000
6	5.242069000	3.042355000	0.143741000
1	6.253013000	3.406824000	0.300394000
1	0.009579000	1.646777000	4.433051000
6	0.410659000	1.487328000	3.420081000
8	-0.590696000	0.926890000	2.616865000
8	1.589361000	0.697502000	3.491916000
6	1.520367000	-0.413061000	4.388867000
1	1.315555000	-0.075818000	5.413177000
1	0.751287000	-1.134509000	4.087681000
1	2.495349000	-0.903215000	4.356418000
1	0.732592000	2.445003000	2.989715000
1	-0.567103000	-0.424763000	2.478725000
1	-0.439067000	-1.221391000	2.000435000

-2985.273538

23-Co-triphos

1	-6.061830000	-2.103988000	-2.138282000
1	-5.753375000	0.216131000	-2.988383000
6	-5.190828000	-1.527191000	-1.841593000
6	-5.016419000	-0.222629000	-2.322108000

1	-4.370370000	-3.088504000	-0.594396000
6	-4.244181000	-2.079546000	-0.976132000
6	-3.896482000	0.520220000	-1.944839000
1	-3.779262000	1.532975000	-2.319866000
1	-2.743881000	5.682740000	-1.521784000
1	-3.491921000	6.063029000	0.820261000
1	-2.419228000	-6.668627000	0.290813000
1	-1.677736000	-6.031000000	-1.997255000
6	-3.126263000	-1.331996000	-0.591978000
6	-2.682205000	4.880634000	-0.792209000
6	-3.103472000	5.093332000	0.523307000
6	-2.937407000	-0.032674000	-1.077381000
1	-1.857844000	3.495521000	-2.205203000
6	-1.832143000	-5.767593000	0.140172000
6	-2.175596000	3.635629000	-1.177344000
6	-1.416982000	-5.408575000	-1.146363000
1	-2.402597000	-1.756897000	0.090901000
6	-3.017247000	4.054972000	1.457194000
1	-3.337928000	4.213846000	2.482658000
1	-1.814972000	-5.231243000	2.232638000
6	-1.492902000	-4.960648000	1.231413000
6	-2.077970000	2.594627000	-0.242407000
1	-1.316059000	0.969574000	-3.064348000
6	-2.502506000	2.813961000	1.079611000
6	-0.668135000	-4.245036000	-1.345581000
1	-0.356465000	-3.987814000	-2.352835000
1	-0.726023000	-1.554026000	-2.401918000
1	-2.418984000	2.021986000	1.818810000
1	0.038666000	-0.277602000	-4.633581000
15	-1.423798000	0.925926000	-0.634712000
6	-0.752175000	-3.793629000	1.033154000
6	-0.556223000	1.099107000	-2.287927000
6	-0.337996000	-3.423906000	-0.255691000
1	-0.515827000	-3.151678000	1.876399000
1	-0.191599000	2.127643000	-2.366687000
1	0.992594000	1.207126000	-4.450473000
6	0.329192000	-1.344516000	-2.200371000
6	0.880027000	0.175929000	-4.099125000
1	0.900183000	-2.002278000	-2.861028000
6	0.640135000	0.140096000	-2.571863000
1	1.789664000	-0.375478000	-4.360438000
15	0.627819000	-1.871692000	-0.434894000
27	0.039264000	-0.058568000	0.818521000
1	2.663940000	-2.996374000	-2.416456000
1	0.066783000	5.288553000	1.947689000
1	0.409976000	2.856063000	1.761536000

6	0.626709000	4.889864000	1.107845000
6	0.823136000	3.511995000	1.000769000
6	1.947111000	0.654462000	-1.898160000
6	3.108959000	-2.928616000	-1.429060000
1	2.339387000	1.496211000	-2.473257000
6	2.376716000	-2.435438000	-0.337414000
1	0.964049000	6.816386000	0.197358000
6	1.126149000	5.745294000	0.121988000
1	2.708240000	-0.129710000	-1.937015000
15	1.763420000	1.148827000	-0.118255000
6	1.523383000	2.972678000	-0.090568000
1	4.992826000	-3.713946000	-2.112037000
6	4.433310000	-3.341641000	-1.258947000
6	1.826987000	5.217401000	-0.967635000
6	2.029390000	3.838548000	-1.072676000
6	2.990029000	-2.370531000	0.923758000
1	2.217371000	5.876913000	-1.737072000
1	2.440638000	-1.969222000	1.770187000
1	2.584076000	3.456472000	-1.923605000
6	5.035108000	-3.276068000	0.002488000
6	3.412447000	0.920251000	0.649195000
6	4.309655000	-2.792131000	1.094956000
1	2.535294000	0.763620000	2.620401000
1	4.597274000	1.029047000	-1.163976000
1	6.066057000	-3.592409000	0.130242000
6	3.457473000	0.767693000	2.044484000
6	4.606747000	0.906042000	-0.085572000
1	4.774142000	-2.721721000	2.073399000
6	4.679965000	0.601042000	2.697259000
6	5.828653000	0.727348000	0.569046000
1	4.703573000	0.478532000	3.775999000
1	6.748570000	0.706434000	-0.007754000
6	5.867685000	0.574963000	1.958764000
1	6.818800000	0.432825000	2.463181000
1	-4.005144000	-0.263887000	1.935577000
6	-3.839751000	-0.226620000	3.023400000
8	-2.497266000	0.116739000	3.300513000
8	-4.238624000	-1.445570000	3.614060000
6	-3.636776000	-2.597920000	3.024051000
1	-3.847801000	-2.646187000	1.947545000
1	-2.550534000	-2.604725000	3.175411000
1	-4.069045000	-3.471718000	3.514967000
1	-4.470074000	0.540004000	3.478468000
1	-1.911707000	-0.267571000	2.614456000
1	-1.078342000	-0.874062000	1.390555000

-2985.288539

1-Ru-triphos

1	-1.610119000	-6.443349000	-0.489345000
1	-1.378446000	-5.500298000	1.801629000
6	-1.069022000	-5.514867000	-0.334176000
6	-0.941918000	-4.984120000	0.951706000
1	-0.595310000	-5.248232000	-2.424974000
6	-0.499314000	-4.843663000	-1.421838000
6	-0.253493000	-3.783136000	1.154614000
1	-0.163158000	-3.401490000	2.165571000
1	5.714051000	-3.107944000	1.471628000
1	6.574495000	-3.107421000	-0.864597000
1	-5.588572000	-4.432714000	-0.823351000
1	-5.699013000	-3.221402000	1.350025000
6	0.181997000	-3.643678000	-1.222308000
6	5.072962000	-2.792923000	0.653511000
6	5.555087000	-2.794485000	-0.659033000
6	0.309001000	-3.098265000	0.068841000
1	3.409495000	-2.408899000	1.946995000
6	-4.890510000	-3.627608000	-0.613525000
6	3.762082000	-2.386887000	0.921155000
6	-4.952242000	-2.947270000	0.610016000
1	0.611541000	-3.125595000	-2.076105000
6	4.719098000	-2.390482000	-1.705471000
1	5.085579000	-2.387871000	-2.727877000
1	-3.868345000	-3.801641000	-2.507953000
6	-3.927015000	-3.271636000	-1.561271000
6	2.924726000	-1.962057000	-0.123351000
1	1.163158000	-1.825501000	2.606639000
6	3.412932000	-1.974918000	-1.438394000
6	-4.053524000	-1.914139000	0.882610000
1	-4.117223000	-1.391866000	1.833657000
1	-1.454838000	-1.550968000	2.203670000
1	2.778326000	-1.629554000	-2.248622000
1	-0.207795000	-0.888781000	4.389821000
15	1.172771000	-1.474354000	0.186284000
6	-3.023122000	-2.241129000	-1.285783000
6	1.162872000	-0.938746000	1.966500000
6	-3.078130000	-1.555705000	-0.063891000
1	-2.263808000	-1.982381000	-2.018315000
1	2.125424000	-0.442669000	2.131094000
1	1.085513000	0.324849000	4.315560000
6	-1.385117000	-0.475561000	2.023542000
6	0.078324000	0.078492000	3.962803000
1	-2.119512000	-0.010810000	2.685335000

6	0.031103000	0.030086000	2.418226000
1	-0.612750000	0.837301000	4.345296000
15	-1.868388000	-0.204439000	0.244570000
44	0.123738000	-0.022781000	-1.159759000
1	-3.588738000	1.273440000	2.306024000
1	5.641827000	1.160976000	-1.055934000
1	3.223995000	0.664626000	-1.260161000
6	4.930068000	1.681952000	-0.421801000
6	3.566404000	1.391718000	-0.535305000
6	0.274228000	1.484685000	1.912484000
6	-3.633676000	1.788838000	1.352329000
1	1.022890000	1.960410000	2.550375000
6	-2.925313000	1.311956000	0.238349000
1	6.429196000	2.857274000	0.592844000
6	5.370626000	2.632056000	0.502490000
1	-0.655442000	2.046764000	2.036406000
15	0.826439000	1.666860000	0.137239000
6	2.631723000	2.038207000	0.282364000
1	-4.953054000	3.302089000	2.129855000
6	-4.416037000	2.944101000	1.256151000
6	4.439994000	3.300815000	1.308653000
6	3.079866000	3.007701000	1.199229000
6	-3.026142000	2.013493000	-0.975817000
1	4.772875000	4.051261000	2.020048000
1	-2.479220000	1.671939000	-1.850074000
1	2.374914000	3.550494000	1.823017000
6	-4.507189000	3.633653000	0.043337000
6	0.126472000	3.262782000	-0.453210000
6	-3.812318000	3.162569000	-1.074794000
1	0.642773000	2.786138000	-2.500581000
1	-0.515393000	4.057380000	1.462760000
1	-5.109878000	4.534263000	-0.027862000
6	0.188034000	3.515978000	-1.835528000
6	-0.456312000	4.218456000	0.392003000
1	-3.866189000	3.697276000	-2.018169000
6	-0.334229000	4.698647000	-2.361778000
6	-0.978486000	5.401541000	-0.138337000
1	-0.284823000	4.879946000	-3.431489000
1	-1.434021000	6.130001000	0.525851000
6	-0.922654000	5.643127000	-1.513721000
1	-1.335246000	6.560681000	-1.922641000
1	1.447057000	0.146163000	-2.107549000

-2703.915940

2-Ru-triphos

1	2.120695000	6.680727000	-1.210823000
1	0.827895000	6.544768000	0.914199000
6	1.621902000	5.756345000	-0.934970000
6	0.898008000	5.679820000	0.261207000
1	2.265077000	4.691234000	-2.697731000
6	1.701350000	4.640816000	-1.771214000
6	0.260062000	4.490772000	0.616758000
1	-0.308728000	4.449101000	1.541451000
1	-5.187200000	2.365704000	2.024097000
1	-6.036148000	3.289935000	-0.125411000
1	5.514689000	3.913542000	-0.850448000
1	4.566077000	3.800914000	1.446985000
6	1.065422000	3.447257000	-1.415387000
6	-4.513159000	2.506584000	1.184498000
6	-4.988687000	3.023216000	-0.021328000
6	0.345757000	3.361232000	-0.216365000
1	-2.830653000	1.756817000	2.267873000
6	4.859823000	3.094049000	-0.570042000
6	-3.164798000	2.156874000	1.317724000
6	4.326339000	3.031818000	0.718609000
1	1.147684000	2.594363000	-2.080063000
6	-4.109475000	3.191681000	-1.098465000
1	-4.470893000	3.593069000	-2.040707000
1	4.948823000	2.139188000	-2.506532000
6	4.540876000	2.098108000	-1.500790000
6	-2.280145000	2.317554000	0.243671000
1	0.842134000	2.216119000	2.240885000
6	-2.767936000	2.836464000	-0.967931000
6	3.476334000	1.980635000	1.081481000
1	3.084312000	1.958686000	2.092406000
1	2.311524000	0.175655000	2.813473000
1	-2.097839000	2.954135000	-1.814579000
15	-0.508448000	1.808239000	0.284572000
6	3.685504000	1.056779000	-1.143238000
6	-0.074706000	1.640004000	2.094301000
6	3.146738000	0.982907000	0.155301000
1	3.434429000	0.294289000	-1.877020000
1	-0.842472000	2.147350000	2.683567000
6	1.534691000	-0.366099000	2.265522000
1	1.602992000	-1.402566000	2.609047000
6	0.140239000	0.202960000	2.651296000
15	1.956348000	-0.392913000	0.452236000
44	0.011633000	-0.015386000	-0.937265000
1	4.511187000	-1.150485000	1.737218000
1	-5.601168000	-0.086827000	-1.766171000
1	-3.129202000	-0.057660000	-1.548116000

6	-5.129075000	-0.577177000	-0.920138000
6	-3.735866000	-0.561173000	-0.803738000
6	-1.021354000	-0.757063000	2.265391000
6	4.228340000	-1.959253000	1.068596000
1	-1.962487000	-0.306394000	2.592046000
6	3.049184000	-1.866662000	0.307785000
1	-6.991184000	-1.214894000	-0.036313000
6	-5.908723000	-1.207023000	0.052493000
1	-0.921326000	-1.687793000	2.831329000
15	-1.276574000	-1.199369000	0.461416000
6	-3.112499000	-1.174500000	0.287968000
1	5.957834000	-3.146104000	1.553878000
6	5.049742000	-3.082416000	0.961402000
6	-5.290766000	-1.828078000	1.145241000
6	-3.900062000	-1.815664000	1.261480000
6	2.711166000	-2.909382000	-0.564568000
1	-5.890087000	-2.323933000	1.903203000
1	1.799860000	-2.855836000	-1.147559000
1	-3.436017000	-2.313916000	2.108234000
6	4.705591000	-4.121571000	0.086332000
6	-0.912587000	-2.997308000	0.309630000
6	3.538707000	-4.032120000	-0.676143000
1	-2.236095000	-3.212801000	-1.392562000
1	0.474812000	-3.151533000	1.969115000
1	5.346761000	-4.994072000	0.000773000
6	-1.506743000	-3.702566000	-0.753161000
6	-0.005360000	-3.664546000	1.144188000
1	3.263804000	-4.836434000	-1.352054000
6	-1.188954000	-5.042248000	-0.980155000
6	0.303055000	-5.009548000	0.923577000
1	-1.655510000	-5.573170000	-1.804564000
1	1.009332000	-5.510343000	1.578538000
6	-0.281253000	-5.699599000	-0.141109000
1	-0.035106000	-6.742678000	-0.315357000
1	-1.252567000	0.372430000	-1.908499000
6	-0.561021000	-1.879563000	-3.343823000
8	0.414623000	-1.722210000	-2.703932000
8	-1.507994000	-2.065272000	-3.992919000
6	0.123671000	0.314120000	4.194826000
1	0.358402000	-0.650891000	4.656474000
1	0.865196000	1.044343000	4.535976000
1	-0.859598000	0.634844000	4.554591000

-2892.507823

TS1-Ru-triphos

Frequency = - 261.0818 cm⁻¹

1	0.275757000	7.021382000	-1.032437000
1	-0.931523000	6.514123000	1.085602000
6	0.038284000	5.993667000	-0.774153000
6	-0.637789000	5.709084000	0.418591000
1	0.935494000	5.166123000	-2.554067000
6	0.406825000	4.953478000	-1.630034000
6	-0.939999000	4.388458000	0.753318000
1	-1.474193000	4.183978000	1.676994000
1	-5.632291000	0.799114000	2.037224000
1	-6.685313000	1.494553000	-0.108251000
1	4.295124000	5.190929000	-0.864813000
1	3.381931000	4.858029000	1.425361000
6	0.106970000	3.629567000	-1.295889000
6	-5.016752000	1.140507000	1.210469000
6	-5.606179000	1.529074000	0.006865000
6	-0.561656000	3.337097000	-0.100054000
1	-3.199865000	0.865068000	2.303367000
6	3.877778000	4.230323000	-0.578483000
6	-3.625657000	1.177842000	1.357215000
6	3.365009000	4.043942000	0.706891000
1	0.407003000	2.837111000	-1.972256000
6	-4.799521000	1.958606000	-1.054451000
1	-5.250061000	2.262034000	-1.994777000
1	4.239977000	3.312774000	-2.500982000
6	3.845381000	3.175926000	-1.498515000
6	-2.812373000	1.602509000	0.299093000
1	0.201058000	2.308139000	2.341787000
6	-3.413419000	1.990898000	-0.910655000
6	2.818650000	2.810285000	1.076996000
1	2.429550000	2.697143000	2.082920000
1	2.167325000	0.776428000	2.826791000
1	-2.796166000	2.310693000	-1.745443000
15	-0.970767000	1.604140000	0.358207000
6	3.295107000	1.947480000	-1.133969000
6	-0.518195000	1.504844000	2.163368000
6	2.780600000	1.750664000	0.161175000
1	3.266565000	1.137060000	-1.858262000
1	-1.401070000	1.758606000	2.755033000
6	1.582423000	0.027206000	2.285525000
1	1.950908000	-0.941786000	2.632709000
6	0.084663000	0.166140000	2.676813000
15	1.974031000	0.125711000	0.471370000
44	0.032378000	0.025303000	-0.945859000
1	4.400335000	-0.523947000	2.056156000

1	-5.351213000	-1.531112000	-1.708878000
1	-3.002066000	-0.795508000	-1.486906000
6	-4.731038000	-1.946310000	-0.920547000
6	-3.402152000	-1.529415000	-0.798982000
6	-0.757823000	-1.065735000	2.239974000
6	4.390359000	-1.163612000	1.177919000
1	-1.796013000	-0.902447000	2.540814000
6	3.347845000	-1.070937000	0.239769000
1	-6.293234000	-3.199046000	-0.118896000
6	-5.259518000	-2.879268000	-0.025847000
1	-0.420936000	-1.948066000	2.791667000
15	-0.841290000	-1.528665000	0.426083000
6	-2.594129000	-2.045580000	0.219140000
1	6.226486000	-2.148146000	1.719016000
6	5.426994000	-2.079070000	0.987161000
6	-4.453663000	-3.403286000	0.993183000
6	-3.125999000	-2.992279000	1.113799000
6	3.364522000	-1.894932000	-0.894224000
1	-4.856992000	-4.133103000	1.688890000
1	2.560503000	-1.844825000	-1.618505000
1	-2.506506000	-3.416480000	1.899370000
6	5.437481000	-2.901362000	-0.146564000
6	0.064495000	-3.116515000	0.243125000
6	4.409102000	-2.804019000	-1.087127000
1	-1.062136000	-3.656244000	-1.528468000
1	1.372069000	-2.903462000	1.961009000
1	6.243959000	-3.613902000	-0.292723000
6	-0.245013000	-3.925275000	-0.865099000
6	1.104917000	-3.503725000	1.099779000
1	4.408554000	-3.443464000	-1.964773000
6	0.476871000	-5.093631000	-1.110652000
6	1.821882000	-4.677758000	0.856937000
1	0.226083000	-5.709578000	-1.968958000
1	2.626049000	-4.961679000	1.528672000
6	1.514324000	-5.471692000	-0.250427000
1	2.076870000	-6.380422000	-0.442095000
1	-1.266096000	0.152797000	-1.974470000
6	-0.541170000	-1.266420000	-3.029522000
8	0.640608000	-1.291747000	-2.776877000
8	-1.515599000	-1.597237000	-3.609450000
6	0.033803000	0.214030000	4.222314000
1	0.521386000	-0.665432000	4.655877000
1	0.546077000	1.106900000	4.596081000
1	-1.001119000	0.241561000	4.578751000

