Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic supporting information for

Effect of chelating ring size in catalytic ketone hydrogenation: Facile synthesis of ruthenium(II) precatalysts containing an N-heterocyclic carbene with a primary amine donor for ketone hydrogenation and a DFT study of mechanisms

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Section 1 Synthesis of imidazolium salt 2

This procedure was slightly modified and the yields obtained for the imidazolium product were similar.[1] Under an argon atmosphere, 1-methylimidazole (5.20 mL, 65.4 mmol) and 2-chloroethylamine hydrochloride (1.50 g, 13.0 mmol) were dissolved in toluene (8 mL). The reaction mixture was refluxed for 3 h with constant stirring. On completion, the solution was cooled to room temperature and the toluene layer was decanted. The crude oil that obtained was washed with diethyl ether (3 × 10 mL) and dried in vacuo. To this was added dry acetone (38 mL) and KPF_6 (2.87 g, 15.7 mmol) at room temperature and the resultant mixture was stirred for 24 h. An off-white solid was collected by filtration, washed with dry acetone (3 × 5 mL), and dried in vacuo. Yield: 2.27 g, 60%. ^{1}H NMR (DMSO-d_6, δ): 9.32 (s, 2-CH of imid., 1H), 8.80 (br, NH_2, 2H), 7.86 (t, J_{HH} = 1.78 Hz, 4-CH of imid., 1H), 7.74 (t, J_{HH} = 1.78 Hz, 5-CH of imid., 1H), 4.56 (t, J_{HH} = 5.76 Hz, CH_2, 2H), 3.85 (s, CH_3, 3H), 3.31 (t, J_{HH} = 5.76 Hz, CH_2, 2H). ^{19}F NMR (DMSO-d_6, δ): -70.6 (d, J_{PF} = 713 Hz). ^{13}C{^{1}H} NMR (DMSO-d_6, δ): 137.4 (N*C*N), 123.6 ($C_{imid.}$), 122.4 ($C_{imid.}$), 46.0 (CH_2), 38.3 (CH_3), 35.7 (CH_2 adjacent to NH_2). MS (ESI, methanol/water; *m/z*): 126.1 ($[M]^+$). HRMS (ESI, methanol/water; *m/z*): calcd for $C_6H_{12}N_3^+$ ($[M]^+$): 126.1022, found: 126.1025. Anal. Calcd for $C_6H_{12}N_3F_6P \cdot 0.5(HCl)$: C, 24.90; H, 4.35; N, 14.52. Found: C, 24.81; H, 4.26; N, 14.20.

1. R. D. Singer, *Private Communication*.

Section 2 Hydrogenation of acetophenone catalyzed by complexes $4 \cdot PF_6$ and 5

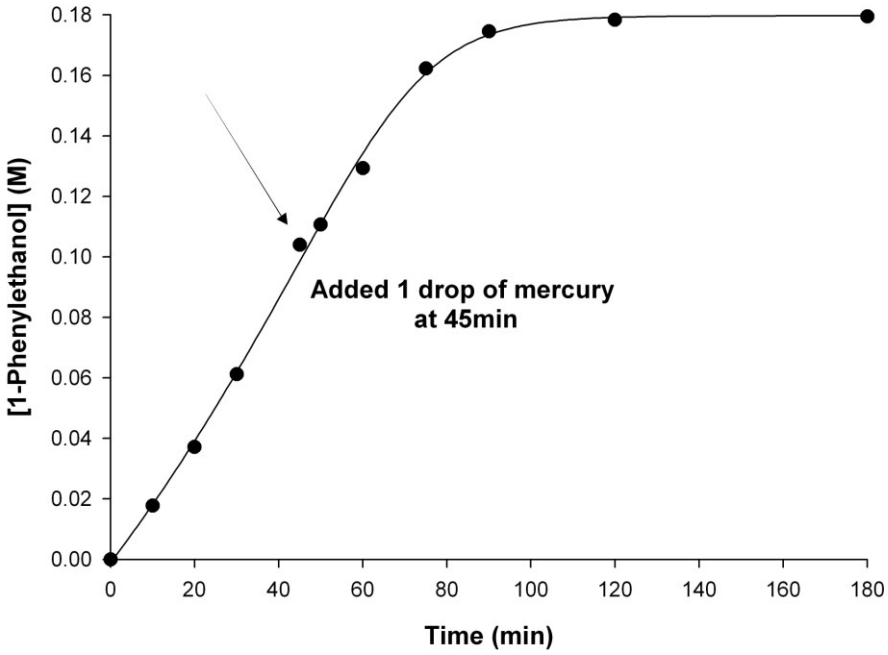


Fig. S1 Transfer hydrogenation of acetophenone (1.1 mmol) to 1-phenylethanol in 2-propanol (6 mL) catalyzed by $\mathbf{4 \cdot PF_6}$ (5.5 μmol) in the presence of potassium *tert*-butoxide (45 μmol). Mercury poisoning test was conducted by adding a drop of mercury to the reaction mixture at 45 min.