-2892.501954

3-Ru-triphos

1	7.032996000	-1.238249000	-0.951373000
1	6.682505000	-0.075253000	1.221598000
6	6.046612000	-0.871145000	-0.683845000
6	5.849836000	-0.219991000	0.539695000
1	5.116866000	-1.560689000	-2.505602000
6	4.972127000	-1.049766000	-1.558734000
6	4.581755000	0.250071000	0.885845000
1	4.446510000	0.765280000	1.832598000
1	1.583098000	5.584713000	1.652051000
1	2.294916000	6.328362000	-0.613290000
1	4.476782000	-4.919148000	-1.048766000
1	4.390083000	-3.931563000	1.232161000
6	3.700286000	-0.586319000	-1.212015000
6	1.828648000	4.852741000	0.888642000
6	2.228362000	5.269465000	-0.382969000
6	3.495758000	0.062446000	0.014018000
1	1.418359000	3.199549000	2.181914000
6	3.607694000	-4.348780000	-0.735459000
6	1.732692000	3.489956000	1.185976000
6	3.559637000	-3.795530000	0.546322000
1	2.875910000	-0.753482000	-1.897611000
6	2.538672000	4.317266000	-1.360558000
1	2.851089000	4.632789000	-2.351494000
1	2.567936000	-4.589602000	-2.614269000
6	2.536355000	-4.162398000	-1.616588000
6	2.042079000	2.529924000	0.212856000
1	2.362676000	-0.384514000	2.528699000
6	2.444390000	2.956896000	-1.066256000
6	2.448285000	-3.050749000	0.949949000
1	2.442004000	-2.625075000	1.946654000
1	0.573542000	-2.161756000	2.766597000
1	2.690671000	2.226465000	-1.832481000
15	1.837372000	0.718076000	0.450371000
6	1.423546000	-3.423259000	-1.216119000
6	1.655732000	0.408855000	2.270804000
6	1.370159000	-2.863548000	0.074201000
1	0.593773000	-3.283384000	-1.904021000
1	1.978944000	1.292889000	2.826602000
6	-0.103557000	-1.458392000	2.273732000
1	-1.105538000	-1.718120000	2.622416000
6	0.235834000	-0.014383000	2.736186000
15	-0.090999000	-1.820276000	0.444435000
44	0.066062000	0.010007000	-0.872034000
1	-0.900357000	-4.210836000	1.901997000

1	-0.856722000	5.354185000	-1.981249000
1	-0.398357000	2.981564000	-1.585896000
6	-1.326771000	4.855739000	-1.139420000
6	-1.072798000	3.499513000	-0.914340000
6	-0.849815000	1.016292000	2.309725000
6	-1.625404000	-4.058204000	1.107138000
1	-0.495435000	2.023777000	2.543003000
6	-1.500923000	-2.972963000	0.220348000
1	-2.358503000	6.620586000	-0.453622000
6	-2.166247000	5.566206000	-0.278990000
1	-1.748381000	0.867702000	2.914585000
15	-1.375057000	1.062521000	0.518235000
6	-1.662847000	2.844640000	0.174678000
1	-2.774879000	-5.791898000	1.656085000
6	-2.682658000	-4.957635000	0.967039000
6	-2.760452000	4.916879000	0.810150000
6	-2.515701000	3.561613000	1.033196000
6	-2.432655000	-2.805406000	-0.811883000
1	-3.417583000	5.462569000	1.480544000
1	-2.338999000	-1.971646000	-1.497315000
1	-2.997136000	3.063967000	1.870343000
6	-3.616862000	-4.785365000	-0.062424000
6	-3.074318000	0.361503000	0.470632000
6	-3.486301000	-3.714710000	-0.949598000
1	-3.532567000	1.371084000	-1.388807000
1	-2.973564000	-0.784867000	2.311723000
1	-4.440367000	-5.485268000	-0.169838000
6	-3.882273000	0.672310000	-0.636624000
6	-3.563622000	-0.523652000	1.441943000
1	-4.209755000	-3.574781000	-1.747110000
6	-5.146405000	0.099763000	-0.773320000
6	-4.832923000	-1.091998000	1.307383000
1	-5.757044000	0.347848000	-1.636089000
1	-5.193974000	-1.779117000	2.066367000
6	-5.623659000	-0.788215000	0.197388000
1	-6.606021000	-1.237680000	0.088636000
1	-1.727317000	1.437457000	-2.986436000
6	-1.789440000	0.370885000	-3.289401000
8	-1.237441000	-0.476882000	-2.481480000
8	-2.366330000	0.077247000	-4.341458000
6	0.254877000	-0.031619000	4.282041000
1	-0.695841000	-0.400802000	4.680130000
1	1.055344000	-0.680394000	4.652450000
1	0.421779000	0.975704000	4.677437000

-2892.527001

4-Ru-triphos

1	-2.775837000	6.385590000	0.585430000
1	-3.904291000	4.861138000	2.199750000
6	-2.572256000	5.319123000	0.559670000
6	-3.205027000	4.462996000	1.470480000
1	-1.188187000	5.453527000	-1.090590000
6	-1.684070000	4.796832000	-0.382320000
6	-2.943162000	3.092879000	1.440150000
1	-3.459375000	2.443613000	2.141350000
1	-6.163912000	-1.575096000	0.628810000
1	-6.598696000	-1.268480000	-1.801040000
1	3.062204000	6.267863000	-1.304910000
1	1.794836000	6.040449000	0.824730000
6	-1.415276000	3.424235000	-0.413220000
6	-5.441298000	-1.055868000	0.006550000
6	-5.684470000	-0.884241000	-1.358590000
6	-2.035527000	2.564488000	0.504080000
1	-4.096782000	-0.721494000	1.640660000
6	2.760974000	5.286179000	-0.951740000
6	-4.262813000	-0.570315000	0.580030000
6	2.050666000	5.159292000	0.244160000
1	-0.723552000	3.032242000	-1.148440000
6	-4.745587000	-0.218531000	-2.154530000
1	-4.928088000	-0.080643000	-3.216130000
1	3.639966000	4.232929000	-2.622410000
6	3.085187000	4.143263000	-1.693340000
6	-3.315750000	0.091215000	-0.213240000
1	-2.017089000	0.951609000	2.834820000
6	-3.567022000	0.266932000	-1.586830000
6	1.654499000	3.897658000	0.699070000
1	1.093770000	3.832332000	1.623940000
1	0.266689000	2.087403000	2.265870000
1	-2.844408000	0.782630000	-2.214930000
1	-0.337830000	0.962296000	4.577490000
15	-1.725057000	0.751172000	0.421230000
6	2.695910000	2.883849000	-1.239760000
6	-1.552191000	0.204033000	2.187930000
6	1.974471000	2.750491000	-0.040170000
1	2.959599000	2.003102000	-1.817470000
1	-2.109722000	-0.725882000	2.322730000
1	-0.791331000	-0.752928000	4.573760000
6	0.832938000	1.156469000	2.179470000
6	-0.070929000	-0.024981000	4.185900000
1	1.681307000	1.250828000	2.859920000
6	-0.079839000	-0.020131000	2.642560000

1	0.921804000	-0.288070000	4.566070000
15	1.481090000	1.050426000	0.443920000
44	-0.005860000	0.066460000	-0.945970000
1	3.625121000	0.937119000	2.545590000
1	-3.676938000	-3.827609000	-2.002980000
1	-1.625663000	-2.493487000	-1.797540000
6	-3.200880000	-3.727134000	-1.032630000
6	-2.036098000	-2.969772000	-0.911470000
6	0.463506000	-1.401115000	2.171900000
6	3.928297000	0.323742000	1.703960000
1	0.060344000	-2.188819000	2.812290000
6	3.107309000	0.185303000	0.570810000
1	-4.676887000	-4.913730000	0.002580000
6	-3.763023000	-4.334620000	0.094480000
1	1.548856000	-1.421853000	2.306690000
15	0.137030000	-1.811879000	0.392180000
6	-1.411429000	-2.813135000	0.339040000
1	5.784293000	-0.213898000	2.647640000
6	5.164114000	-0.323775000	1.763010000
6	-3.149105000	-4.185964000	1.340380000
6	-1.977073000	-3.432831000	1.462870000
6	3.559637000	-0.588802000	-0.508920000
1	-3.579150000	-4.653068000	2.221400000
1	2.945288000	-0.699859000	-1.393010000
1	-1.521194000	-3.341646000	2.442540000
6	5.600393000	-1.107680000	0.688960000
6	1.426633000	-3.032295000	-0.075920000
6	4.798854000	-1.231279000	-0.447900000
1	1.166119000	-2.638418000	-2.187650000
1	1.944640000	-3.656799000	1.938040000
1	6.558838000	-1.615730000	0.740040000
6	1.685855000	-3.230612000	-1.441650000
6	2.132871000	-3.781957000	0.876870000
1	5.124860000	-1.839625000	-1.285820000
6	2.646325000	-4.158922000	-1.847200000
6	3.098791000	-4.705267000	0.466820000
1	2.846197000	-4.297660000	-2.905590000
1	3.647367000	-5.273941000	1.211850000
6	3.358543000	-4.894494000	-0.894000000
1	4.113071000	-5.608956000	-1.209560000
1	1.115589000	1.057502000	-4.329600000
8	1.293934000	-0.269936000	-2.777590000
6	0.824532000	0.787719000	-3.303670000
8	0.025464000	1.535890000	-2.661890000

-2892.539543

5-Ru-triphos

1	3.481876269	6.170302413	-0.862696461
1	4.984127269	4.344505413	-1.644936461
6	3.164161269	5.134624413	-0.789556461
6	4.008955269	4.107590413	-1.229966461
1	1.245113269	5.603154413	0.086443539
6	1.913639269	4.819150413	-0.255956461
6	3.607009269	2.774812413	-1.132736461
1	4.282205269	1.992168413	-1.465406461
1	6.170255269	-1.821441587	-0.818956461
1	6.609386269	-1.643273587	1.622983539
1	-2.694951731	6.505274413	0.987373539
1	-2.399974731	5.967633413	-1.424506461
6	1.509572269	3.482432413	-0.163926461
6	5.461197269	-1.313197587	-0.172556461
6	5.706648269	-1.213728587	1.199023539
6	2.346557269	2.447708413	-0.599866461
1	4.132760269	-0.858360587	-1.790546461
6	-2.452966731	5.492193413	0.680783539
6	4.298450269	-0.766371587	-0.723016461
6	-2.286618731	5.190832413	-0.674376461
1	0.524311269	3.267438413	0.226823539
6	4.782851269	-0.564243587	2.025123539
1	4.964522269	-0.486014587	3.092973539
1	-2.431290731	4.708993413	2.694793539
6	-2.304272731	4.484942413	1.640033539
6	3.368354269	-0.117526587	0.099883539
1	2.121789269	0.967519413	-2.908336461
6	3.619274269	-0.020227587	1.480723539
6	-1.967375731	3.890100413	-1.073526461
1	-1.835296731	3.687810413	-2.130746461
1	-0.133714731	2.165321413	-2.368496461
1	2.904967269	0.478965413	2.129313539
1	0.467750269	1.038348413	-4.689706461
15	1.829148269	0.674611413	-0.515326461
6	-1.986098731	3.184890413	1.243783539
6	1.627785269	0.201522413	-2.304096461
6	-1.809960731	2.876190413	-0.114756461
1	-1.859112731	2.414550413	1.994513539
1	2.154760269	-0.738550587	-2.482236461
1	0.854661269	-0.692953587	-4.702696461
6	-0.724578731	1.246424413	-2.302586461
6	0.158665269	0.057559413	-4.313246461
1	-1.566448731	1.357708413	-2.990456461
6	0.151535269	0.044919413	-2.769106461

1	-0.839316731	-0.162134587	-4.706796461
15	-1.409359731	1.139448413	-0.574026461
44	0.014935269	0.070790413	0.825193539
1	-3.645995731	1.834539413	-2.373406461
1	3.485793269	-4.028347587	1.875183539
1	1.476791269	-2.633916587	1.670973539
6	3.056784269	-3.852025587	0.893803539
6	1.918389269	-3.055539587	0.773003539
6	-0.459982731	-1.315046587	-2.322636461
6	-3.958900731	0.985461413	-1.773546461
1	-0.091496731	-2.113648587	-2.970346461
6	-3.097773731	0.424346413	-0.811566461
1	4.543858269	-5.015552587	-0.151246461
6	3.650832269	-4.405138587	-0.244706461
1	-1.543931731	-1.279441587	-2.468886461
15	-0.184354731	-1.785328587	-0.550136461
6	1.356250269	-2.800416587	-0.490306461
1	-5.892130731	0.906551413	-2.710576461
6	-5.239872731	0.466507413	-1.962196461
6	3.095733269	-4.162015587	-1.502966461
6	1.952837269	-3.366219587	-1.626376461
6	-3.556708731	-0.642200587	-0.030696461
1	3.550501269	-4.586167587	-2.393186461
1	-2.916140731	-1.080334587	0.718843539
1	1.543828269	-3.201557587	-2.616856461
6	-5.683388731	-0.613439587	-1.187476461
6	-1.449491731	-3.070541587	-0.188726461
6	-4.841381731	-1.161684587	-0.219136461
1	-1.173020731	-2.893963587	1.949073539
1	-1.976153731	-3.500089587	-2.252856461
1	-6.680010731	-1.017564587	-1.337846461
6	-1.681302731	-3.423370587	1.151223539
6	-2.141214731	-3.741898587	-1.208616461
1	-5.170905731	-1.997702587	0.390073539
6	-2.605178731	-4.422395587	1.463883539
6	-3.065239731	-4.741193587	-0.889786461
1	-2.785389731	-4.678294587	2.503783539
1	-3.600052731	-5.249470587	-1.686636461
6	-3.301901731	-5.081602587	0.445183539
1	-4.024685731	-5.854088587	0.690403539
1	-2.929811269	0.498934587	2.568656461
8	-1.258457269	-0.654224413	2.466176461
6	-2.311695269	-0.254108413	3.096226461
8	-2.664567269	-0.654086413	4.211616461
8	0.328803013	1.523773624	2.547273784
6	1.237971663	2.459794055	3.174310745

1	2.262631317	2.095500906	3.067063972
1	1.141205543	3.451749273	2.722802404
1	0.962107491	2.507580442	4.225537224
1	-0.359623540	1.130187510	3.100816368

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6-Ru-triphos

1	1.782419000	6.731333000	-0.260599000
1	3.246901000	5.486888000	-1.844417000
6	1.768805000	5.645334000	-0.274507000
6	2.590592000	4.946499000	-1.168569000
1	0.298884000	5.475910000	1.296886000
6	0.937908000	4.941319000	0.599927000
6	2.569933000	3.551228000	-1.192959000
1	3.225215000	3.029386000	-1.884429000
1	6.536669000	-0.131902000	-0.789277000
1	6.875390000	-0.424900000	1.658886000
1	-3.795422000	6.024941000	0.777153000
1	-3.172423000	5.549527000	-1.587087000
6	0.912328000	3.542441000	0.580343000
6	5.707935000	0.012398000	-0.102489000
6	5.898244000	-0.150427000	1.272839000
6	1.720145000	2.840341000	-0.326335000
1	4.334495000	0.475747000	-1.676362000
6	-3.347789000	5.071580000	0.511950000
6	4.450030000	0.357070000	-0.604532000
6	-2.995835000	4.806632000	-0.814820000
1	0.268574000	2.991866000	1.261440000
6	4.824639000	0.040048000	2.148265000
1	4.961704000	-0.084492000	3.218349000
1	-3.386684000	4.302804000	2.529116000
6	-3.119990000	4.103225000	1.495185000
6	3.365344000	0.538829000	0.268026000
1	2.137914000	1.350201000	-2.699003000
6	3.567324000	0.383158000	1.648486000
6	-2.414794000	3.582448000	-1.157216000
1	-2.164428000	3.402857000	-2.196501000
1	-0.312681000	2.189339000	-2.301760000
1	2.742504000	0.519076000	2.336930000
1	0.625316000	1.328930000	-4.570652000
15	1.684322000	0.998323000	-0.327961000
6	-2.537298000	2.879173000	1.159700000
6	1.702315000	0.524322000	-2.131384000
6	-2.171764000	2.613152000	-0.170122000
1	-2.308521000	2.158228000	1.934752000

1	2.372979000	-0.331368000	-2.247514000
1	1.288142000	-0.315760000	-4.641726000
6	-0.760150000	1.190660000	-2.292610000
6	0.450101000	0.288232000	-4.278031000
1	-1.573862000	1.216977000	-3.020540000
6	0.318960000	0.166858000	-2.744116000
1	-0.462381000	-0.058554000	-4.774705000
15	-1.479834000	0.960181000	-0.597676000
44	-0.000780000	-0.018632000	0.837889000
1	-3.099619000	-0.034623000	-2.996827000
1	4.383909000	-3.250463000	1.547802000
1	2.203405000	-2.144199000	1.430451000
6	3.819553000	-3.286292000	0.621433000
6	2.576647000	-2.653771000	0.548271000
6	-0.084295000	-1.304604000	-2.432559000
6	-3.586058000	-0.330988000	-2.074979000
1	0.461525000	-1.976521000	-3.097811000
6	-3.037207000	-0.010560000	-0.823918000
1	5.311705000	-4.420760000	-0.447567000
6	4.339485000	-3.939736000	-0.498450000
1	-1.141589000	-1.440601000	-2.666275000
15	0.192898000	-1.817743000	-0.668892000
6	1.832511000	-2.666678000	-0.643495000
1	-5.188365000	-1.296694000	-3.137171000
6	-4.783191000	-1.049782000	-2.160439000
6	3.601735000	-3.971289000	-1.686492000
6	2.354399000	-3.345907000	-1.757000000
6	-3.727995000	-0.399334000	0.336186000
1	3.994161000	-4.483766000	-2.559837000
1	-3.334553000	-0.139629000	1.310693000
1	1.799753000	-3.400669000	-2.687670000
6	-5.449319000	-1.450936000	-1.000166000
6	-0.979368000	-3.200855000	-0.324084000
6	-4.921444000	-1.115327000	0.251091000
1	0.244989000	-3.933465000	1.312158000
1	-2.459320000	-2.749066000	-1.844360000
1	-6.373614000	-2.016337000	-1.069245000
6	-0.693217000	-4.037288000	0.774843000
6	-2.191262000	-3.379188000	-1.006618000
1	-5.434419000	-1.413950000	1.160251000
6	-1.601123000	-5.019962000	1.178964000
6	-3.093059000	-4.369840000	-0.605784000
1	-1.362895000	-5.651752000	2.029308000
1	-4.026469000	-4.487044000	-1.147606000
6	-2.806756000	-5.188310000	0.489041000
1	-3.513891000	-5.949734000	0.803369000

1	-1.655805000	-0.002987000	3.702921000
8	-1.385722000	-1.351823000	2.242413000
6	-1.861762000	-1.055116000	3.481005000
8	-2.427382000	-1.861314000	4.180400000
8	-0.354074000	1.358907000	2.376659000
6	0.555765000	1.449014000	3.438706000
1	1.420521000	2.096680000	3.203511000
1	0.057067000	1.884332000	4.321161000
1	0.962349000	0.468043000	3.759769000
1	-1.564720000	-2.288236000	2.013561000

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7-Ru-triphos

1	4.288868000	5.772450000	-0.070140000
1	5.593819000	3.892281000	-1.051950000
6	3.873428000	4.769220000	-0.080660000
6	4.607089000	3.712390000	-0.635700000
1	2.033178000	5.336850000	0.898100000
6	2.610108000	4.526550000	0.462420000
6	4.074839000	2.422760000	-0.652480000
1	4.663169000	1.612230000	-1.073660000
1	6.176101000	-2.452569000	0.067410000
1	6.148981000	-2.546309000	2.553400000
1	-2.087302000	6.771228000	0.585220000
1	-1.766322000	6.152708000	-1.803750000
6	2.076059000	3.233470000	0.445890000
6	5.406921000	-1.926819000	0.625160000
6	5.391441000	-1.978399000	2.021540000
6	2.797109000	2.174640000	-0.118780000
1	4.466650000	-1.180590000	-1.147980000
6	-1.860512000	5.744238000	0.314820000
6	4.429580000	-1.203590000	-0.064400000
6	-1.679492000	5.397438000	-1.028260000
1	1.094579000	3.061299000	0.865270000
6	4.394550000	-1.300350000	2.731330000
1	4.374020000	-1.338930000	3.816490000
1	-1.877522000	5.029568000	2.353010000
6	-1.744332000	4.765908000	1.307890000
6	3.423900000	-0.528530000	0.642870000
1	2.896550000	0.696210000	-2.460750000
6	3.413780000	-0.580580000	2.047770000
6	-1.386012000	4.076998000	-1.380160000
1	-1.256941000	3.829458000	-2.429010000
1	0.729679000	2.236809000	-2.307060000
1	2.628340000	-0.073790000	2.602170000

1	1.663559000	1.098069000	-4.505730000
15	2.111270000	0.462790000	-0.175730000
6	-1.443651000	3.446308000	0.961770000
6	2.174950000	0.025580000	-1.986480000
6	-1.260571000	3.094548000	-0.384850000
1	-1.311911000	2.698288000	1.737200000
1	2.567780000	-0.990650000	-2.078000000
1	1.808260000	-0.670261000	-4.543290000
6	0.033159000	1.396899000	-2.398370000
6	1.154250000	0.160679000	-4.258340000
1	-0.641101000	1.647749000	-3.220430000
6	0.821890000	0.100579000	-2.752260000
1	0.240250000	0.097549000	-4.858290000
15	-0.929661000	1.336938000	-0.815000000
44	0.100040000	0.097969000	0.774550000
1	-2.553210000	1.039808000	-3.388690000
1	2.769371000	-4.430510000	2.139100000
1	1.104501000	-2.688031000	1.667750000
6	2.457811000	-4.253310000	1.114440000
6	1.511801000	-3.264421000	0.842820000
6	-0.033740000	-1.179441000	-2.515270000
6	-3.138070000	0.696208000	-2.542600000
1	0.369711000	-2.000601000	-3.110810000
6	-2.619280000	0.726178000	-1.239530000
1	3.763432000	-5.754690000	0.277300000
6	3.017182000	-4.993830000	0.068930000
1	-1.045920000	-1.001342000	-2.885670000
15	-0.165630000	-1.681651000	-0.732240000
6	1.105091000	-3.001381000	-0.476580000
1	-4.813900000	0.186777000	-3.792690000
6	-4.429220000	0.213247000	-2.777520000
6	2.615782000	-4.745480000	-1.246530000
6	1.662161000	-3.759191000	-1.517940000
6	-3.420950000	0.278338000	-0.176410000
1	3.042812000	-5.316770000	-2.065560000
1	-3.035120000	0.283188000	0.837270000
1	1.365641000	-3.598461000	-2.548510000
6	-5.216910000	-0.236653000	-1.714690000
6	-1.740079000	-2.615312000	-0.566400000
6	-4.710740000	-0.197313000	-0.411990000
1	-1.582749000	-2.588132000	1.593440000
1	-2.211319000	-2.817802000	-2.673830000
1	-6.215850000	-0.619633000	-1.900120000
6	-2.161349000	-2.926512000	0.737790000
6	-2.512529000	-3.040082000	-1.655900000
1	-5.315080000	-0.551303000	0.417540000

6	-3.328359000	-3.662762000	0.945850000
6	-3.693329000	-3.758312000	-1.443260000
1	-3.635219000	-3.915102000	1.956870000
1	-4.290449000	-4.070913000	-2.294780000
6	-4.102009000	-4.074543000	-0.145150000
1	-5.016459000	-4.637213000	0.017150000
1	-0.202616493	-1.933098160	2.898207970
8	-1.749243270	-0.672648166	2.866358853
6	-1.110879402	-1.683820375	3.461927207
8	-1.475532274	-2.256571664	4.469525725
8	0.382330000	1.078009000	2.515080000
6	-2.989005175	-0.227492228	3.485286744
1	-3.335778581	0.589278587	2.852889032
1	-3.706212522	-1.052005134	3.499773837
1	-2.791771586	0.104727024	4.506928772
1	1.017779000	1.798829000	2.612360000

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8-Ru-triphos

1	-4.488997000	-5.026095000	0.296500000
1	-3.176007000	-4.803409000	2.401040000
6	-3.591135000	-4.415828000	0.317430000
6	-2.857135000	-4.287500000	1.500320000
1	-3.731313000	-3.838627000	-1.758300000
6	-3.165983000	-3.752559000	-0.836000000
6	-1.705982000	-3.496244000	1.531840000
1	-1.150682000	-3.430786000	2.460800000
1	4.743796000	-3.928996000	0.794200000
1	4.337561000	-5.537485000	-1.064230000
1	-6.632435000	-1.503277000	-1.707530000
1	-6.201985000	-1.436129000	0.742060000
6	-2.021890000	-2.953653000	-0.804000000
6	3.792846000	-3.932093000	0.270580000
6	3.565823000	-4.830912000	-0.774100000
6	-1.280850000	-2.810956000	0.381940000
1	3.030042000	-2.315021000	1.437280000
6	-5.712174000	-1.069690000	-1.327600000
6	2.806110000	-3.015200000	0.642240000
6	-5.470604000	-1.032471000	0.048240000
1	-1.722328000	-2.440814000	-1.711360000
6	2.339223000	-4.813748000	-1.446530000
1	2.151001000	-5.506547000	-2.261110000
1	-4.942042000	-0.574943000	-3.284640000
6	-4.762672000	-0.549634000	-2.213880000
6	1.568820000	-2.997595000	-0.018840000

1	0.153543000	-1.985871000	2.783710000
6	1.346337000	-3.906935000	-1.070640000
6	-4.283672000	-0.482745000	0.541210000
1	-4.122232000	-0.468576000	1.613700000
1	-2.055792000	-0.654563000	2.160810000
1	0.396227000	-3.918621000	-1.594660000
1	-0.793372000	-0.494957000	4.443930000
15	0.245484000	-1.774561000	0.359210000
6	-3.574670000	-0.005508000	-1.723980000
6	0.534596000	-1.219252000	2.106350000
6	-3.322160000	0.029221000	-0.341820000
1	-2.839659000	0.385360000	-2.422570000
1	1.613216000	-1.185356000	2.270540000
1	0.901680000	0.032357000	4.441230000
6	-1.543639000	0.297435000	1.998730000
6	-0.092399000	0.237600000	4.029990000
1	-2.056306000	1.046317000	2.607830000
6	-0.073019000	0.161650000	2.488140000
1	-0.402206000	1.233801000	4.362770000
15	-1.730367000	0.772306000	0.204110000
44	0.070910000	0.022670000	-1.116500000
1	-3.826622000	2.270403000	1.643030000
1	5.430156000	-1.050799000	-1.662170000
1	3.139110000	-0.130131000	-1.702420000
6	5.000158000	-0.643487000	-0.752120000
6	3.710660000	-0.110633000	-0.779800000
6	0.802705000	1.347387000	1.978940000
6	-3.241260000	2.992131000	1.080150000
1	1.632875000	1.518614000	2.667670000
6	-2.162681000	2.567307000	0.282050000
1	-0.457215000	1.450011000	-2.249680000
1	6.719446000	-1.109453000	0.467850000
6	5.722738000	-0.679260000	0.444120000
1	0.196928000	2.258219000	1.999150000
15	1.458824000	1.180245000	0.254820000
6	3.132331000	0.410989000	0.390040000
1	-4.419384000	4.655645000	1.766530000
6	-3.585055000	4.342312000	1.145970000
6	5.152439000	-0.166468000	1.612670000
6	3.868031000	0.385657000	1.585840000
6	-1.452808000	3.519195000	-0.459480000
1	5.703819000	-0.191600000	2.547810000
1	-0.619699000	3.223162000	-1.083300000
1	3.460903000	0.786868000	2.506900000
6	-2.860112000	5.288780000	0.409550000
6	1.882600000	2.885573000	-0.288790000

6	-1.797583000	4.874066000	-0.395000000
1	2.343418000	2.221032000	-2.299200000
1	1.546833000	3.884075000	1.610550000
1	-3.127478000	6.339971000	0.462130000
6	2.285921000	3.068562000	-1.622420000
6	1.841154000	3.991784000	0.572840000
1	-1.227831000	5.597804000	-0.969790000
6	2.620015000	4.339351000	-2.091830000
6	2.176878000	5.263892000	0.099600000
1	2.925175000	4.467180000	-3.125960000
1	2.132261000	6.113713000	0.774040000
6	2.560099000	5.442371000	-1.232170000
1	2.813632000	6.432610000	-1.598370000
8	1.142377000	-0.905594000	-2.594010000
1	0.258044000	1.275129000	-2.521950000
1	1.583734000	-1.720136000	-2.317470000

-2780.340523

TS2-Ru-triphos

Frequency = - 1004.1244 cm⁻¹

1	-4.089508000	5.299303000	-0.731038000
1	-3.070266000	4.891279000	1.502286000
6	-3.694572000	4.318866000	-0.482969000
6	-3.122592000	4.090709000	0.770571000
1	-4.191895000	3.451216000	-2.397638000
6	-3.749557000	3.281497000	-1.420552000
6	-2.600569000	2.833311000	1.088274000
1	-2.157234000	2.689990000	2.066734000
1	-6.116457000	-2.189702000	1.634263000
1	-6.256079000	-3.426889000	-0.520262000
1	-0.052806000	7.056821000	-0.877228000
1	1.243307000	6.443167000	1.157799000
6	-3.229740000	2.025614000	-1.106242000
6	-5.347274000	-2.057400000	0.878981000
6	-5.425541000	-2.751936000	-0.334938000
6	-2.650640000	1.789228000	0.154492000
1	-4.241214000	-0.648040000	2.062659000
6	0.149310000	6.013088000	-0.655582000
6	-4.281620000	-1.188266000	1.120894000
6	0.876198000	5.668828000	0.490668000
1	-3.275944000	1.226522000	-1.841681000
6	-4.436095000	-2.574240000	-1.305670000
1	-4.492383000	-3.112465000	-2.247346000
1	-0.894847000	5.271504000	-2.392473000

6	-0.318910000	5.012081000	-1.509612000
6	-3.280807000	-1.017528000	0.149316000
1	-2.022634000	0.743696000	2.778132000
6	-3.362426000	-1.711496000	-1.065203000
6	1.135691000	4.327952000	0.777614000
1	1.713855000	4.076270000	1.662389000
1	0.037308000	2.223174000	2.401503000
1	-2.579116000	-1.582953000	-1.805253000
1	-0.391599000	0.934996000	4.551950000
15	-1.880297000	0.137951000	0.409950000
6	-0.066620000	3.667907000	-1.221350000
6	-1.469813000	-0.013495000	2.215240000
6	0.661294000	3.316609000	-0.075976000
1	-0.466804000	2.906613000	-1.884112000
1	-1.867693000	-0.976348000	2.549381000
1	-0.401178000	-0.838035000	4.543139000
6	0.687033000	1.388635000	2.124116000
6	0.100237000	0.047768000	4.139204000
1	1.619309000	1.544869000	2.672062000
6	0.033317000	0.059604000	2.594303000
1	1.138695000	0.040736000	4.486246000
15	1.024524000	1.555866000	0.299298000
44	-0.043262000	-0.011328000	-1.027937000
1	3.344438000	0.651189000	2.069007000
1	-0.370625000	-5.736817000	-2.149526000
1	1.006373000	-3.739924000	-1.679265000
6	-0.598559000	-5.118714000	-1.286412000
6	0.174214000	-3.985955000	-1.024239000
6	0.820983000	-1.189812000	2.106320000
6	3.719444000	0.974645000	1.104779000
1	0.465908000	-2.072776000	2.645877000
6	2.857968000	1.476372000	0.120735000
1	1.247682000	-0.048388000	-2.323824000
1	-2.262315000	-6.336475000	-0.644033000
6	-1.658768000	-5.457903000	-0.437114000
1	1.871585000	-1.067994000	2.383696000
15	0.836671000	-1.609245000	0.282163000
6	-0.108138000	-3.175745000	0.091121000
1	5.744147000	0.462441000	1.623698000
6	5.091461000	0.864325000	0.854522000
6	-1.939140000	-4.661489000	0.675362000
6	-1.170301000	-3.524433000	0.935917000
6	3.392279000	1.865153000	-1.120057000
1	-2.763808000	-4.911719000	1.335525000
1	2.734374000	2.244738000	-1.897159000
1	-1.416732000	-2.918713000	1.798780000

6	5.614712000	1.255672000	-0.378703000
6	2.566857000	-2.171866000	-0.000421000
6	4.760354000	1.760168000	-1.367002000
1	2.946708000	-0.975206000	-1.754460000
1	2.515097000	-3.498829000	1.715683000
1	6.678865000	1.162976000	-0.573656000
6	3.343413000	-1.711288000	-1.068162000
6	3.110145000	-3.114813000	0.891789000
1	5.158665000	2.064971000	-2.330169000
6	4.649137000	-2.179698000	-1.243408000
6	4.414875000	-3.576951000	0.718122000
1	5.244223000	-1.804034000	-2.069955000
1	4.824537000	-4.305213000	1.411724000
6	5.187773000	-3.109992000	-0.352764000
1	6.203804000	-3.469267000	-0.486591000
8	-0.650482000	-1.263746000	-2.765215000
1	0.599929000	-0.644265000	-2.653408000
1	-0.573851000	-2.212663000	-2.589450000

-2780.326598

9-Ru-triphos

1	-5.215933000	4.649581000	0.535808000
1	-5.455779000	2.902591000	2.294433000
6	-4.587592000	3.764041000	0.512650000
6	-4.720034000	2.783512000	1.504373000
1	-3.534728000	4.351081000	-1.279188000
6	-3.647342000	3.596833000	-0.506242000
6	-3.910243000	1.646706000	1.478183000
1	-4.040845000	0.888986000	2.245600000
1	-4.314434000	-4.410486000	0.828989000
1	-5.563756000	-4.097361000	-1.301838000
1	-0.656669000	6.808009000	-1.852052000
1	-0.558187000	6.445450000	0.607542000
6	-2.833742000	2.459196000	-0.529523000
6	-4.187489000	-3.500702000	0.249995000
6	-4.887283000	-3.326043000	-0.946145000
6	-2.948498000	1.478105000	0.466330000
1	-2.774770000	-2.686305000	1.634519000
6	-0.344642000	5.846445000	-1.455312000
6	-3.309608000	-2.513294000	0.709365000
6	-0.290018000	5.642772000	-0.073126000
1	-2.104904000	2.354588000	-1.324959000
6	-4.710902000	-2.149346000	-1.683645000
1	-5.252990000	-1.998352000	-2.612586000
1	-0.033089000	4.959079000	-3.400129000

6	0.004258000	4.807675000	-2.325315000
6	-3.119945000	-1.333728000	-0.023392000
1	-2.042824000	0.176222000	2.814016000
6	-3.834513000	-1.162579000	-1.226650000
6	0.102517000	4.403685000	0.441468000
1	0.131254000	4.270460000	1.517893000
1	-0.550517000	2.180968000	2.017131000
1	-3.712141000	-0.249819000	-1.804547000
1	-0.438531000	0.992598000	4.414187000
15	-1.881755000	-0.028350000	0.380031000
6	0.397669000	3.569157000	-1.813650000
6	-1.342119000	-0.321729000	2.139130000
6	0.443021000	3.354071000	-0.425075000
1	0.664613000	2.765480000	-2.495391000
1	-1.412702000	-1.390552000	2.350486000
1	-0.078246000	-0.743672000	4.457565000
6	0.371440000	1.597060000	1.935498000
6	0.214968000	0.212087000	4.009752000
1	1.108708000	2.080823000	2.579572000
6	0.104079000	0.155268000	2.469522000
1	1.242701000	0.433350000	4.317186000
15	0.946346000	1.684431000	0.164621000
44	0.025685000	0.040579000	-1.112145000
1	2.776591000	3.182120000	2.012766000
1	-0.940487000	-5.443493000	-1.891240000
1	0.210179000	-3.264215000	-1.845709000
6	-0.729163000	-4.966762000	-0.938668000
6	-0.087578000	-3.728701000	-0.912532000
6	1.191814000	-0.844362000	1.974389000
6	3.382183000	2.643277000	1.290482000
1	1.229980000	-1.704159000	2.647409000
6	2.785173000	1.847419000	0.295981000
1	1.293939000	0.082945000	-2.153572000
1	-1.602587000	-6.551359000	0.241162000
6	-1.097002000	-5.590652000	0.258743000
1	2.170173000	-0.358905000	2.051986000
15	1.055535000	-1.449032000	0.216834000
6	0.191586000	-3.085568000	0.306020000
1	5.217591000	3.380436000	2.137212000
6	4.771351000	2.765587000	1.361000000
6	-0.806645000	-4.971411000	1.475680000
6	-0.166029000	-3.727703000	1.500440000
6	3.606438000	1.203224000	-0.638549000
1	-1.082327000	-5.448251000	2.411657000
1	3.151538000	0.600791000	-1.414956000
1	0.042491000	-3.278450000	2.464491000