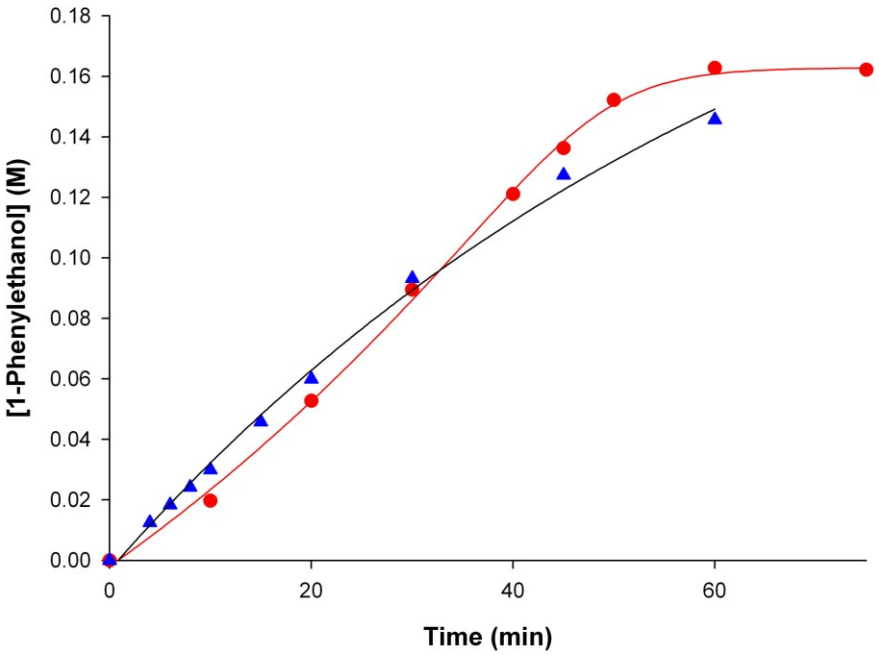


Fig. S2 H_2-Hydrogenation of acetophenone (0.17 M) to 1-phenylethanol in THF catalyzed by complex **1a** (0.84 mM, in blue triangles) or complex **4·PF$_6$** (0.84 mM, in red circles) in the presence of potassium *tert*-butoxide (7 mM) under 25 bar of H_2 pressure at 50˚C. The H_2-hydrogenation result for complex **1a** was reported in ref 2.