6	5.584228000	2.099781000	0.435418000
6	2.767927000	-2.009276000	-0.189556000
6	4.997723000	1.324799000	-0.567978000
1	2.481404000	-1.775216000	-2.313331000
1	3.387249000	-2.366129000	1.862099000
1	6.664867000	2.189920000	0.496345000
6	3.159808000	-2.104955000	-1.532756000
6	3.664019000	-2.411052000	0.814064000
1	5.617465000	0.804777000	-1.292672000
6	4.429401000	-2.580143000	-1.868401000
6	4.938700000	-2.876059000	0.477320000
1	4.721916000	-2.641114000	-2.912660000
1	5.626835000	-3.170818000	1.264208000
6	5.325153000	-2.961326000	-0.863743000
1	6.316679000	-3.320289000	-1.123474000
8	-1.064367000	-1.167376000	-2.674612000
1	-0.558187000	-1.603025000	-3.372848000
1	-1.787078000	-1.762336000	-2.417418000

-2780.354847

10-Ru-triphos

1	6.081551000	2.887452000	0.563083000
1	4.675546000	3.509890000	2.519114000
6	5.014041000	2.688938000	0.549530000
6	4.224801000	3.035651000	1.652550000
1	5.035976000	1.802784000	-1.419126000
6	4.428640000	2.083709000	-0.564637000
6	2.852242000	2.778839000	1.642826000
1	2.257165000	3.073572000	2.501116000
1	-3.015722000	5.404133000	0.176932000
1	-1.752656000	6.750475000	-1.497047000
1	6.905190000	-1.581454000	-0.838712000
1	6.195396000	-1.101305000	1.497600000
6	3.058802000	1.811578000	-0.574420000
6	-2.042428000	5.072934000	-0.171490000
6	-1.334833000	5.825067000	-1.112224000
6	2.263144000	2.155014000	0.531002000
1	-2.093854000	3.311718000	1.037300000
6	5.849698000	-1.516566000	-0.592002000
6	-1.510227000	3.879291000	0.323965000
6	5.451762000	-1.246236000	0.719684000
1	2.614142000	1.319102000	-1.433337000
6	-0.085194000	5.379342000	-1.557407000
1	0.473415000	5.956427000	-2.288099000
1	5.182523000	-1.914136000	-2.608626000

6	4.882970000	-1.702904000	-1.586503000
6	-0.253731000	3.432218000	-0.111672000
1	0.464969000	2.059684000	2.831536000
6	0.452958000	4.190557000	-1.062798000
6	4.094675000	-1.152768000	1.040544000
1	3.819342000	-0.937415000	2.066426000
1	1.986499000	-0.021795000	2.358644000
1	1.425720000	3.863290000	-1.415227000
1	0.705128000	0.382019000	4.531633000
15	0.463071000	1.827406000	0.422415000
6	3.527852000	-1.609095000	-1.270151000
6	-0.156012000	1.490746000	2.134984000
6	3.122265000	-1.327989000	0.045130000
1	2.788565000	-1.742055000	-2.051066000
1	-1.161824000	1.905670000	2.220946000
1	-1.059468000	0.554512000	4.476590000
6	1.159866000	-0.703414000	2.143071000
6	-0.213941000	-0.034191000	4.105861000
1	1.309207000	-1.588725000	2.765449000
6	-0.165300000	-0.006696000	2.561034000
1	-0.325964000	-1.060945000	4.469476000
15	1.317616000	-1.243684000	0.364549000
44	-0.003501000	0.102666000	-0.989244000
1	2.167755000	-3.501101000	2.052954000
1	-5.034233000	2.822448000	-1.752767000
1	-3.346575000	1.035856000	-1.734528000
6	-4.697792000	2.414555000	-0.804480000
6	-3.736099000	1.404131000	-0.789512000
6	-1.421992000	-0.781226000	2.054240000
6	1.413394000	-3.872588000	1.365269000
1	-2.254071000	-0.610601000	2.741495000
6	0.829106000	-3.020306000	0.409123000
1	-5.946897000	3.709153000	0.389804000
6	-5.210702000	2.911222000	0.398416000
1	-1.212448000	-1.854411000	2.100104000
15	-1.984581000	-0.447098000	0.312295000
6	-3.277524000	0.864513000	0.425218000
1	1.497596000	-5.863028000	2.173861000
6	1.041810000	-5.215273000	1.430910000
6	-4.769484000	2.375598000	1.611240000
6	-3.814827000	1.352724000	1.626030000
6	-0.103503000	-3.542213000	-0.495795000
1	-5.165321000	2.750373000	2.550438000
1	-0.527518000	-2.907986000	-1.259893000
1	-3.499973000	0.956189000	2.584547000
6	0.086056000	-5.724534000	0.541470000

6	-2.974074000	-1.923129000	-0.151425000
6	-0.478327000	-4.888262000	-0.422805000
1	-2.598332000	-1.613625000	-2.257833000
1	-3.521375000	-2.529968000	1.860242000
1	-0.207951000	-6.768381000	0.599578000
6	-3.113491000	-2.217170000	-1.517488000
6	-3.606662000	-2.740025000	0.798796000
1	-1.217284000	-5.271819000	-1.119787000
6	-3.873493000	-3.315797000	-1.926269000
6	-4.358085000	-3.843534000	0.386157000
1	-3.968547000	-3.539662000	-2.984729000
1	-4.837473000	-4.474577000	1.128791000
6	-4.493463000	-4.133299000	-0.975793000
1	-5.075517000	-4.993313000	-1.293517000
1	0.880963000	-1.395937000	-4.346672000
8	0.095724000	-1.184792000	-2.487631000
6	0.843689000	-0.765866000	-3.443784000
8	1.496939000	0.296898000	-3.370376000
1	-0.469363000	1.388038000	-2.250029000
1	-1.142625000	1.184641000	-1.943112000

-2893.697161

TS3-Ru-triphos

Frequency = - 356.8107 cm⁻¹

1	-6.742974000	0.301456000	0.965372000
1	-5.660549000	-1.070223000	2.741255000
6	-5.711440000	-0.019216000	0.853522000
6	-5.103154000	-0.786031000	1.853681000
1	-5.446563000	0.927912000	-1.067305000
6	-4.985954000	0.329341000	-0.287329000
6	-3.774573000	-1.192923000	1.716301000
1	-3.338380000	-1.799745000	2.501989000
1	-1.382926000	-6.393274000	0.653782000
1	-2.001131000	-6.674030000	-1.739477000
1	-5.086250000	4.887874000	-0.681243000
1	-4.647709000	4.178151000	1.664144000
6	-3.654275000	-0.070774000	-0.429180000
6	-1.520426000	-5.522557000	0.019851000
6	-1.868135000	-5.679356000	-1.324886000
6	-3.033681000	-0.827286000	0.577499000
1	-1.069901000	-4.148420000	1.602744000
6	-4.219615000	4.275779000	-0.449727000
6	-1.341544000	-4.244174000	0.557137000
6	-3.975244000	3.875904000	0.866839000

1	-3.100895000	0.218213000	-1.313482000
6	-2.045135000	-4.552322000	-2.136367000
1	-2.319354000	-4.667734000	-3.180546000
1	-3.523611000	4.194198000	-2.493057000
6	-3.342529000	3.886033000	-1.467602000
6	-1.505544000	-3.113523000	-0.256623000
1	-1.370370000	-1.841635000	2.744021000
6	-1.865023000	-3.274416000	-1.606195000
6	-2.865588000	3.081143000	1.167108000
1	-2.700714000	2.791341000	2.198604000
1	-1.771660000	0.864333000	2.362957000
1	-1.997650000	-2.403409000	-2.242495000
1	-0.965453000	-0.275881000	4.530122000
15	-1.291728000	-1.397953000	0.351600000
6	-2.234936000	3.089992000	-1.172275000
6	-0.582124000	-1.520702000	2.060657000
6	-1.993526000	2.672358000	0.146374000
1	-1.577111000	2.771053000	-1.970871000
1	0.159160000	-2.325261000	2.047338000
1	0.513831000	-1.256415000	4.491661000
6	-0.705088000	1.056489000	2.221499000
6	0.062915000	-0.316655000	4.156088000
1	-0.448731000	1.869056000	2.904917000
6	0.087307000	-0.222010000	2.615536000
1	0.623850000	0.510898000	4.603041000
15	-0.501370000	1.652415000	0.474250000
44	0.027175000	-0.103660000	-0.979534000
1	0.910791000	3.309228000	2.598497000
1	2.072286000	-5.440908000	-0.534133000
1	1.073259000	-3.212805000	-0.715841000
6	2.560784000	-4.598879000	-0.053293000
6	1.992933000	-3.324180000	-0.156969000
6	1.577029000	-0.120604000	2.179613000
6	1.320122000	3.543342000	1.622053000
1	2.183723000	-0.798737000	2.785435000
6	0.849318000	2.905319000	0.465191000
1	4.185435000	-5.771447000	0.745009000
6	3.743435000	-4.782844000	0.665082000
1	1.932095000	0.893603000	2.375987000
15	1.872935000	-0.526749000	0.390625000
6	2.596674000	-2.223493000	0.462188000
1	2.693628000	4.982342000	2.441345000
6	2.333450000	4.502602000	1.536215000
6	4.360697000	-3.685798000	1.280017000
6	3.792712000	-2.415956000	1.178775000
6	1.401796000	3.254105000	-0.780380000

1	5.284548000	-3.818791000	1.834997000
1	1.054490000	2.777330000	-1.692220000
1	4.290308000	-1.573628000	1.651323000
6	2.880724000	4.839064000	0.295630000
6	3.297234000	0.489030000	-0.166702000
6	2.409460000	4.214971000	-0.863357000
1	2.989334000	-0.099109000	-2.234308000
1	3.895910000	1.273191000	1.766671000
1	3.673980000	5.577681000	0.232132000
6	3.592897000	0.481437000	-1.542283000
6	4.097558000	1.244610000	0.701756000
1	2.834554000	4.463403000	-1.830723000
6	4.668884000	1.219324000	-2.036869000
6	5.173680000	1.983160000	0.201893000
1	4.883818000	1.207956000	-3.101196000
1	5.781382000	2.570090000	0.883881000
6	5.461227000	1.973816000	-1.165192000
1	6.295114000	2.553097000	-1.550176000
1	-1.717823000	0.763963000	-4.451432000
8	0.214964000	0.281601000	-4.031508000
6	-0.963043000	0.493669000	-3.690162000
8	-1.427998000	0.427271000	-2.491403000
1	0.511161000	-1.170108000	-2.493328000
1	0.516559000	-1.677184000	-1.890412000

-2893.698455

11-Ru-triphos

1	-1.171845000	-6.658323000	-0.983177000
1	-2.760382000	-5.336050000	-2.375064000
6	-1.246622000	-5.582918000	-0.851316000
6	-2.136921000	-4.839526000	-1.637336000
1	0.228412000	-5.499384000	0.723719000
6	-0.463402000	-4.935139000	0.105231000
6	-2.229350000	-3.456964000	-1.473816000
1	-2.939458000	-2.903321000	-2.081260000
1	-6.403739000	-0.075746000	-1.266688000
1	-7.083167000	-0.448772000	1.098684000
1	4.323333000	-5.781196000	0.724992000
1	3.849517000	-5.169428000	-1.640480000
6	-0.555208000	-3.548672000	0.270131000
6	-5.659935000	-0.333908000	-0.518725000
6	-6.040982000	-0.543636000	0.808714000
6	-1.425202000	-2.794714000	-0.527371000
1	-4.052389000	-0.275495000	-1.930529000
6	3.832180000	-4.840728000	0.493123000

6	-4.316971000	-0.447302000	-0.893451000
6	3.564305000	-4.498012000	-0.835748000
1	0.052324000	-3.065563000	1.021069000
6	-5.073223000	-0.878511000	1.763518000
1	-5.360070000	-1.048299000	2.797109000
1	3.665763000	-4.227249000	2.557670000
6	3.463295000	-3.967685000	1.522543000
6	-3.340662000	-0.766497000	0.061211000
1	-1.778762000	-1.124895000	-2.762977000
6	-3.733529000	-0.989795000	1.390877000
6	2.928683000	-3.289662000	-1.137580000
1	2.736543000	-3.046268000	-2.177168000
1	0.711980000	-1.933817000	-2.287857000
1	-2.992093000	-1.240236000	2.141342000
1	-0.139796000	-0.868241000	-4.529168000
15	-1.553634000	-0.955867000	-0.345065000
6	2.822539000	-2.763367000	1.223618000
6	-1.406865000	-0.338854000	-2.100833000
6	2.546230000	-2.415179000	-0.108825000
1	2.513463000	-2.106282000	2.029527000
1	-2.084421000	0.513641000	-2.207901000
1	-0.858111000	0.754101000	-4.475432000
6	1.109560000	-0.920779000	-2.166895000
6	-0.023765000	0.140647000	-4.118818000
1	1.952484000	-0.837326000	-2.857367000
6	0.008256000	0.102193000	-2.575137000
1	0.905751000	0.565962000	-4.512599000
15	1.714016000	-0.800710000	-0.413683000
44	-0.048346000	0.033363000	1.017314000
1	3.664002000	0.201626000	-2.545814000
1	-4.872031000	3.013896000	0.833222000
1	-2.772217000	1.734496000	1.056364000
6	-4.021845000	3.266606000	0.206634000
6	-2.835417000	2.535482000	0.330786000
6	0.336393000	1.544656000	-2.085112000
6	3.910273000	0.647587000	-1.587961000
1	-0.169146000	2.263355000	-2.734283000
6	3.158366000	0.354016000	-0.440360000
1	-5.035918000	4.870469000	-0.820959000
6	-4.113746000	4.305403000	-0.721715000
1	1.409923000	1.719133000	-2.189384000
15	-0.146881000	1.890407000	-0.320592000
6	-1.731031000	2.830737000	-0.478450000
1	5.561065000	1.751716000	-2.418143000
6	4.995411000	1.526796000	-1.518578000
6	-3.007576000	4.621435000	-1.521119000

6	-1.824594000	3.891838000	-1.398277000
6	3.526005000	0.946498000	0.779790000
1	-3.065027000	5.436853000	-2.236182000
1	2.955271000	0.739921000	1.680502000
1	-0.973678000	4.165381000	-2.015559000
6	5.350779000	2.112123000	-0.299745000
6	1.018396000	3.174169000	0.289068000
6	4.616201000	1.814743000	0.851733000
1	0.373250000	2.859295000	2.330923000
1	1.886629000	3.739664000	-1.617957000
1	6.189966000	2.799490000	-0.249076000
6	1.033512000	3.419765000	1.673663000
6	1.872948000	3.907443000	-0.546521000
1	4.877214000	2.272235000	1.801011000
6	1.894136000	4.377997000	2.211691000
6	2.734343000	4.865226000	-0.004317000
1	1.899841000	4.555860000	3.283094000
1	3.398108000	5.420395000	-0.660421000
6	2.749120000	5.101459000	1.373110000
1	3.423737000	5.842663000	1.791234000
1	-0.277106000	-2.224736000	4.467198000
8	-1.259322000	-0.530673000	3.979053000
6	-0.414126000	-1.479755000	3.677785000
8	0.193509000	-1.567079000	2.602640000
1	-1.305154000	0.091427000	3.156550000
1	-1.252628000	0.734342000	1.944680000

-2893.696658

12-Ru-triphos

1	3.235515000	5.835626000	-0.010769000
1	2.173521000	5.305759000	2.177848000
6	2.474430000	5.063834000	0.054168000
6	1.880981000	4.764308000	1.282926000
1	2.551017000	4.577966000	-2.048278000
6	2.089473000	4.359376000	-1.090286000
6	0.912048000	3.760206000	1.371122000
1	0.471171000	3.552687000	2.339717000
1	-4.808491000	4.431736000	1.236536000
1	-5.410368000	4.727913000	-1.161019000
1	6.189124000	3.044427000	-1.345307000
1	5.635500000	2.959014000	1.078132000
6	1.123807000	3.356402000	-1.002319000
6	-4.194550000	3.984594000	0.460131000
6	-4.531384000	4.152187000	-0.886372000
6	0.527416000	3.039595000	0.230669000

1	-2.820819000	3.136077000	1.867862000
6	5.369121000	2.424283000	-0.995315000
6	-3.065104000	3.240664000	0.815986000
6	5.058587000	2.375878000	0.366251000
1	0.843449000	2.814428000	-1.901294000
6	-3.731478000	3.573550000	-1.877919000
1	-3.986285000	3.697522000	-2.926532000
1	4.838447000	1.722264000	-2.968346000
6	4.611952000	1.680456000	-1.906845000
6	-2.270200000	2.642180000	-0.173753000
1	-0.793105000	2.064359000	2.667894000
6	-2.609619000	2.822222000	-1.522979000
6	4.003157000	1.579323000	0.821475000
1	3.785032000	1.554461000	1.884382000
1	1.664650000	1.220653000	2.316447000
1	-2.010806000	2.346628000	-2.293460000
1	0.271620000	0.842041000	4.477695000
15	-0.742759000	1.693613000	0.238988000
6	3.550317000	0.895347000	-1.455416000
6	-0.977906000	1.206610000	2.017355000
6	3.240922000	0.828752000	-0.084903000
1	2.950625000	0.343379000	-2.174830000
1	-2.037397000	0.957655000	2.135195000
1	-1.264949000	-0.038670000	4.362772000
6	1.385722000	0.177920000	2.141425000
6	-0.218335000	-0.034292000	4.039430000
1	1.990186000	-0.433851000	2.817454000
6	-0.122262000	0.000079000	2.497815000
1	0.267536000	-0.931725000	4.437241000
15	1.846533000	-0.275852000	0.385434000
44	-0.080355000	-0.041105000	-1.088564000
1	4.461679000	-1.055272000	1.592351000
1	-5.652136000	0.609968000	-1.299903000
1	-3.229259000	0.127987000	-1.455186000
6	-5.169069000	0.027610000	-0.520831000
6	-3.800669000	-0.241841000	-0.612607000
6	-0.696431000	-1.354614000	1.971533000
6	3.956432000	-1.964818000	1.281183000
1	-1.494309000	-1.680930000	2.642182000
6	2.706486000	-1.896531000	0.640594000
1	-6.965093000	-0.216435000	0.651909000
6	-5.903754000	-0.433409000	0.573957000
1	0.084177000	-2.119595000	2.024275000
15	-1.338993000	-1.349434000	0.221603000
6	-3.146796000	-0.973326000	0.388377000
1	5.531791000	-3.237200000	2.010318000