2. W. W. N. O, A. J. Lough and R. H. Morris, *Organometallics*, 2011, **30**, 1236-1252.

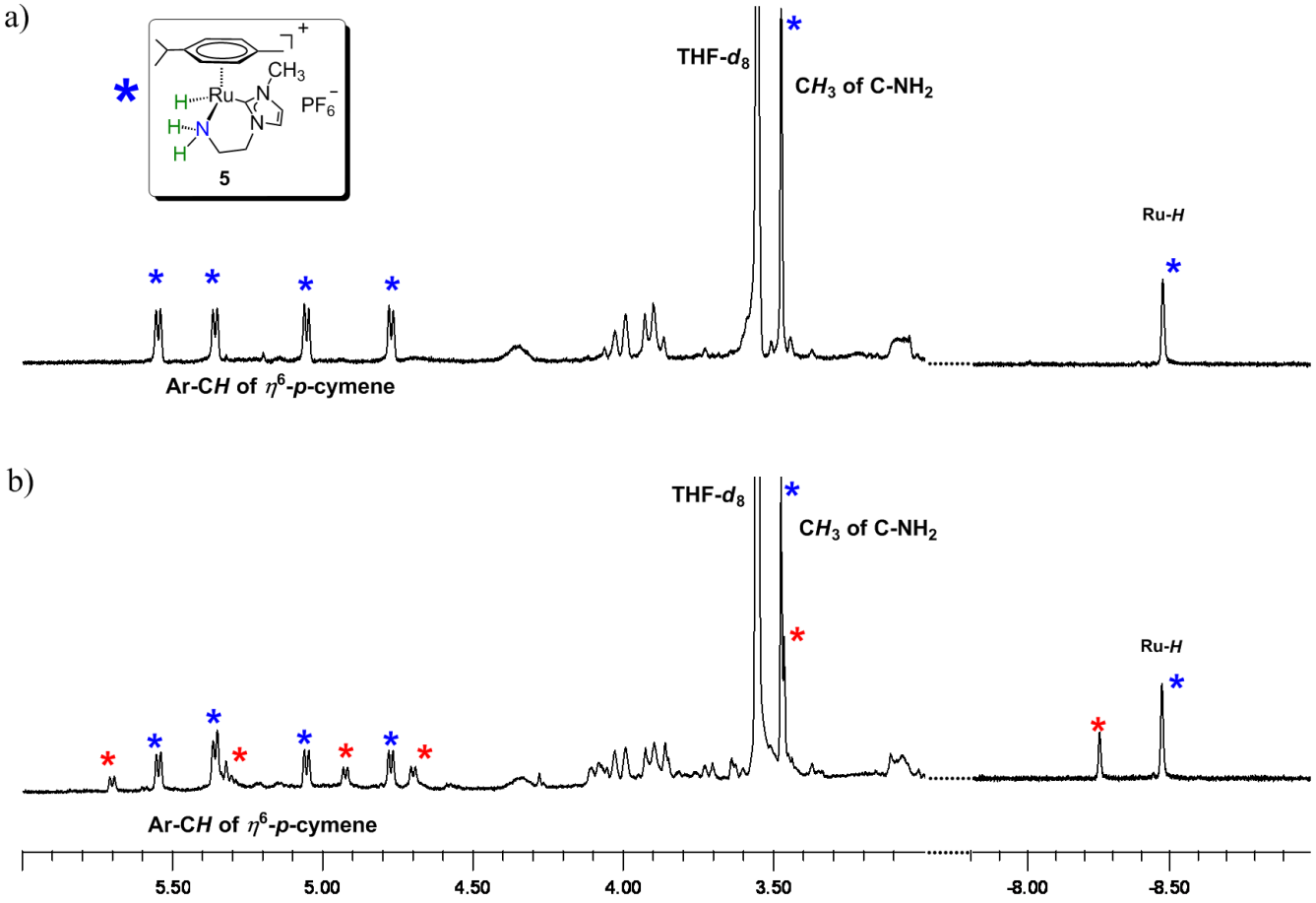
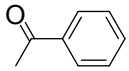
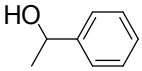
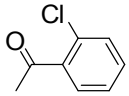
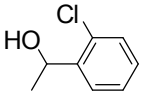
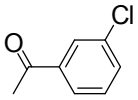
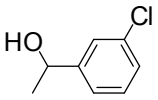
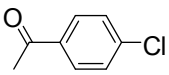
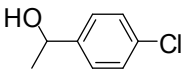
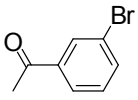
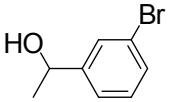
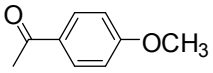
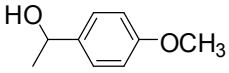
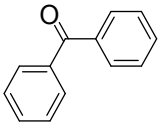
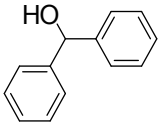
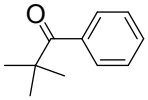
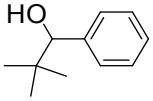


Fig. S3 Partial ^{1}H NMR (400 MHz) spectra in THF-d_8 showing (a) the hydride-amine complex **5**; (b) isolated products from the reaction of complex **4**·$\mathbf{PF_6}$ and 10 equiv of sodium 2-propoxide in 2-propanol, these included complex **5** (noted in blue asterisk) and a structurally similar species (noted in red asterisk).

Section 3 GC conditions for all of the ketone substrates and alcohol products

Table S1 The oven temperatures, retention times (t_R, t_p, /min) for all the substrates and alcohol products reported from GC analyses

Substrates/Alcohol Products		Oven Temperature (^oC)	t_R (min)	t_P (min)
		130	4.56	7.58, 8.03
		145	4.63	10.34, 12.16
		140	6.46	14.81, 16.05
		145	5.96	11.03, 12.09
		145	8.22	18.97, 20.40
		140	10.61	13.50, 14.28
		180	7.94	12.57
		140	5.67	13.15, 13.78

Section 4 Computed outer-sphere bifunctional mechanism for the transfer hydrogenation of acetophenone in 2-propanol

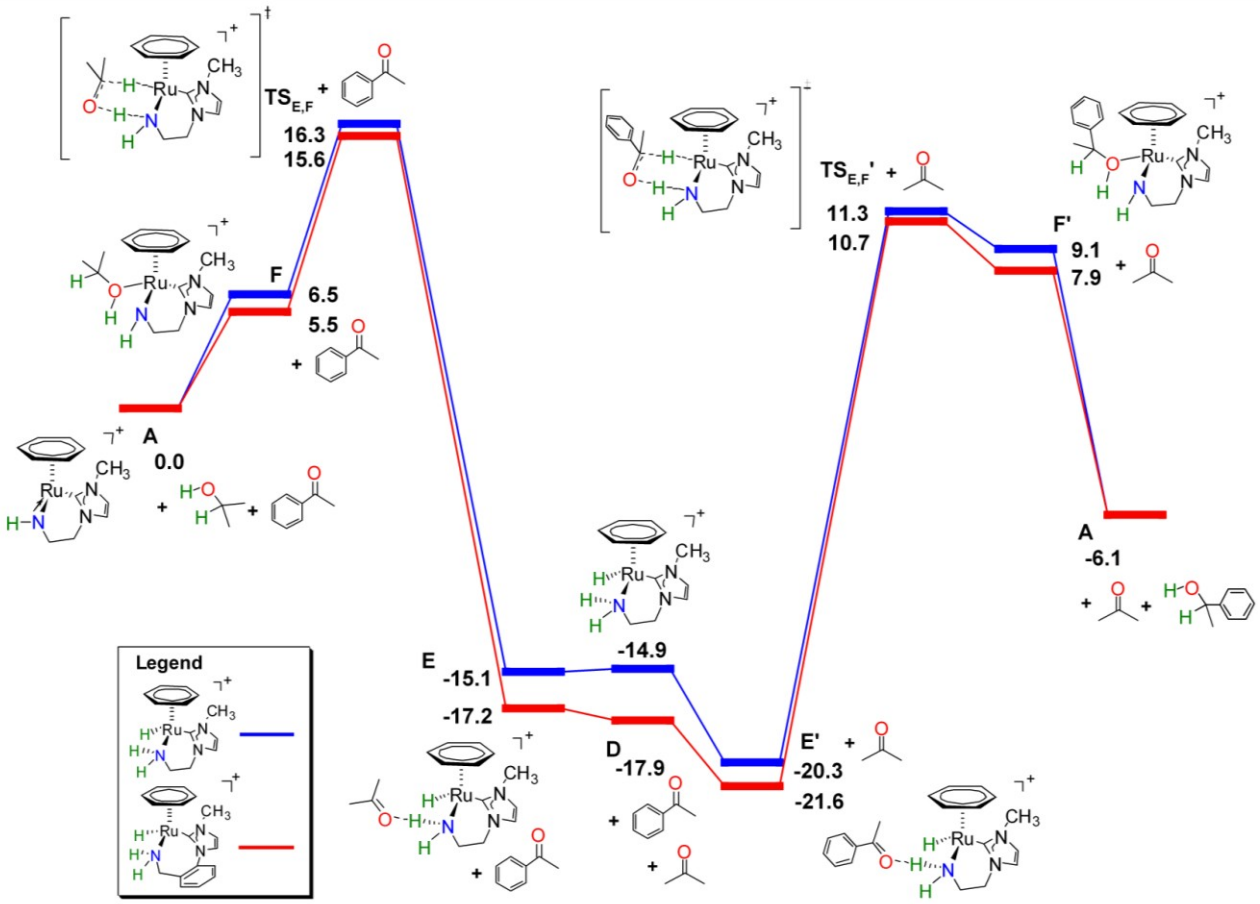


Fig. S4 The free energy profile for the outer-sphere bifunctional mechanism in the transfer hydrogenation of acetophenone in 2-propanol starting from **A** and moving to the right. Pathway colored in blue represents catalysis involving the 6-membered-chelating ring system ($\mathbf{A_6}$) and the one in red represents catalysis involving the 7-membered-chelating ring system ($\mathbf{A_7}$). The gas phase free energies (1 atm, 298 K) are reported relative to **A**, 2-propanol and acetophenone in kcal/mol.