6	4.564887000	-3.199476000	1.516766000
6	-5.264679000	-1.180397000	1.570503000
6	-3.898175000	-1.453049000	1.476554000
6	2.087927000	-3.087142000	0.238022000
1	-5.828174000	-1.552117000	2.421318000
1	1.132295000	-3.057257000	-0.268900000
1	-3.436008000	-2.047742000	2.257435000
6	3.932337000	-4.384370000	1.119039000
6	-1.380502000	-3.126629000	-0.266773000
6	2.691807000	-4.325536000	0.479260000
1	-1.527891000	-2.625654000	-2.360188000
1	-1.263790000	-3.971998000	1.729918000
1	4.406660000	-5.343608000	1.304600000
6	-1.477631000	-3.431144000	-1.634263000
6	-1.332491000	-4.174396000	0.666490000
1	2.190490000	-5.235940000	0.163823000
6	-1.507913000	-4.759421000	-2.064230000
6	-1.360945000	-5.503388000	0.234131000
1	-1.577865000	-4.981032000	-3.125090000
1	-1.314709000	-6.305570000	0.964750000
6	-1.443401000	-5.799248000	-1.130187000
1	-1.459211000	-6.832805000	-1.462964000
1	-1.352550000	0.184717000	-2.093394000
8	0.770047000	-1.148934000	-2.860527000
6	1.696066000	-2.247527000	-3.013433000
1	1.205350000	-3.197251000	-2.781681000
1	2.088295000	-2.259794000	-4.033830000
1	2.506984000	-2.076024000	-2.307623000
1	0.098133000	-1.190552000	-3.553179000

-2819.627406

13-Ru-triphos

1	4.006560000	-5.522564000	0.582558000
1	3.271147000	-5.162193000	-1.768617000
6	3.203285000	-4.825713000	0.362767000
6	2.791573000	-4.622443000	-0.957345000
1	2.902690000	-4.262989000	2.425793000
6	2.581282000	-4.121518000	1.398423000
6	1.761041000	-3.721609000	-1.243014000
1	1.459740000	-3.591174000	-2.276631000
1	-3.808273000	-5.029488000	-1.910866000
1	-4.751004000	-5.290543000	0.378630000
1	6.632691000	-2.135521000	1.899037000
1	6.469333000	-1.882461000	-0.571546000
6	1.558383000	-3.216356000	1.113266000

6	-3.371728000	-4.489777000	-1.075558000
6	-3.899492000	-4.637777000	0.210606000
6	1.135506000	-3.006932000	-0.210713000
1	-1.886725000	-3.553359000	-2.302309000
6	5.766711000	-1.651888000	1.456847000
6	-2.280378000	-3.643921000	-1.295521000
6	5.675126000	-1.509536000	0.068591000
1	1.098289000	-2.666578000	1.930678000
6	-3.326969000	-3.939622000	1.279180000
1	-3.731963000	-4.045170000	2.281318000
1	4.788155000	-1.298130000	3.349615000
6	4.733452000	-1.179139000	2.271454000
6	-1.715170000	-2.925038000	-0.230509000
1	0.077354000	-2.259843000	-2.859943000
6	-2.242602000	-3.088513000	1.059180000
6	4.561176000	-0.888631000	-0.504273000
1	4.515078000	-0.791367000	-1.584215000
1	2.341316000	-1.095444000	-2.191187000
1	-1.826414000	-2.523811000	1.887128000
1	1.248936000	-0.994268000	-4.555508000
15	-0.257604000	-1.821032000	-0.468151000
6	3.617332000	-0.567117000	1.698240000
6	-0.295448000	-1.411187000	-2.281653000
6	3.521476000	-0.406134000	0.306611000
1	2.810905000	-0.228724000	2.340476000
1	-1.351290000	-1.301183000	-2.547978000
1	-0.379213000	-0.305318000	-4.715378000
6	1.912095000	-0.091856000	-2.125846000
6	0.600636000	-0.167469000	-4.245685000
1	2.531870000	0.562200000	-2.745464000
6	0.469129000	-0.124406000	-2.707181000
1	1.033418000	0.765481000	-4.622421000
15	2.044871000	0.479733000	-0.350724000
44	-0.031631000	0.054501000	0.836763000
1	4.405019000	1.693405000	-1.725946000
1	-5.467200000	-1.265342000	0.228680000
1	-3.171582000	-0.538545000	0.716326000
6	-4.939166000	-0.650784000	-0.494029000
6	-3.632573000	-0.239573000	-0.214944000
6	-0.322316000	1.174285000	-2.351448000
6	3.844553000	2.493369000	-1.251429000
1	-1.042293000	1.388014000	-3.144010000
6	2.676565000	2.210024000	-0.520174000
1	-6.562210000	-0.609721000	-1.916322000
6	-5.550571000	-0.283096000	-1.694019000
1	0.377166000	2.014630000	-2.335520000

15	-1.218993000	1.155228000	-0.722921000
6	-2.920590000	0.546811000	-1.129781000
1	5.208849000	4.009234000	-1.937530000
6	4.306363000	3.804691000	-1.368808000
6	-4.853841000	0.516164000	-2.608603000
6	-3.552346000	0.934359000	-2.326405000
6	1.989088000	3.263253000	0.097619000
1	-5.323687000	0.818500000	-3.539929000
1	1.088980000	3.064306000	0.665417000
1	-3.047735000	1.572708000	-3.044161000
6	3.609200000	4.852969000	-0.752837000
6	-1.571459000	2.909867000	-0.299143000
6	2.452638000	4.578838000	-0.020678000
1	-2.867336000	2.297060000	1.323490000
1	-0.370151000	3.870642000	-1.828947000
1	3.968837000	5.873617000	-0.845259000
6	-2.421467000	3.136627000	0.798440000
6	-1.029098000	4.008027000	-0.979684000
1	1.901441000	5.384194000	0.455854000
6	-2.710581000	4.435418000	1.215713000
6	-1.324419000	5.310709000	-0.563351000
1	-3.366233000	4.594150000	2.066750000
1	-0.895396000	6.152259000	-1.099056000
6	-2.158532000	5.528268000	0.535849000
1	-2.381562000	6.540668000	0.859073000
1	-1.421478000	-0.381275000	1.607964000
8	0.126451000	1.825916000	2.276291000
6	1.175500000	1.879635000	3.266600000
1	1.041112000	2.759510000	3.901192000
1	1.179703000	0.972428000	3.879728000
1	2.116019000	1.967862000	2.722425000
1	-0.724030000	1.976767000	2.716309000
1	-1.936758000	0.207970000	2.755931000
8	-2.285721000	0.771274000	3.523386000
8	-4.204451000	-0.384334000	3.200761000
6	-3.561041000	0.467699000	3.781176000
1	-3.958586000	1.093728000	4.592637000

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14-Ru-triphos

1	1.856651000	-6.448721000	-0.526194000
1	1.871462000	-5.085662000	-2.608762000
6	1.290686000	-5.523658000	-0.577613000
6	1.300890000	-4.757986000	-1.745050000
1	0.510520000	-5.691749000	1.431284000

6	0.539561000	-5.096472000	0.523651000
6	0.585549000	-3.558044000	-1.808540000
1	0.615050000	-2.990134000	-2.730427000
1	-5.434297000	-3.396529000	-2.006512000
1	-6.341537000	-3.486270000	0.311156000
1	6.304215000	-3.482548000	-0.206239000
1	6.643880000	-1.245427000	-1.245379000
6	-0.179855000	-3.903756000	0.456880000
6	-4.835122000	-3.046035000	-1.171355000
6	-5.343388000	-3.098544000	0.130651000
6	-0.151754000	-3.109166000	-0.703761000
1	-3.176065000	-2.536458000	-2.424241000
6	5.473843000	-2.787013000	-0.285410000
6	-3.551484000	-2.546129000	-1.406350000
6	5.665135000	-1.529502000	-0.869708000
1	-0.778258000	-3.601239000	1.309768000
6	-4.559802000	-2.649056000	1.197362000
1	-4.944619000	-2.683519000	2.212315000
1	4.052804000	-4.113599000	0.657927000
6	4.212225000	-3.141635000	0.200916000
6	-2.766149000	-2.074237000	-0.340559000
1	-1.000855000	-1.680231000	-3.072122000
6	-3.281764000	-2.138299000	0.960858000
6	4.599205000	-0.631645000	-0.968836000
1	4.765062000	0.344049000	-1.414461000
1	1.581345000	-1.142729000	-2.646383000
1	-2.695554000	-1.756157000	1.788965000
1	0.238306000	-0.504532000	-4.803063000
15	-1.037647000	-1.491054000	-0.636486000
6	3.145668000	-2.244494000	0.103577000
6	-1.091037000	-0.837692000	-2.381482000
6	3.327296000	-0.983903000	-0.486055000
1	2.175158000	-2.528458000	0.493236000
1	-2.101804000	-0.438695000	-2.517165000
1	-1.176141000	0.556551000	-4.653238000
6	1.391183000	-0.091332000	-2.420860000
6	-0.144360000	0.401155000	-4.320200000
1	2.072980000	0.473450000	-3.061760000
6	-0.075398000	0.272081000	-2.781164000
1	0.457040000	1.250344000	-4.661844000
15	1.879664000	0.148357000	-0.639730000
44	-0.078937000	-0.040765000	0.798179000
1	3.117507000	2.112645000	-2.642957000
1	-5.664710000	0.744401000	1.159774000
1	-3.201316000	0.526635000	1.215336000
6	-5.061739000	1.270743000	0.425751000

6	-3.670452000	1.140097000	0.457472000
6	-0.480826000	1.655193000	-2.188764000
6	3.143892000	2.537723000	-1.645404000
1	-1.282375000	2.075239000	-2.799030000
6	2.635856000	1.829873000	-0.544899000
1	-6.750992000	2.161427000	-0.580762000
6	-5.669863000	2.063245000	-0.550448000
1	0.371562000	2.333697000	-2.274878000
15	-1.026697000	1.641599000	-0.405662000
6	-2.869151000	1.788872000	-0.490617000
1	4.078139000	4.347031000	-2.343019000
6	3.695975000	3.811833000	-1.478691000
6	-4.877114000	2.736385000	-1.487533000
6	-3.487540000	2.603726000	-1.456782000
6	2.693707000	2.429818000	0.725645000
1	-5.338858000	3.366003000	-2.242401000
1	2.280417000	1.921184000	1.591425000
1	-2.900095000	3.152028000	-2.186273000
6	3.754092000	4.392989000	-0.209315000
6	-0.531110000	3.274247000	0.287086000
6	3.253244000	3.696478000	0.894499000
1	-0.802924000	2.588848000	2.328701000
1	-0.168849000	4.289615000	-1.598033000
1	4.175870000	5.385540000	-0.082462000
6	-0.534494000	3.421915000	1.685468000
6	-0.178310000	4.368722000	-0.516533000
1	3.274494000	4.146659000	1.881907000
6	-0.181236000	4.641315000	2.266307000
6	0.175056000	5.587161000	0.069427000
1	-0.180716000	4.739512000	3.347968000
1	0.454656000	6.424009000	-0.563647000
6	0.176843000	5.726419000	1.460110000
1	0.458173000	6.672840000	1.912339000
1	-1.418976000	-0.116452000	1.739454000
8	0.986389000	-1.271028000	2.566434000
6	2.338743000	-0.945908000	3.026399000
1	2.265923000	-0.354962000	3.940009000
1	2.892163000	-1.867429000	3.205020000
1	2.795618000	-0.376356000	2.224033000
1	-1.854255000	0.883357000	4.570257000
1	-1.219718000	0.454019000	3.224453000
8	-1.002240000	0.751912000	4.133286000
8	0.685392000	-2.446399000	4.482999000
6	0.253239000	-2.000231000	3.449529000
1	-0.768598000	-2.118484000	3.078487000

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15-Ru-triphos

1	0.338444000	6.729108000	0.260691000
1	0.300342000	5.762474000	-2.031581000
6	0.598033000	5.686531000	0.104167000
6	0.574270000	5.143400000	-1.182486000
1	0.982240000	5.295421000	2.194457000
6	0.958106000	4.881213000	1.190908000
6	0.899313000	3.798209000	-1.387424000
1	0.879472000	3.407769000	-2.398580000
1	6.503251000	1.469765000	-1.444149000
1	7.198226000	1.292647000	0.940320000
1	-4.671107000	5.482082000	0.087035000
1	-5.528897000	3.751663000	-1.482724000
6	1.281254000	3.539504000	0.988763000
6	5.755826000	1.361288000	-0.663727000
6	6.145460000	1.264427000	0.675278000
6	1.249003000	2.981483000	-0.303755000
1	4.128171000	1.414908000	-2.053298000
6	-4.118527000	4.558534000	-0.058961000
6	4.400850000	1.320893000	-1.007421000
6	-4.601074000	3.585178000	-0.943037000
1	1.553253000	2.922213000	1.840704000
6	5.172572000	1.130966000	1.671552000
1	5.465407000	1.054890000	2.714677000
1	-2.543828000	5.084184000	1.324283000
6	-2.927370000	4.335829000	0.637303000
6	3.420911000	1.165185000	-0.013730000
1	1.795436000	1.562948000	-2.839089000
6	3.820367000	1.079931000	1.328441000
6	-3.894480000	2.395007000	-1.132068000
1	-4.287552000	1.644320000	-1.810924000
1	-0.799833000	1.922880000	-2.497309000
1	3.072549000	0.941656000	2.102856000
1	0.336497000	0.964036000	-4.697530000
15	1.620432000	1.178928000	-0.426140000
6	-2.221001000	3.144738000	0.448802000
6	1.562148000	0.692995000	-2.218438000
6	-2.693114000	2.167572000	-0.439197000
1	-1.296727000	2.977790000	0.990184000
1	2.384033000	-0.016433000	-2.361713000
1	1.289183000	-0.528357000	-4.575924000
6	-1.016860000	0.857215000	-2.389850000
6	0.357317000	-0.042914000	-4.266600000
1	-1.799667000	0.640001000	-3.120917000

6	0.252974000	0.022352000	-2.726072000
1	-0.480093000	-0.610917000	-4.685681000
15	-1.690067000	0.639076000	-0.668491000
44	0.139995000	0.087311000	0.859126000
1	-3.372704000	-0.553414000	-2.938083000
1	5.171451000	-2.435747000	1.231443000
1	2.919719000	-1.404222000	1.260223000
6	4.431785000	-2.737380000	0.495606000
6	3.163992000	-2.147263000	0.512495000
6	0.129918000	-1.445815000	-2.214307000
6	-3.613698000	-1.047456000	-2.002953000
1	0.791140000	-2.078840000	-2.809931000
6	-2.971009000	-0.686854000	-0.807863000
1	5.730157000	-4.156787000	-0.483300000
6	4.744618000	-3.700767000	-0.465803000
1	-0.890583000	-1.790240000	-2.398779000
15	0.514260000	-1.737260000	-0.406609000
6	2.199881000	-2.502172000	-0.438349000
1	-5.060527000	-2.328852000	-2.950760000
6	-4.578754000	-2.059722000	-2.015254000
6	3.777851000	-4.082987000	-1.404278000
6	2.513995000	-3.490665000	-1.389693000
6	-3.316769000	-1.368713000	0.371552000
1	4.006506000	-4.842190000	-2.146482000
1	-2.807383000	-1.137895000	1.299849000
1	1.777597000	-3.817689000	-2.117653000
6	-4.919946000	-2.721746000	-0.832641000
6	-0.538557000	-3.160423000	0.101581000
6	-4.286954000	-2.371108000	0.363346000
1	-0.151052000	-2.773941000	2.193262000
1	-1.118704000	-3.838016000	-1.877745000
1	-5.664173000	-3.512465000	-0.845225000
6	-0.662086000	-3.412291000	1.478641000
6	-1.195554000	-4.001460000	-0.808326000
1	-4.527164000	-2.893101000	1.284273000
6	-1.438707000	-4.476610000	1.938102000
6	-1.973450000	-5.066579000	-0.346054000
1	-1.530185000	-4.655054000	3.005469000
1	-2.485778000	-5.704196000	-1.060376000
6	-2.100653000	-5.304655000	1.025081000
1	-2.712324000	-6.128660000	1.380233000
1	1.345848000	-0.361554000	1.862076000
8	-1.198367000	0.093875000	2.999171000
6	-2.466806000	0.778229000	3.239467000
1	-3.206964000	0.061099000	3.597373000
1	-2.317014000	1.566988000	3.977968000

1	-2.757224000	1.198910000	2.281470000
8	-1.123100000	-0.487563000	5.190370000
6	-0.632142000	-0.487075000	4.086852000
1	0.325540000	-0.938674000	3.801724000

-2932.959775

16-Ru-triphos

1	-6.520053000	-1.714136000	-0.980207000
1	-5.779961000	-0.179167000	-2.794713000
6	-5.585928000	-1.168651000	-0.884206000
6	-5.168178000	-0.308447000	-1.906680000
1	-5.100291000	-2.004596000	1.047755000
6	-4.794326000	-1.328022000	0.255998000
6	-3.963054000	0.388925000	-1.790860000
1	-3.667231000	1.056950000	-2.593673000
1	-3.178433000	5.769806000	-1.260377000
1	-3.401555000	6.319812000	1.156581000
1	-4.153379000	-5.622885000	0.789397000
1	-3.689267000	-5.114424000	-1.600575000
6	-3.586220000	-0.636179000	0.366183000
6	-2.926527000	5.029299000	-0.506885000
6	-3.052653000	5.337716000	0.851363000
6	-3.155884000	0.225171000	-0.653337000
1	-2.387800000	3.550502000	-1.962313000
6	-3.384603000	-4.902536000	0.525719000
6	-2.473602000	3.767207000	-0.902498000
6	-3.124686000	-4.616059000	-0.817947000
1	-2.960317000	-0.788355000	1.238402000
6	-2.723872000	4.378366000	1.815338000
1	-2.816165000	4.611621000	2.872095000
1	-2.853491000	-4.470384000	2.574927000
6	-2.654415000	-4.255528000	1.528931000
6	-2.130510000	2.805054000	0.060127000
1	-1.635707000	1.457103000	-2.818019000
6	-2.262168000	3.120453000	1.421129000
6	-2.141206000	-3.683777000	-1.162588000
1	-1.958742000	-3.476197000	-2.212060000
1	-1.495583000	-1.230399000	-2.416105000
1	-1.980501000	2.387130000	2.170985000
1	-0.804269000	0.049835000	-4.568986000
15	-1.560836000	1.115680000	-0.394872000
6	-1.676731000	-3.319480000	1.188039000
6	-0.824860000	1.332946000	-2.095565000
6	-1.415476000	-3.024081000	-0.160519000
1	-1.126062000	-2.800020000	1.966478000