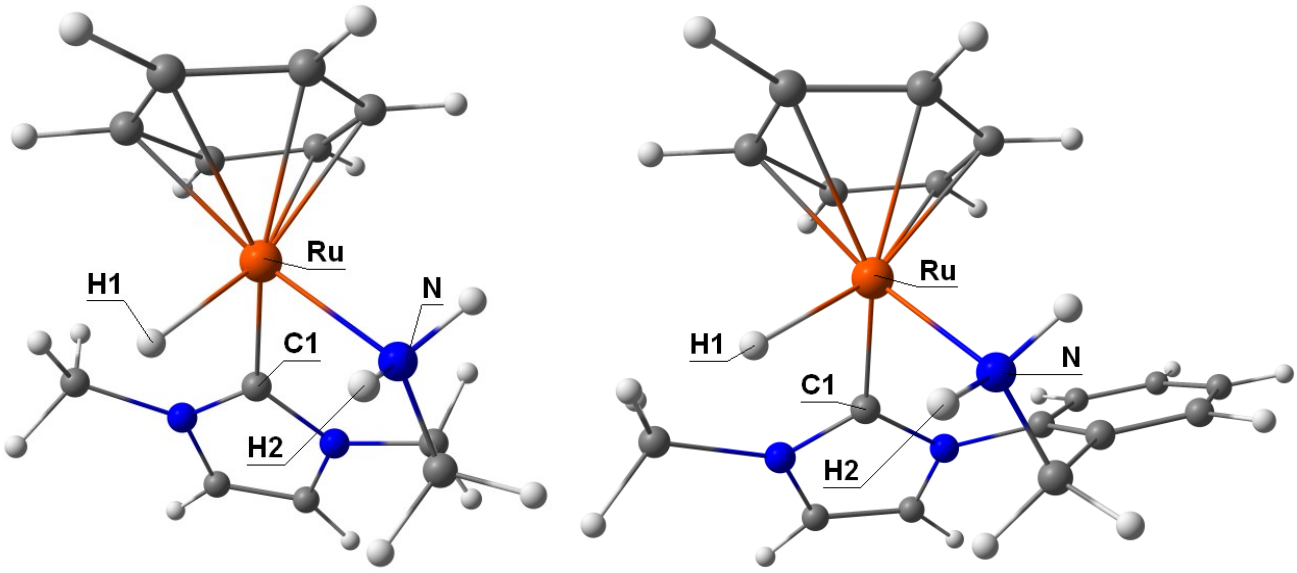


Fig. S5 Computed structures of $[Ru(\eta^6\text{-}C_6H_6)(C\text{–}NH_2)H]^+$ ($\mathbf{D_6}$, left; $\mathbf{D_7}$, right). The color codes for the atoms are: ruthenium (orange), nitrogen (blue), carbon (grey) and hydrogen (white). Selected bond distances (Å) and angles (deg): $\mathbf{D_6}$, Ru–C1, 2.02; Ru–N1, 2.17; Ru–H1, 1.58; N–H2, 1.02; H1–H2, 2.45; H1–Ru–C1, 83.1; $\mathbf{D_7}$, Ru–C1, 2.03; Ru–N1, 2.16; Ru–H1, 1.72; Ru–H2, 1.58; N–H2, 1.02; H1–H2, 2.32; H1–Ru–C1, 81.2.

Section 5 Computed outer-sphere bifunctional mechanism for the H_2-hydrogenation of acetophenone