1	-0.280158000	2.282253000	-2.076751000
1	0.430107000	1.320360000	-4.453381000
6	-0.414493000	-1.213457000	-2.249745000
6	0.170196000	0.304124000	-4.137983000
1	0.019431000	-1.940210000	-2.940767000
6	0.128827000	0.204178000	-2.595743000
1	0.916466000	-0.383389000	-4.550693000
15	-0.114764000	-1.772327000	-0.500941000
44	-0.026621000	0.067839000	0.887553000
1	1.103470000	-3.695156000	-2.499781000
1	0.751853000	5.566212000	0.946212000
1	0.492567000	3.107847000	1.077172000
6	1.387977000	4.925529000	0.342315000
6	1.234580000	3.536559000	0.414777000
6	1.592105000	0.394239000	-2.093949000
6	1.755926000	-3.617897000	-1.635620000
1	2.079606000	1.161060000	-2.702209000
6	1.426460000	-2.783279000	-0.554947000
1	2.470065000	6.558461000	-0.562978000
6	2.350033000	5.480595000	-0.504264000
1	2.135668000	-0.540451000	-2.262220000
15	1.803919000	0.855747000	-0.290944000
6	2.031513000	2.690091000	-0.366212000
1	3.181976000	-5.005645000	-2.455965000
6	2.933466000	-4.368867000	-1.611914000
6	3.165706000	4.641063000	-1.274776000
6	3.008400000	3.256096000	-1.205574000
6	2.283020000	-2.730425000	0.555187000
1	3.924012000	5.065190000	-1.926583000
1	2.035990000	-2.087791000	1.391898000
1	3.658008000	2.620023000	-1.800631000
6	3.788603000	-4.301763000	-0.505118000
6	3.495903000	0.275578000	0.135902000
6	3.458070000	-3.486129000	0.579738000
1	3.067519000	0.466422000	2.243078000
1	4.254072000	-0.035656000	-1.873021000
1	4.707189000	-4.881083000	-0.492356000
6	3.813893000	0.197236000	1.501742000
6	4.466068000	-0.086001000	-0.810277000
1	4.120170000	-3.419004000	1.437411000
6	5.073005000	-0.237927000	1.916697000
6	5.725558000	-0.529261000	-0.394754000
1	5.301050000	-0.298474000	2.976820000
1	6.464846000	-0.815163000	-1.137306000
6	6.031600000	-0.608470000	0.966803000
1	7.008543000	-0.959037000	1.286228000

1	-0.004079000	1.317176000	1.693065000
6	0.430353000	-0.203704000	3.599284000
8	0.363843000	-1.026293000	2.678530000
8	-0.535605000	0.048711000	4.453034000
6	-1.814627000	-0.603988000	4.216760000
1	-2.219734000	-0.251868000	3.266095000
1	-1.685296000	-1.686848000	4.196144000
1	-2.449202000	-0.299313000	5.045760000
1	1.329290000	0.375418000	3.829637000

-2932.970708

TS4-Ru-triphos

Frequency = - 534.0712 cm⁻¹

1	-6.484640000	-1.957489000	-1.004374000
1	-5.798105000	-0.377764000	-2.801721000
6	-5.562602000	-1.391854000	-0.908740000
6	-5.175032000	-0.506360000	-1.921606000
1	-5.040733000	-2.240567000	1.008536000
6	-4.757692000	-1.547785000	0.222271000
6	-3.986053000	0.217565000	-1.806217000
1	-3.714670000	0.904967000	-2.601182000
1	-3.248152000	5.615742000	-1.353595000
1	-3.508783000	6.183966000	1.055536000
1	-3.868875000	-5.815968000	1.047333000
1	-3.438769000	-5.396573000	-1.365701000
6	-3.566020000	-0.827958000	0.333492000
6	-2.999032000	4.884517000	-0.590335000
6	-3.146308000	5.202978000	0.763186000
6	-3.164410000	0.056083000	-0.678163000
1	-2.423803000	3.400655000	-2.025857000
6	-3.137442000	-5.071598000	0.746913000
6	-2.527238000	3.624396000	-0.969212000
6	-2.896627000	-4.835550000	-0.610227000
1	-2.936452000	-0.977268000	1.202515000
6	-2.821490000	4.255063000	1.739564000
1	-2.930152000	4.495371000	2.793018000
1	-2.623328000	-4.521558000	2.772309000
6	-2.437614000	-4.344908000	1.716917000
6	-2.188234000	2.673877000	0.006066000
1	-1.675734000	1.255429000	-2.864118000
6	-2.343507000	2.998336000	1.362775000
6	-1.961435000	-3.873237000	-1.002647000
1	-1.790961000	-3.703090000	-2.061001000
1	-1.441384000	-1.404241000	-2.357691000

1	-2.071737000	2.278505000	2.128950000
1	-0.773430000	-0.183054000	-4.563649000
15	-1.593680000	0.991831000	-0.438006000
6	-1.507569000	-3.379077000	1.329308000
6	-0.861688000	1.188872000	-2.137932000
6	-1.266975000	-3.135875000	-0.033514000
1	-0.980352000	-2.796021000	2.079888000
1	-0.352832000	2.157690000	-2.151184000
1	0.409466000	1.137743000	-4.485450000
6	-0.360885000	-1.343881000	-2.196763000
6	0.186528000	0.124350000	-4.134964000
1	0.094372000	-2.078674000	-2.864890000
6	0.135371000	0.079934000	-2.590825000
1	0.962791000	-0.548004000	-4.515845000
15	-0.036335000	-1.839775000	-0.437002000
44	-0.077762000	-0.011052000	0.914854000
1	1.347997000	-3.668008000	-2.406348000
1	0.498531000	5.478738000	1.077495000
1	0.419807000	3.011532000	1.176388000
6	1.125313000	4.894370000	0.410360000
6	1.078107000	3.497613000	0.466573000
6	1.583245000	0.352160000	-2.083454000
6	1.972703000	-3.551152000	-1.526596000
1	2.037722000	1.118723000	-2.716510000
6	1.568195000	-2.741366000	-0.452040000
1	2.002155000	6.612206000	-0.556731000
6	1.966306000	5.527907000	-0.506902000
1	2.173104000	-0.559657000	-2.215946000
15	1.765762000	0.878544000	-0.295623000
6	1.862186000	2.720214000	-0.396002000
1	3.501455000	-4.842534000	-2.316691000
6	3.194872000	-4.225216000	-1.477394000
6	2.768638000	4.759763000	-1.361394000
6	2.719424000	3.366020000	-1.304802000
6	2.395698000	-2.633921000	0.676541000
1	3.433275000	5.246596000	-2.069148000
1	2.093108000	-2.007552000	1.507647000
1	3.359866000	2.788735000	-1.965711000
6	4.020053000	-4.105550000	-0.352749000
6	3.492808000	0.412638000	0.130932000
6	3.615402000	-3.314025000	0.724628000
1	3.064587000	0.517754000	2.247602000
1	4.261352000	0.193553000	-1.886634000
1	4.973155000	-4.625177000	-0.320530000
6	3.823020000	0.333196000	1.493736000
6	4.482434000	0.140789000	-0.825886000

1	4.254016000	-3.205865000	1.595692000
6	5.115178000	-0.010178000	1.894210000
6	5.774343000	-0.212003000	-0.424509000
1	5.352333000	-0.073522000	2.952120000
1	6.528643000	-0.428079000	-1.175526000
6	6.094004000	-0.288766000	0.934295000
1	7.097082000	-0.567632000	1.243164000
1	-0.156710000	1.209505000	1.840760000
6	0.299706000	0.335438000	3.168287000
8	0.482304000	-0.824309000	2.661012000
8	-0.700103000	0.606444000	4.031672000
6	-1.855646000	-0.256345000	3.991200000
1	-2.409818000	-0.081997000	3.063980000
1	-1.561269000	-1.305128000	4.056973000
1	-2.465277000	0.029768000	4.846731000
1	1.136672000	1.013710000	3.356064000

-2932.950260

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1	-3.861125000	5.707014000	-0.115079000
1	-3.992926000	4.575464000	2.097681000
6	-3.525506000	4.680094000	-0.006699000
6	-3.597446000	4.046014000	1.235861000
1	-2.944316000	4.476013000	-2.077109000
6	-3.011866000	3.988763000	-1.109169000
6	-3.158918000	2.725153000	1.380401000
1	-3.232368000	2.260333000	2.357431000
1	-6.440922000	-2.013734000	0.566481000
1	-6.476183000	-2.548214000	-1.864139000
1	0.758186000	6.697759000	-1.352439000
1	-0.520304000	6.159621000	0.714151000
6	-2.566188000	2.675313000	-0.963889000
6	-5.611262000	-1.718344000	-0.069079000
6	-5.631182000	-2.017414000	-1.435699000
6	-2.634198000	2.028003000	0.283131000
1	-4.533841000	-0.804695000	1.545661000
6	0.792555000	5.695459000	-0.935739000
6	-4.524731000	-1.036575000	0.485081000
6	0.076905000	5.395390000	0.226431000
1	-2.155618000	2.157312000	-1.827029000
6	-4.559022000	-1.634425000	-2.246959000
1	-4.564662000	-1.868715000	-3.307329000
1	2.112605000	4.925848000	-2.464319000
6	1.552404000	4.700039000	-1.561659000
6	-3.441151000	-0.656796000	-0.323159000

1	-2.601780000	0.417863000	2.729901000
6	-3.468051000	-0.960846000	-1.692699000
6	0.111054000	4.105290000	0.762441000
1	-0.470246000	3.897221000	1.652421000
1	-0.557308000	2.061021000	2.495011000
1	-2.634681000	-0.682087000	-2.331519000
1	-1.158700000	0.727601000	4.650961000
15	-2.012860000	0.291502000	0.345441000
6	1.596523000	3.411149000	-1.028249000
6	-1.914960000	-0.187758000	2.134591000
6	0.872883000	3.106379000	0.140781000
1	2.196342000	2.648598000	-1.518849000
1	-2.273731000	-1.217468000	2.209241000
1	-1.202541000	-1.044359000	4.574431000
6	0.187451000	1.267960000	2.397211000
6	-0.633000000	-0.157369000	4.277041000
1	0.967691000	1.477699000	3.132161000
6	-0.486540000	-0.094189000	2.741391000
1	0.348710000	-0.202050000	4.760301000
15	0.948971000	1.364039000	0.703651000
44	-0.014380000	0.015010000	-0.825609000
1	2.884852000	2.341917000	2.754631000
1	-2.271655000	-4.666628000	-2.393339000
1	-0.579683000	-2.947399000	-1.888289000
6	-2.068545000	-4.401628000	-1.360209000
6	-1.111204000	-3.429509000	-1.072359000
6	0.411278000	-1.293950000	2.318361000
6	3.415411000	1.693057000	2.063941000
1	0.142498000	-2.175740000	2.905241000
6	2.747411000	1.082997000	0.986541000
1	-3.530836000	-5.766276000	-0.547219000
6	-2.776395000	-5.018317000	-0.322859000
1	1.448769000	-1.059481000	2.577131000
15	0.427388000	-1.756490000	0.518871000
6	-0.843193000	-3.064499000	0.258991000
1	5.290142000	1.955715000	3.085901000
6	4.782571000	1.483105000	2.250191000
6	-2.511455000	-4.665377000	1.002791000
6	-1.546254000	-3.696208000	1.294731000
6	3.470850000	0.287717000	0.089211000
1	-3.054745000	-5.140477000	1.814141000
1	2.962510000	-0.154023000	-0.757599000
1	-1.358124000	-3.449759000	2.333701000
6	5.496640000	0.668525000	1.361451000
6	2.002047000	-2.682892000	0.298871000
6	4.839900000	0.078445000	0.279631000

1	2.032587000	-2.357812000	-1.835119000
1	2.289587000	-3.175002000	2.398281000
1	6.559230000	0.502094000	1.512471000
6	2.517257000	-2.847812000	-0.997729000
6	2.669267000	-3.269883000	1.386811000
1	5.385379000	-0.550015000	-0.417929000
6	3.691096000	-3.577994000	-1.196729000
6	3.845356000	-3.996624000	1.180401000
1	4.088456000	-3.687654000	-2.201739000
1	4.356255000	-4.440604000	2.029691000
6	4.360386000	-4.150804000	-0.110389000
1	5.277115000	-4.711595000	-0.267449000
1	0.925361000	1.386669000	-3.282389000
6	1.608880000	0.519709000	-3.288899000
8	1.324379000	-0.424401000	-2.325069000
8	2.903441000	1.112647000	-3.125989000
6	3.972650000	0.199646000	-3.360479000
1	3.908539000	-0.674574000	-2.702099000
1	3.971570000	-0.144034000	-4.405799000
1	4.903330000	0.734525000	-3.158499000
1	1.566020000	0.045989000	-4.287699000

-2932.963230

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1	4.874476000	-4.766126000	0.305548000
1	3.926479000	-4.608068000	-1.991128000
6	3.948469000	-4.225751000	0.133421000
6	3.418402000	-4.134237000	-1.156333000
1	3.694195000	-3.667706000	2.203704000
6	3.285339000	-3.611651000	1.199691000
6	2.232442000	-3.429517000	-1.381795000
1	1.843529000	-3.382935000	-2.392797000
1	-3.300480000	-5.405695000	-1.793119000
1	-3.802207000	-6.031694000	0.564335000
1	6.732870000	-1.167611000	1.840931000
1	6.467108000	-1.171831000	-0.633456000
6	2.105519000	-2.901862000	0.974085000
6	-2.809353000	-4.888800000	-0.973796000
6	-3.089016000	-5.241176000	0.349537000
6	1.567710000	-2.798865000	-0.319641000
1	-1.697517000	-3.621620000	-2.289238000
6	5.811840000	-0.809565000	1.390621000
6	-1.896043000	-3.867887000	-1.252337000
6	5.662757000	-0.811718000	0.001169000
1	1.612348000	-2.417508000	1.811773000

6	-2.445691000	-4.570059000	1.395155000
1	-2.658813000	-4.835758000	2.426685000
1	4.864453000	-0.359838000	3.279326000
6	4.764621000	-0.354914000	2.197874000
6	-1.258451000	-3.181862000	-0.206716000
1	0.279006000	-2.275223000	-2.904422000
6	-1.536022000	-3.546981000	1.120855000
6	4.477268000	-0.355329000	-0.582508000
1	4.391820000	-0.368521000	-1.663697000
1	2.368818000	-0.775111000	-2.297401000
1	-1.076328000	-2.998249000	1.933255000
1	1.234696000	-0.877254000	-4.637956000
15	-0.011249000	-1.859789000	-0.507741000
6	3.578453000	0.093026000	1.615359000
6	-0.186663000	-1.478414000	-2.319906000
6	3.421695000	0.104348000	0.219507000
1	2.768750000	0.420816000	2.256552000
1	-1.255282000	-1.517626000	-2.547615000
1	-0.482160000	-0.445084000	-4.772368000
6	1.795347000	0.152988000	-2.230581000
6	0.474590000	-0.152758000	-4.326314000
1	2.301616000	0.893164000	-2.856240000
6	0.367824000	-0.103882000	-2.787007000
1	0.753612000	0.828256000	-4.725397000
15	1.837124000	0.754413000	-0.464216000
44	-0.022676000	0.065396000	0.792151000
1	4.085694000	2.235241000	-1.704925000
1	-5.071055000	-2.158209000	0.529856000
1	-2.930427000	-0.965934000	0.867754000
6	-4.700882000	-1.494696000	-0.246261000
6	-3.488910000	-0.823768000	-0.052041000
6	-0.599931000	1.064283000	-2.426203000
6	3.374581000	2.968374000	-1.334874000
1	-1.377486000	1.144222000	-3.189097000
6	2.206188000	2.554861000	-0.668645000
1	-6.355180000	-1.860674000	-1.583520000
6	-5.419577000	-1.330164000	-1.431876000
1	-0.040782000	2.003874000	-2.452624000
15	-1.412300000	0.949472000	-0.761666000
6	-2.986567000	0.023620000	-1.051468000
1	4.544850000	4.631794000	-2.036837000
6	3.639321000	4.325506000	-1.521257000
6	-4.929261000	-0.475157000	-2.426474000
6	-3.724089000	0.203230000	-2.235936000
6	1.319049000	3.524442000	-0.184440000
1	-5.484427000	-0.333256000	-3.349115000

1	0.425363000	3.225476000	0.346903000
1	-3.378312000	0.873876000	-3.015807000
6	2.741042000	5.288998000	-1.042903000
6	-2.051274000	2.634075000	-0.398050000
6	1.583645000	4.885469000	-0.374511000
1	-2.914134000	1.942058000	1.454356000
1	-1.332903000	3.649081000	-2.177477000
1	2.947698000	6.345130000	-1.189348000
6	-2.764243000	2.793911000	0.801171000
6	-1.875658000	3.738534000	-1.243586000
1	0.880000000	5.622894000	0.000288000
6	-3.283030000	4.038074000	1.157025000
6	-2.397794000	4.986142000	-0.886042000
1	-3.829100000	4.147842000	2.089245000
1	-2.252491000	5.835445000	-1.546988000
6	-3.096495000	5.140592000	0.314243000
1	-3.496081000	6.111734000	0.590786000
1	-0.607504435	-0.574706510	4.073688941
8	-2.257356496	0.581353471	3.922984048
6	-3.645629760	0.567047870	3.576312704
1	-3.784897869	0.327781664	2.515654902
1	-4.180156942	-0.175039515	4.183517619
1	-4.045760811	1.561237442	3.785954594
8	-1.415910000	-0.736817000	2.166509000
6	-1.555401469	-0.643730419	3.513040142
1	-2.137987929	-1.495665317	3.905965502
8	-0.099677000	1.884644000	2.149837000
6	0.627470976	3.012558459	2.667631582
1	-0.073632407	3.809912922	2.932465763
1	1.213520935	2.735163730	3.551260994
1	1.292876325	3.369922563	1.881921496
1	-0.785414355	1.400770763	2.679933695

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1	6.388396000	2.695852000	-0.183383000
1	5.408383000	2.914494000	2.095184000
6	5.325374000	2.536875000	-0.028996000
6	4.776086000	2.656081000	1.250776000
1	4.920283000	2.093052000	-2.103019000
6	4.501719000	2.202692000	-1.107558000
6	3.409445000	2.442197000	1.452902000
1	3.011516000	2.551152000	2.455757000
1	-0.980928000	6.393540000	1.689628000
1	-1.088606000	7.125027000	-0.686741000