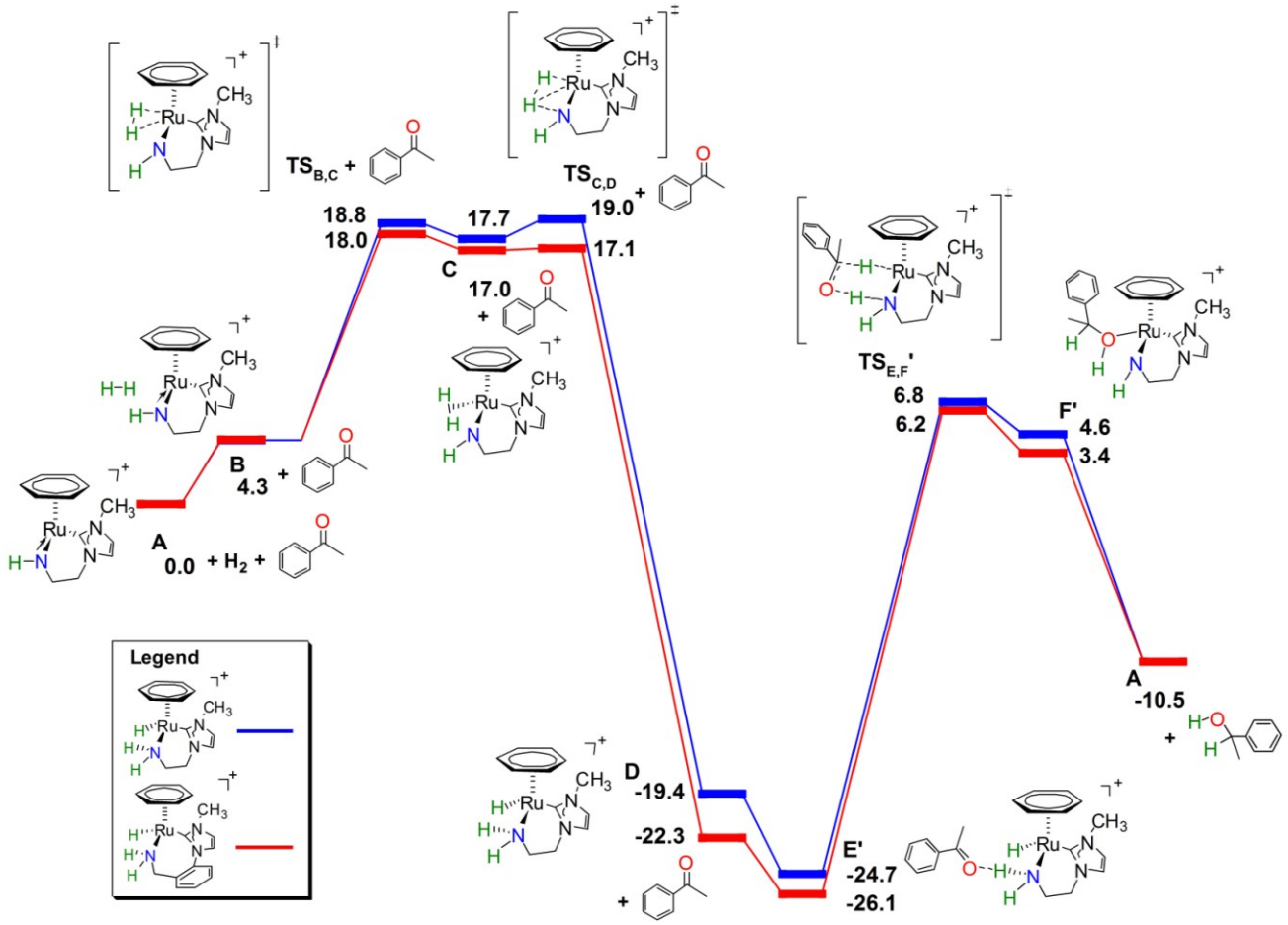


Fig. S6 The free energy profile for the outer-sphere bifunctional mechanism in the H_2-hydrogenation of acetophenone starting from **A** and moving to the right. Pathway colored in blue represents catalysis involving the 6-membered-chelating ring system ($\mathbf{A_6}$) and the one in red represents catalysis involving the 7-membered-chelating ring system ($\mathbf{A_7}$). The gas phase free energies (1 atm, 298 K) are reported relative to **A**, H_2 and acetophenone in kcal/mol.

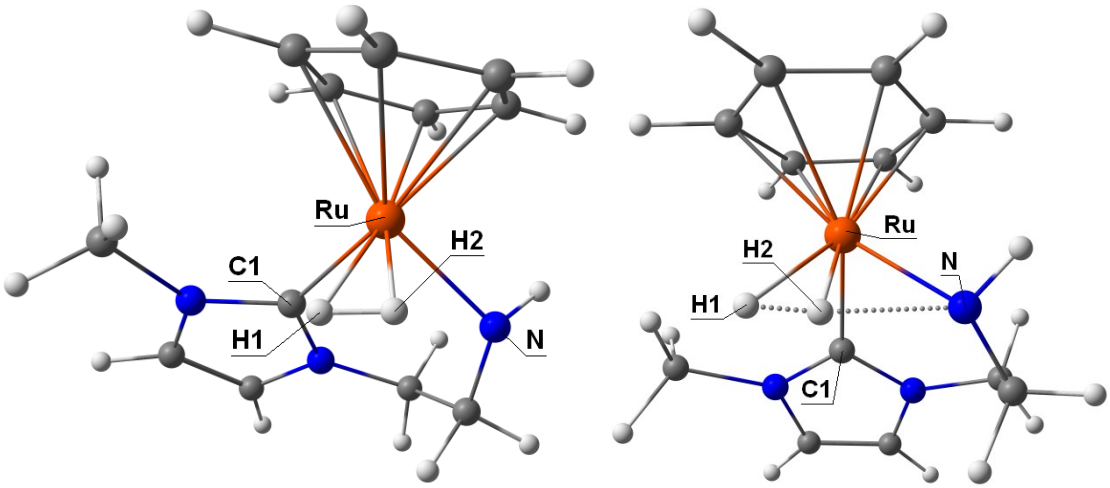


Fig. S7 Computed structure of $[Ru(\eta^6\text{-}C_6H_6)(\eta^2\text{-}H_2)(C\text{–}NH)]^+$ (**C_6**, left) and the transition state structure for the heterolytic splitting of H_2 (**$TS_{C,D(6)}$**, right). The color codes for the atoms are: ruthenium (orange), nitrogen (blue), carbon (grey) and hydrogen (white). Selected bond distances (Å): **C_6**, Ru–C1, 2.06; Ru–N1, 2.06; Ru–H1, 1.75; Ru–H2, 1.75; H1–H2, 0.84; **$TS_{C,D(6)}$**, Ru–C1, 2.04; Ru–N1, 2.11; Ru–H1, 1.72; Ru–H2, 1.71; N–H2, 1.70; H1–H2, 0.90.

Section 6 Computed inner-sphere mechanism for the transfer hydrogenation of acetophenone in 2-propanol

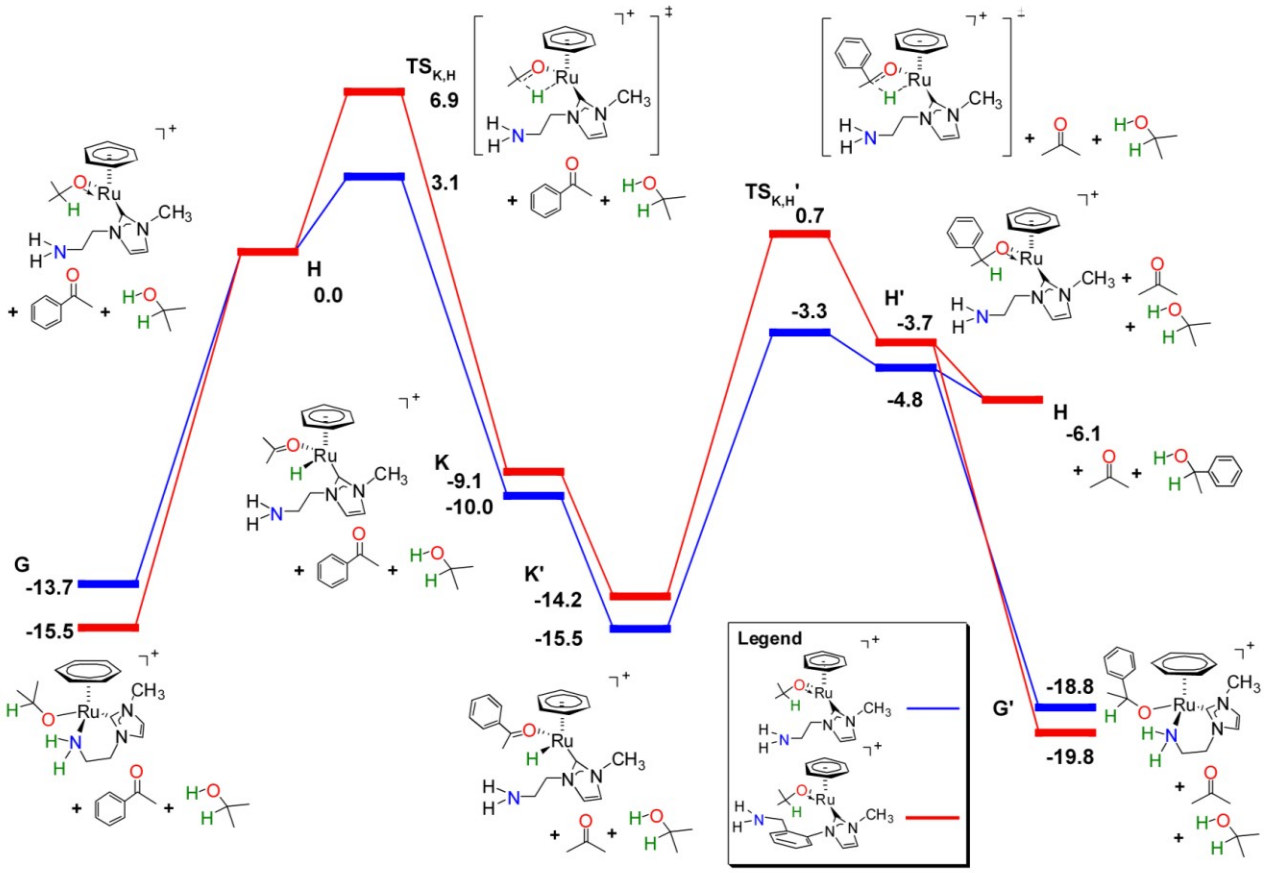


Fig. S8. The free energy profile for the inner-sphere mechanism in the transfer hydrogenation of acetophenone in 2-propanol starting from **H** and moving to the right. Pathway colored in blue represents catalysis involving the 6-membered-chelating ring system ($\mathbf{H_6}$) and the one in red represents catalysis involving the 7-membered-chelating ring system ($\mathbf{H_7}$). The gas phase free energies (1 atm, 298 K) are reported relative to **H**, 2-propanol and acetophenone in kcal/mol.