1	6.779208000	-1.358640000	-1.851061000
1	6.477015000	-1.303688000	0.618757000
6	3.139633000	1.977772000	-0.903645000
6	-0.677642000	5.716767000	0.896242000
6	-0.735515000	6.128689000	-0.438579000
6	2.578099000	2.092295000	0.378682000
1	-0.192575000	4.139286000	2.264207000
6	5.781052000	-1.331774000	-1.424091000
6	-0.229238000	4.432590000	1.220465000
6	5.611421000	-1.300753000	-0.037214000
1	2.521234000	1.694102000	-1.750523000
6	-0.331817000	5.253156000	-1.452312000
1	-0.364607000	5.566601000	-2.491543000
1	4.777547000	-1.343212000	-3.337096000
6	4.658543000	-1.323422000	-2.257664000
6	0.159097000	3.540786000	0.208108000
1	1.125915000	2.092730000	2.945946000
6	0.114135000	3.968849000	-1.130822000
6	4.328609000	-1.262312000	0.516965000
1	4.231821000	-1.243608000	1.596780000
1	2.539781000	-0.102344000	2.195982000
1	0.430849000	3.301071000	-1.926921000
1	1.622637000	0.378047000	4.561948000
15	0.755853000	1.822235000	0.535385000
6	3.377572000	-1.278660000	-1.705383000
6	0.422298000	1.525584000	2.331817000
6	3.198065000	-1.246720000	-0.313786000
1	2.518161000	-1.263243000	-2.363395000
1	-0.569975000	1.929368000	2.553318000
1	-0.124599000	0.599985000	4.780722000
6	1.652439000	-0.735338000	2.124457000
6	0.636977000	-0.010885000	4.284287000
1	1.850390000	-1.625546000	2.725279000
6	0.450588000	0.025828000	2.750624000
1	0.554448000	-1.035357000	4.662359000
15	1.471255000	-1.264464000	0.339545000
44	-0.034825000	0.058507000	-0.818352000
1	2.517300000	-3.486964000	2.054629000
1	-3.732196000	3.941951000	1.106817000
1	-1.889900000	2.417974000	0.631360000
6	-3.902649000	2.870614000	1.158704000
6	-2.847133000	1.995182000	0.894560000
6	-0.887659000	-0.697757000	2.443007000
6	1.811973000	-3.903402000	1.341641000
1	-1.664013000	-0.351581000	3.131896000
6	1.143387000	-3.080442000	0.417288000

1	-5.993438000	3.040202000	1.672529000
6	-5.166786000	2.364765000	1.474001000
1	-0.732020000	-1.760733000	2.642685000
15	-1.589264000	-0.546294000	0.717994000
6	-3.023385000	0.606150000	0.951830000
1	2.109172000	-5.907449000	2.066963000
6	1.591959000	-5.282041000	1.345038000
6	-5.359572000	0.980907000	1.524515000
6	-4.298365000	0.107105000	1.269549000
6	0.272337000	-3.659006000	-0.517630000
1	-6.338334000	0.575026000	1.762747000
1	-0.250453000	-3.017730000	-1.224116000
1	-4.473030000	-0.961781000	1.316383000
6	0.714921000	-5.855114000	0.415237000
6	-2.444385000	-2.140628000	0.396975000
6	0.063997000	-5.042288000	-0.515228000
1	-3.007285000	-1.485339000	-1.583119000
1	-2.078091000	-3.103570000	2.311420000
1	0.544291000	-6.927971000	0.419262000
6	-3.067874000	-2.284397000	-0.855007000
6	-2.533552000	-3.182955000	1.331514000
1	-0.623058000	-5.478013000	-1.234685000
6	-3.753695000	-3.459624000	-1.165067000
6	-3.220063000	-4.358522000	1.015126000
1	-4.227008000	-3.562235000	-2.137527000
1	-3.274866000	-5.159283000	1.746633000
6	-3.827261000	-4.502490000	-0.234748000
1	-4.356424000	-5.418495000	-0.481396000
1	-1.720886000	0.231062000	-3.670710000
8	-3.477753000	0.472808000	-2.752955000
6	-4.465743000	1.418931000	-2.330017000
1	-4.170250000	1.916990000	-1.402130000
1	-4.647484000	2.167971000	-3.112473000
1	-5.381119000	0.853516000	-2.150257000
8	-1.416150000	1.410563000	-2.059867000
6	-2.263628000	1.017490000	-3.158339000
1	-2.412385000	1.901121000	-3.793675000
8	-0.674166000	-1.340088000	-2.233673000
6	0.149353000	-1.486941000	-3.354937000
1	-0.458647000	-1.740122000	-4.241356000
1	0.716429000	-0.570923000	-3.624393000
1	0.891376000	-2.299290000	-3.234048000
1	-1.673518000	2.279309000	-1.719760000

-3048.660961

20-Ru-triphos

1	-5.515554000	-4.575783000	-0.280167000
1	-4.639187000	-4.338557000	2.036733000
6	-4.568508000	-4.074022000	-0.105188000
6	-4.078103000	-3.937832000	1.197583000
1	-4.222596000	-3.638185000	-2.192426000
6	-3.841635000	-3.552469000	-1.179698000
6	-2.863979000	-3.284186000	1.428409000
1	-2.507049000	-3.194537000	2.448979000
1	2.012623000	-5.829172000	2.234032000
1	3.287834000	-6.133055000	0.118730000
1	-6.694511000	-0.887465000	-2.921837000
1	-6.892342000	-0.545595000	-0.466249000
6	-2.633748000	-2.892788000	-0.949105000
6	1.847588000	-5.157405000	1.396721000
6	2.563312000	-5.328531000	0.205598000
6	-2.132407000	-2.752351000	0.355233000
1	0.365283000	-4.009262000	2.441164000
6	-5.834171000	-0.556215000	-2.347998000
6	0.916411000	-4.122557000	1.512452000
6	-5.945873000	-0.365270000	-0.967182000
1	-2.087257000	-2.464696000	-1.784481000
6	2.348040000	-4.459478000	-0.868223000
1	2.908901000	-4.581125000	-1.789777000
1	-4.518367000	-0.475997000	-4.059198000
6	-4.612178000	-0.324637000	-2.988026000
6	0.704012000	-3.243922000	0.437180000
1	-0.889217000	-2.023263000	2.939052000
6	1.423319000	-3.417165000	-0.755565000
6	-4.840426000	0.056117000	-0.223442000
1	-4.948312000	0.203714000	0.846478000
1	-2.973123000	-0.519842000	1.842817000
1	1.291539000	-2.704428000	-1.564905000
1	-2.191551000	-0.569800000	4.316464000
15	-0.520685000	-1.880827000	0.523162000
6	-3.503302000	0.086956000	-2.246919000
6	-0.421930000	-1.280568000	2.287351000
6	-3.610360000	0.277835000	-0.859464000
1	-2.551854000	0.244070000	-2.749344000
1	0.642332000	-1.283785000	2.543249000
1	-0.514887000	-0.139226000	4.707202000
6	-2.353318000	0.380019000	1.817836000
6	-1.384874000	0.139730000	4.103406000
1	-2.921052000	1.164185000	2.323249000
6	-1.031016000	0.125140000	2.599323000
1	-1.713534000	1.136295000	4.416944000

15	-2.116476000	0.843111000	0.037549000
44	-0.177259000	0.006803000	-0.802249000
1	-3.460871000	3.012033000	1.688805000
1	4.583322000	-2.160893000	0.746567000
1	2.479206000	-1.158548000	-0.037721000
6	4.236143000	-1.235535000	1.194693000
6	3.034875000	-0.673495000	0.751878000
6	-0.017858000	1.287679000	2.364845000
6	-2.929966000	3.464651000	0.857705000
1	0.703682000	1.308738000	3.186362000
6	-2.213764000	2.678237000	-0.058188000
1	5.923170000	-1.027386000	2.522603000
6	4.987416000	-0.594582000	2.180903000
1	-0.568730000	2.232670000	2.395565000
15	0.956079000	1.235160000	0.771259000
6	2.569650000	0.525517000	1.302591000
1	-3.525139000	5.452627000	1.427435000
6	-2.973883000	4.853566000	0.708732000
6	4.539805000	0.620118000	2.720052000
6	3.337520000	1.177686000	2.284873000
6	-1.556191000	3.303864000	-1.129736000
1	5.128146000	1.131546000	3.476280000
1	-0.985365000	2.712352000	-1.838966000
1	3.007161000	2.124187000	2.703991000
6	-2.311758000	5.468648000	-0.359104000
6	1.363899000	2.971215000	0.351893000
6	-1.606067000	4.690396000	-1.280766000
1	1.907646000	2.385908000	-1.659278000
1	0.888865000	3.888385000	2.260045000
1	-2.341390000	6.548671000	-0.467900000
6	1.826066000	3.209007000	-0.954297000
6	1.246010000	4.043487000	1.247268000
1	-1.077813000	5.159825000	-2.104487000
6	2.169530000	4.500050000	-1.355664000
6	1.582962000	5.337684000	0.838499000
1	2.523144000	4.672594000	-2.367892000
1	1.480917000	6.163646000	1.536184000
6	2.044769000	5.568527000	-0.460509000
1	2.301357000	6.575633000	-0.775465000
1	-2.100339753	-1.733280254	-5.003001917
8	-0.210415333	-2.573263010	-5.114292880
6	-0.642178866	-3.771188639	-5.750494674
1	0.213072753	-4.159875051	-6.306249909
1	-0.963959587	-4.522185933	-5.013836936
1	-1.470450861	-3.581005235	-6.448604342
8	1.392371529	0.045980024	-1.708192044

6	-1.235252931	-1.958215438	-4.353343041
1	-1.546681086	-2.610983640	-3.526509974
8	-0.733665972	-0.790553591	-3.770446326
6	-0.457711210	0.262660517	-4.707334536
1	-1.373913648	0.539201844	-5.244870557
1	-0.105130670	1.112821421	-4.123450262
1	0.316532976	-0.040160937	-5.416337834
1	2.205499361	0.379106859	-1.293954728

-3048.666401

22-Ru-triphso

1	4.102848000	5.912734000	-0.353020000
1	5.303066000	4.046792000	-1.487050000
6	3.690237000	4.908464000	-0.333700000
6	4.364235000	3.860123000	-0.974180000
1	1.957878000	5.459717000	0.831090000
6	2.489957000	4.655516000	0.332140000
6	3.834344000	2.570294000	-0.950260000
1	4.378262000	1.765553000	-1.437210000
1	6.060016000	-2.291519000	-0.391600000
1	6.308486000	-2.289389000	2.083730000
1	-2.075140000	6.769043000	1.147030000
1	-1.227211000	6.355912000	-1.155760000
6	1.958495000	3.360887000	0.355800000
6	5.352547000	-1.748108000	0.227450000
6	5.491217000	-1.747318000	1.617500000
6	2.618833000	2.309066000	-0.290210000
1	4.214928000	-1.077836000	-1.458180000
6	-1.897222000	5.753833000	0.805490000
6	4.298258000	-1.057717000	-0.377370000
6	-1.420512000	5.522262000	-0.487400000
1	1.022305000	3.194218000	0.871330000
6	4.570378000	-1.049817000	2.406810000
1	4.669358000	-1.044877000	3.488240000
1	-2.525883000	4.840373000	2.661260000
6	-2.147743000	4.671893000	1.657460000
6	3.367699000	-0.362685000	0.407470000
1	2.498051000	0.860296000	-2.641740000
6	3.514589000	-0.363805000	1.805860000
6	-1.181314000	4.217142000	-0.929170000
1	-0.809064000	4.069941000	-1.936490000
1	0.334193000	2.308459000	-2.251500000
1	2.803290000	0.168806000	2.431240000
1	1.023502000	1.212438000	-4.530080000
15	1.952911000	0.586597000	-0.284510000

6	-1.911825000	3.369103000	1.218130000
6	1.863210000	0.158907000	-2.094400000
6	-1.416976000	3.129682000	-0.074900000
1	-2.117426000	2.539063000	1.885450000
1	2.284569000	-0.838034000	-2.241390000
1	1.216289000	-0.550262000	-4.594530000
6	-0.353858000	1.457760000	-2.247650000
6	0.575660000	0.259469000	-4.229420000
1	-1.133328000	1.675591000	-2.982110000
6	0.429110000	0.187149000	-2.693860000
1	-0.401130000	0.170490000	-4.716630000
15	-1.141698000	1.379581000	-0.566220000
44	-0.002500000	0.070800000	0.901410000
1	-3.215147000	2.084494000	-2.575630000
1	2.969093000	-4.342315000	1.985530000
1	1.118826000	-2.747482000	1.679280000
6	2.622194000	-4.111834000	0.983110000
6	1.576205000	-3.205723000	0.807570000
6	-0.359992000	-1.112010000	-2.370220000
6	-3.628538000	1.326235000	-1.917360000
1	-0.033013000	-1.915890000	-3.033920000
6	-2.865839000	0.789664000	-0.863850000
1	4.056942000	-5.396426000	0.009450000
6	3.233433000	-4.702065000	-0.127070000
1	-1.415712000	-0.938368000	-2.596620000
15	-0.294753000	-1.715060000	-0.617680000
6	1.124086000	-2.882222000	-0.483530000
1	-5.519148000	1.315478000	-2.942370000
6	-4.940759000	0.898717000	-2.123170000
6	2.786503000	-4.389024000	-1.413370000
6	1.733775000	-3.486943000	-1.592460000
6	-3.445380000	-0.158015000	-0.008500000
1	3.255693000	-4.842765000	-2.281260000
1	-2.870521000	-0.573846000	0.811910000
1	1.403515000	-3.269522000	-2.602210000
6	-5.509680000	-0.059652000	-1.274050000
6	-1.736264000	-2.847918000	-0.467130000
6	-4.762521000	-0.579873000	-0.216070000
1	-1.489115000	-3.040748000	1.667130000
1	-2.277444000	-2.874457000	-2.574100000
1	-6.529921000	-0.393491000	-1.438680000
6	-2.050085000	-3.367347000	0.800510000
6	-2.496185000	-3.244277000	-1.579270000
1	-5.192422000	-1.324763000	0.446690000
6	-3.118646000	-4.253126000	0.951180000
6	-3.563966000	-4.132335000	-1.422100000

1	-3.359117000	-4.637705000	1.938090000
1	-4.146457000	-4.426154000	-2.290310000
6	-3.881027000	-4.635895000	-0.157610000
1	-4.715018000	-5.321063000	-0.037100000
1	-0.796560000	0.299801000	3.905130000
6	-1.314781000	-0.634408000	3.610420000
8	-1.186582000	-0.915238000	2.262670000
8	-2.673401000	-0.542896000	4.037350000
6	-3.327329000	0.657275000	3.640460000
1	-2.784748000	1.541394000	4.010260000
1	-3.425819000	0.725965000	2.551590000
1	-4.325139000	0.644596000	4.085110000
1	-0.907462000	-1.466619000	4.203470000
1	0.670022000	1.417039000	2.039400000
1	-0.103358000	1.420500000	2.206690000

-2934.125640

TS6-Ru-triphos

Frequency = - 270.0691 cm⁻¹

1	-7.306830601	-1.143758666	1.098559153
1	-6.977339601	0.872217334	-0.327845847
6	-6.303974601	-0.819876666	0.836366153
6	-6.119679601	0.312813334	0.033821153
1	-5.326243601	-2.412220666	1.918445153
6	-5.194161601	-1.529759666	1.299985153
6	-4.830759601	0.732295334	-0.297761847
1	-4.700208601	1.622481334	-0.906450847
1	-1.934064601	5.466939334	-1.575602847
1	-2.166788601	6.207429334	0.786899153
1	-4.088230601	-5.634120666	0.834145153
1	-4.256730601	-4.409331666	-1.325301847
6	-3.902202601	-1.113006666	0.963744153
6	-2.041695601	4.734117334	-0.781777847
6	-2.173875601	5.149121334	0.544476153
6	-3.708319601	0.020067334	0.164351153
1	-1.940644601	3.080546334	-2.137237847
6	-3.308876601	-4.937930666	0.539690153
6	-2.038453601	3.371341334	-1.097422847
6	-3.403114601	-4.252552666	-0.673097847
1	-3.059096601	-1.690850666	1.321130153
6	-2.309272601	4.196706334	1.561158153
1	-2.411959601	4.511630334	2.595280153
1	-2.121726601	-5.258182666	2.317121153
6	-2.205527601	-4.724461666	1.375290153

6	-2.158568601	2.411693334	-0.084921847
1	-2.679862601	-0.581579666	-2.323705847
6	-2.295065601	2.838490334	1.249836153
6	-2.406791601	-3.346353666	-1.049218847
1	-2.517508601	-2.818738666	-1.989449847
1	-0.726572601	-2.233212666	-2.846918847
1	-2.385838601	2.104768334	2.046878153
1	-1.616977601	-0.792700666	-4.599182847
15	-2.031249601	0.595237334	-0.335347847
6	-1.206969601	-3.826267666	0.998632153
6	-2.007444601	0.266660334	-2.165915847
6	-1.301468601	-3.123802666	-0.216969847
1	-0.351859601	-3.671083666	1.650941153
1	-2.463201601	1.110776334	-2.692232847
1	-1.088867601	0.896752334	-4.703630847
6	-0.111219601	-1.466178666	-2.369775847
6	-0.818821601	-0.094868666	-4.325518847
1	0.898046399	-1.612653666	-2.761386847
6	-0.623010601	-0.059517666	-2.792276847
1	0.100342399	-0.412961666	-4.828667847
15	-0.010035601	-1.858091666	-0.546831847
44	-0.112898601	-0.039038666	0.804487153
1	1.002874399	-4.261048666	-1.903698847
1	1.365844399	5.034009334	2.246821153
1	1.045404399	2.635728334	1.710540153
6	1.456194399	4.696070334	1.218724153
6	1.258456399	3.345493334	0.918268153
6	0.418756399	1.057731334	-2.496315847
6	1.761704399	-3.940696666	-1.194712847
1	-0.055968601	2.027378334	-2.661806847
6	1.549155399	-2.813376666	-0.381943847
1	1.909378399	6.656189334	0.440324153
6	1.761682399	5.606437334	0.204241153
1	1.235926399	0.995211334	-3.219162847
15	1.154347399	1.115795334	-0.788676847
6	1.362201399	2.899959334	-0.406999847
1	3.114271399	-5.530931666	-1.718584847
6	2.951773399	-4.661956666	-1.087790847
6	1.878525399	5.162742334	-1.117873847
6	1.683425399	3.814885334	-1.424037847
6	2.526719399	-2.422238666	0.540489153
1	2.122332399	5.863970334	-1.910514847
1	2.363325399	-1.539089666	1.149011153
1	1.789001399	3.487594334	-2.454017847
6	3.930386399	-4.266794666	-0.166369847
6	2.889879399	0.533927334	-0.956714847

6	3.714798399	-3.150873666	0.645647153
1	3.431379399	1.405064334	0.943341153
1	2.691883399	-0.482433666	-2.867065847
1	4.856790399	-4.828016666	-0.085972847
6	3.778330399	0.833788334	0.090529153
6	3.345108399	-0.232432666	-2.039515847
1	4.474340399	-2.836021666	1.354545153
6	5.095816399	0.376640334	0.047708153
6	4.664485399	-0.692090666	-2.076980847
1	5.771784399	0.614306334	0.863789153
1	4.999227399	-1.288063666	-2.920665847
6	5.542334399	-0.390604666	-1.033510847
1	6.566232399	-0.751265666	-1.060877847
1	1.244207399	-1.229309666	3.477341153
6	1.466222399	-0.144883666	3.409550153
8	1.473229399	0.280150334	2.087183153
8	2.712219399	0.100998334	4.048447153
6	3.774002399	-0.715827666	3.560148153
1	3.531431399	-1.783514666	3.672138153
1	3.986072399	-0.508414666	2.506316153
1	4.657996399	-0.485393666	4.158976153
1	0.738774399	0.412512334	4.019261153
1	-0.865729399	-0.634109334	2.461445847
1	-1.192761601	-1.151601666	1.871741153

-2934.130038

23-Ru-triphos

1	6.393351000	0.840142000	2.272800000
1	4.941094000	2.602564000	3.267250000
6	5.354332000	0.924704000	1.968500000
6	4.536993000	1.914125000	2.530970000
1	5.455470000	-0.712987000	0.565150000
6	4.829271000	0.054234000	1.011350000
6	3.200593000	2.021856000	2.144420000
1	2.585804000	2.803947000	2.581390000
1	0.005368000	6.216440000	1.109560000
1	0.617258000	6.680029000	-1.257390000
1	5.031425000	-5.027086000	0.394680000
1	3.805235000	-4.769135000	2.545470000
6	3.491091000	0.166416000	0.619560000
6	0.323147000	5.406929000	0.459260000
6	0.666797000	5.666699000	-0.870060000
6	2.663322000	1.139727000	1.188850000
1	0.104225000	3.934350000	1.995770000
6	4.131975000	-4.420395000	0.440010000

6	0.377875000	4.103449000	0.960260000
6	3.444765000	-4.273844000	1.648780000
1	3.089310000	-0.499784000	-0.130790000
6	1.070506000	4.615749000	-1.699580000
1	1.337936000	4.806868000	-2.734760000
1	4.184036000	-3.889145000	-1.653040000
6	3.656396000	-3.781364000	-0.709940000
6	0.776194000	3.043539000	0.131620000
1	0.732382000	1.423879000	3.129410000
6	1.124834000	3.311899000	-1.204180000
6	2.289546000	-3.488563000	1.711960000
1	1.769967000	-3.401572000	2.660350000
1	1.087059000	-1.169411000	2.750820000
1	1.435723000	2.509648000	-1.865940000
1	-0.096430000	-0.152260000	4.758630000
15	0.888632000	1.297519000	0.703930000
6	2.507297000	-2.991433000	-0.646750000
6	-0.006508000	1.237270000	2.345710000
6	1.818317000	-2.830302000	0.564670000
1	2.160398000	-2.470723000	-1.532960000
1	-0.719567000	2.065341000	2.371900000
1	-1.533039000	0.858182000	4.507580000
6	0.072649000	-1.340550000	2.375010000
6	-1.036570000	-0.069289000	4.203200000
1	-0.321902000	-2.192720000	2.935790000
6	-0.779330000	-0.073769000	2.678950000
1	-1.678751000	-0.909618000	4.488220000
15	0.271788000	-1.826880000	0.594800000
44	0.003850000	-0.102380000	-0.815250000
1	-1.970133000	-3.252538000	2.124290000
1	-2.471274000	4.637463000	-2.202790000
1	-1.863497000	2.268902000	-1.916480000
6	-2.721685000	4.128543000	-1.277200000
6	-2.377976000	2.786663000	-1.111660000
6	-2.169940000	-0.103838000	1.984250000
6	-1.961744000	-3.575488000	1.089310000
1	-2.850389000	0.554613000	2.528870000
6	-1.003473000	-3.092569000	0.187770000
1	-3.618633000	5.867634000	-0.365440000
6	-3.362964000	4.819234000	-0.244080000
1	-2.598821000	-1.105547000	2.060820000
15	-2.173359000	0.335802000	0.175510000
6	-2.675147000	2.110073000	0.084290000
1	-3.666775000	-4.857356000	1.375090000
6	-2.926425000	-4.496587000	0.667320000
6	-3.663315000	4.157134000	0.949260000

6	-3.324386000	2.809904000	1.112300000
6	-1.018604000	-3.558389000	-1.140300000
1	-4.159344000	4.686215000	1.757800000
1	-0.282583000	-3.196470000	-1.853590000
1	-3.573547000	2.325364000	2.050220000
6	-2.938555000	-4.948557000	-0.654380000
6	-3.649900000	-0.547966000	-0.470290000
6	-1.976975000	-4.481248000	-1.557030000
1	-2.612701000	-1.244977000	-2.231830000
1	-4.967590000	-0.017674000	1.167700000
1	-3.692386000	-5.658676000	-0.980420000
6	-3.554691000	-1.227226000	-1.692280000
6	-4.872060000	-0.546244000	0.223460000
1	-1.979515000	-4.826988000	-2.586350000
6	-4.663192000	-1.900265000	-2.215270000
6	-5.977211000	-1.222103000	-0.296980000
1	-4.575172000	-2.430915000	-3.158610000
1	-6.917111000	-1.218852000	0.247330000
6	-5.874082000	-1.900363000	-1.518320000
1	-6.734122000	-2.427092000	-1.921330000
1	3.804292000	1.283925000	-1.998870000
6	3.701132000	1.220786000	-3.093520000
8	2.365682000	0.926537000	-3.439680000
8	4.631541000	0.289884000	-3.610180000
6	4.553869000	-1.000665000	-3.007490000
1	4.693689000	-0.939326000	-1.919790000
1	3.591259000	-1.483334000	-3.217490000
1	5.355479000	-1.603836000	-3.437760000
1	3.959873000	2.175915000	-3.555510000
1	1.962281000	0.372898000	-2.732580000
1	1.490230000	-0.387032000	-1.467230000

-2934.132778

24-Ru-triphos

1	3.073062000	6.424835000	-0.928351000
1	4.557808000	4.727650000	-1.985148000
6	2.818865000	5.370303000	-0.874748000
6	3.653752000	4.415678000	-1.470151000
1	1.007128000	5.688019000	0.259582000
6	1.661998000	4.959113000	-0.208773000
6	3.328549000	3.059556000	-1.403741000
1	3.988721000	2.330909000	-1.865440000
1	6.009548000	-1.460520000	-1.835090000
1	6.674255000	-1.670022000	0.552536000
1	-2.807514000	6.236901000	2.100091000

1	-2.693706000	6.098659000	-0.381766000
6	1.340765000	3.599430000	-0.138969000
6	5.361386000	-1.076037000	-1.053040000
6	5.734130000	-1.194767000	0.288392000
6	2.163013000	2.637598000	-0.739126000
1	3.883971000	-0.385983000	-2.446913000
6	-2.591818000	5.288530000	1.617068000
6	4.150497000	-0.467332000	-1.398316000
6	-2.527260000	5.211483000	0.222073000
1	0.446361000	3.297851000	0.389896000
6	4.886367000	-0.709018000	1.289976000
1	5.163279000	-0.806760000	2.335811000
1	-2.427552000	4.192662000	3.471522000
6	-2.377358000	4.140650000	2.387899000
6	3.296552000	0.022131000	-0.400565000
1	1.712659000	1.353976000	-3.097161000
6	3.672843000	-0.112051000	0.947611000
6	-2.243154000	3.994218000	-0.403437000
1	-2.193352000	3.960833000	-1.486742000
1	-0.473792000	2.487802000	-2.079185000
1	3.007119000	0.239559000	1.730403000
1	-0.126534000	1.694041000	-4.625205000
15	1.684100000	0.849962000	-0.710370000
6	-2.089694000	2.923696000	1.766033000
6	1.269348000	0.546052000	-2.508195000
6	-2.014296000	2.842412000	0.365727000
1	-1.911801000	2.037240000	2.367415000
1	1.751668000	-0.382580000	-2.824459000
1	0.243571000	-0.017790000	-4.908197000
6	-1.075928000	1.575069000	-2.121526000
6	-0.403454000	0.669872000	-4.352825000
1	-1.950123000	1.808659000	-2.733082000
6	-0.253170000	0.450993000	-2.830993000
1	-1.437765000	0.498321000	-4.670187000
15	-1.633978000	1.203276000	-0.382364000
44	-0.089234000	0.018680000	0.720239000
1	-3.906190000	1.761490000	-2.253729000
1	3.390288000	-4.080329000	1.078556000
1	1.335053000	-2.726679000	1.154905000
6	2.894380000	-3.807475000	0.151783000
6	1.735487000	-3.031724000	0.192464000
6	-0.827629000	-0.961196000	-2.516865000
6	-4.211001000	0.974643000	-1.571724000
1	-0.498575000	-1.669670000	-3.280696000
6	-3.335240000	0.491806000	-0.582386000
1	4.331984000	-4.811849000	-1.107179000

6	3.422525000	-4.219350000	-1.075681000
1	-1.918872000	-0.918425000	-2.588361000
15	-0.430292000	-1.618395000	-0.826833000
6	1.088528000	-2.654781000	-0.997797000
1	-6.162492000	0.837496000	-2.465798000
6	-5.502362000	0.456783000	-1.691940000
6	2.777671000	-3.860221000	-2.261795000
6	1.615501000	-3.083621000	-2.224465000
6	-3.793644000	-0.498918000	0.297028000
1	3.179582000	-4.176532000	-3.219944000
1	-3.129599000	-0.875549000	1.064880000
1	1.138459000	-2.821352000	-3.162270000
6	-5.943121000	-0.545022000	-0.819442000
6	-1.710363000	-2.902406000	-0.501668000
6	-5.087147000	-1.014974000	0.179030000
1	-2.416608000	-3.118665000	-2.542887000
1	-1.234146000	-2.955809000	1.601301000
1	-6.945460000	-0.951385000	-0.917921000
6	-2.507577000	-3.453689000	-1.515082000
6	-1.846601000	-3.378364000	0.811877000
1	-5.415343000	-1.793182000	0.861667000
6	-3.445938000	-4.445816000	-1.211633000
6	-2.777149000	-4.373463000	1.112212000
1	-4.067362000	-4.855428000	-2.002604000
1	-2.875924000	-4.727491000	2.134349000
6	-3.585707000	-4.905523000	0.100770000
1	-4.317804000	-5.672870000	0.334525000
6	1.261635000	2.279889000	2.973639000
1	2.039522000	2.502018000	2.243810000
1	0.517605000	3.082477000	2.966656000
1	1.708508000	2.192945000	3.968181000
8	0.850661000	-2.395731000	3.445679000
6	2.102313000	-1.811840000	3.823501000
1	2.057661000	-0.718653000	3.802004000
1	2.400691000	-2.149771000	4.824372000
1	2.838223000	-2.148039000	3.091457000
6	-0.227628000	-2.076881000	4.293382000
1	0.074854000	-2.105977000	5.346815000
1	-0.994183000	-2.832884000	4.095109000
8	0.659198000	1.029325000	2.600080000
1	-1.303901000	-0.600813000	1.646331000
8	-0.752197000	-0.776583000	4.066419000
1	-1.133134000	-0.771570000	3.152688000
1	0.224496000	0.598967000	3.365536000

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25-Ru-triphos

1	2.587440000	6.289811000	-2.016941000
1	4.238544000	4.563427000	-2.722285000
6	2.415994000	5.243664000	-1.780792000
6	3.344738000	4.272437000	-2.177811000
1	0.542732000	5.601329000	-0.764443000
6	1.271609000	4.859799000	-1.078284000
6	3.126811000	2.927413000	-1.874147000
1	3.858287000	2.186015000	-2.183462000
1	6.065972000	-1.657219000	-1.289903000
1	6.861572000	-0.911103000	0.946561000
1	-3.174808000	6.168328000	0.821288000
1	-3.260499000	5.469362000	-1.565528000
6	1.057449000	3.511064000	-0.771720000
6	5.439013000	-1.021278000	-0.671905000
6	5.885095000	-0.603792000	0.583918000
6	1.977013000	2.531588000	-1.166973000
1	3.861079000	-0.973583000	-2.119206000
6	-2.912023000	5.152074000	0.542328000
6	4.180212000	-0.631125000	-1.141854000
6	-2.958839000	4.760300000	-0.800102000
1	0.166195000	3.232058000	-0.225066000
6	5.063962000	0.208651000	1.375541000
1	5.399471000	0.536620000	2.355297000
1	-2.473512000	4.521142000	2.567119000
6	-2.521812000	4.233150000	1.521850000
6	3.349468000	0.175653000	-0.354182000
1	1.729169000	0.809338000	-3.247996000
6	3.805634000	0.589943000	0.910334000
6	-2.608419000	3.457764000	-1.165056000
1	-2.641951000	3.180103000	-2.213589000
1	-0.617155000	1.889444000	-2.496960000
1	3.168962000	1.213444000	1.531858000
1	-0.076473000	0.711285000	-4.845838000
15	1.657096000	0.740865000	-0.811453000
6	-2.173068000	2.929466000	1.159836000
6	1.332838000	0.083271000	-2.532324000
6	-2.204889000	2.534274000	-0.186894000
1	-1.852525000	2.230348000	1.925433000
1	1.900916000	-0.840157000	-2.668293000
1	0.456879000	-0.980490000	-4.819103000
6	-1.116578000	0.922496000	-2.380725000
6	-0.270736000	-0.273059000	-4.406406000
1	-1.990206000	0.943940000	-3.035718000
6	-0.160381000	-0.212836000	-2.866816000

1	-1.272268000	-0.594192000	-4.712448000
15	-1.692208000	0.814483000	-0.605731000
44	-0.094460000	-0.021391000	0.715251000
1	-3.959653000	0.871324000	-2.574017000
1	3.646100000	-3.687321000	1.938318000
1	1.522142000	-2.469708000	1.676888000
6	3.182527000	-3.623441000	0.958345000
6	1.982650000	-2.928659000	0.806274000
6	-0.607944000	-1.600619000	-2.324446000
6	-4.220339000	0.191833000	-1.769221000
1	-0.176089000	-2.393190000	-2.940833000
6	-3.332501000	-0.047188000	-0.704449000
1	4.729101000	-4.757067000	-0.034120000
6	3.790189000	-4.223947000	-0.149244000
1	-1.694323000	-1.684587000	-2.433447000
15	-0.235189000	-1.908070000	-0.531571000
6	1.370158000	-2.822830000	-0.455782000
1	-6.138819000	-0.241161000	-2.640716000
6	-5.468279000	-0.433913000	-1.808309000
6	3.186883000	-4.128582000	-1.405492000
6	1.982566000	-3.434228000	-1.558774000
6	-3.734417000	-0.906248000	0.327269000
1	3.652336000	-4.590039000	-2.271555000
1	-3.058434000	-1.092389000	1.152930000
1	1.537444000	-3.381647000	-2.546285000
6	-5.852993000	-1.301690000	-0.779576000
6	-1.415328000	-3.238826000	-0.040858000
6	-4.984824000	-1.530078000	0.290578000
1	-1.860055000	-3.941311000	-2.046644000
1	-1.187419000	-2.807355000	2.060384000
1	-6.821785000	-1.791489000	-0.813526000
6	-2.034912000	-4.072729000	-0.984023000
6	-1.650378000	-3.458531000	1.325287000
1	-5.270058000	-2.202209000	1.094601000
6	-2.898278000	-5.090847000	-0.566446000
6	-2.504283000	-4.481497000	1.741042000
1	-3.382920000	-5.720236000	-1.307201000
1	-2.683531000	-4.634888000	2.801337000
6	-3.136899000	-5.296544000	0.795429000
1	-3.810554000	-6.085078000	1.117814000
6	0.949536000	2.597551000	2.720466000
1	1.267260000	2.940436000	1.738669000
1	0.137621000	3.229113000	3.091590000
1	1.798596000	2.626915000	3.412553000
8	0.650800000	-0.716031000	3.812374000
6	2.072769000	-0.795415000	3.973866000

1	2.589573000	-0.406101000	3.092801000
1	2.396441000	-0.243183000	4.866116000
1	2.313586000	-1.852819000	4.095600000
6	0.138306000	0.575962000	3.797591000
1	0.530339000	1.177854000	4.629222000
1	-0.946706000	0.498251000	3.847888000
8	0.492731000	1.240473000	2.562992000
1	-1.248750000	-0.594582000	1.700460000
8	-2.031876000	2.815104000	4.440326000
1	-1.884766000	2.903521000	5.391614000
1	-2.980801000	2.652658000	4.349478000

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26-Ru-triphos

1	3.789411000	5.814568000	-1.505266000
1	5.048273000	3.853588000	-2.384432000
6	3.414624000	4.808524000	-1.341102000
6	4.122385000	3.705472000	-1.836003000
1	1.668941000	5.453213000	-0.242672000
6	2.227495000	4.607422000	-0.633007000
6	3.641686000	2.411232000	-1.626917000
1	4.203524000	1.565596000	-2.013499000
1	5.663499000	-2.527044000	-1.701605000
1	6.483415000	-2.464325000	0.646198000
1	-1.959144000	6.615842000	1.673237000
1	-2.022586000	6.244117000	-0.786044000
6	1.750390000	3.309416000	-0.420368000
6	5.133945000	-1.943100000	-0.954461000
6	5.594273000	-1.908292000	0.363868000
6	2.445592000	2.199146000	-0.918328000
1	3.655142000	-1.275130000	-2.354116000
6	-1.882909000	5.609310000	1.272851000
6	3.987096000	-1.231594000	-1.322658000
6	-1.917933000	5.400650000	-0.109974000
1	0.832019000	3.173407000	0.136819000
6	4.899137000	-1.159520000	1.320529000
1	5.244820000	-1.130379000	2.349935000
1	-1.721498000	4.671987000	3.212595000
6	-1.748179000	4.517930000	2.137817000
6	3.281888000	-0.483353000	-0.370515000
1	1.783430000	0.763642000	-3.127605000
6	3.749612000	-0.458961000	0.955449000
6	-1.814238000	4.107407000	-0.630155000
1	-1.839296000	3.970643000	-1.706307000
1	-0.224957000	2.258446000	-2.174839000

1	3.206623000	0.106750000	1.706790000
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6	-5.453983000	0.821450000	-1.607013000
6	2.179001000	-4.471695000	-1.754109000
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-2973.415962

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