Section 7 Computed inner-sphere mechanism for the H_2-hydrogenation of acetone

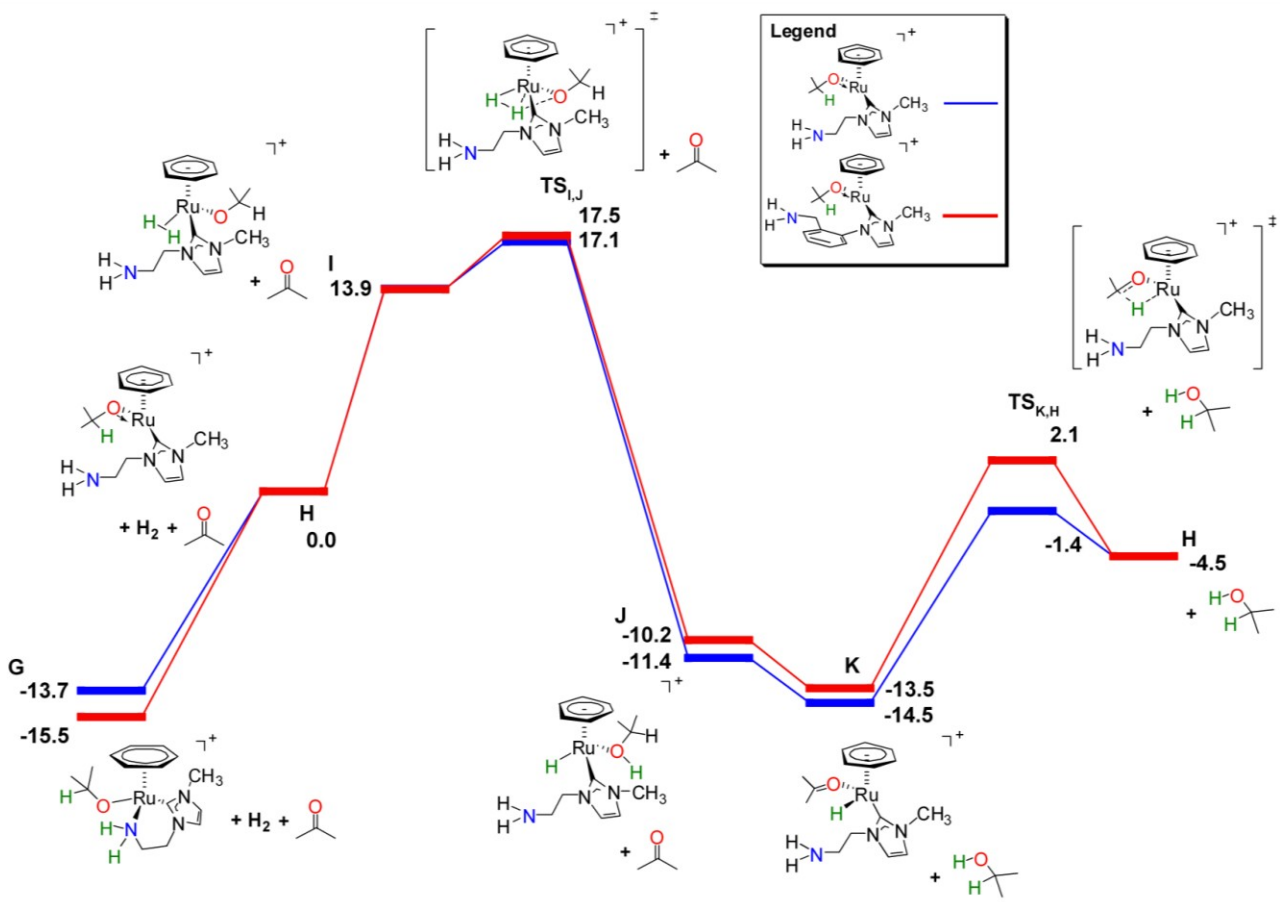


Fig. S9 The free energy profile for the inner-sphere mechanism in the H_2-hydrogenation of acetone starting from **H** and moving to the right. Pathway colored in blue represents catalysis involving the 6-membered-chelating ring system (**H$_6$**) and the one in red represents catalysis involving the 7-membered-chelating ring system (**H$_7$**). The gas phase free energies (1 atm, 298 K) are reported relative to **H**, H_2 and acetone in kcal/mol.

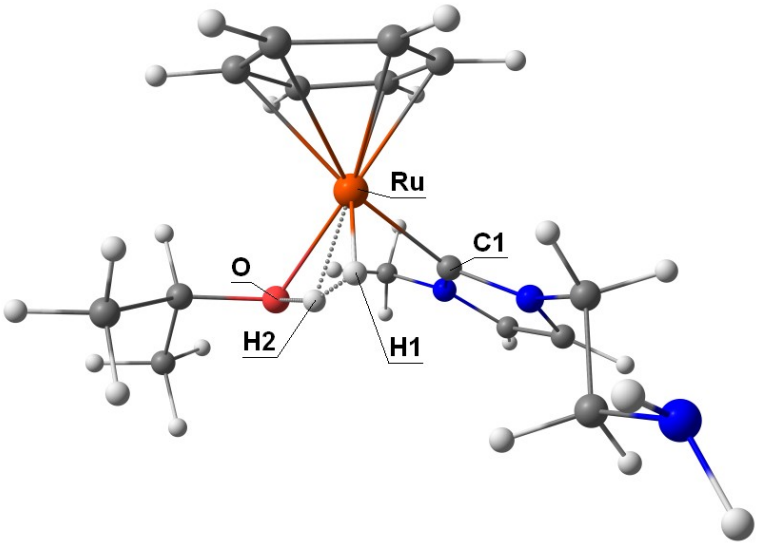


Fig. S10 Computed transition state structure for the heterolytic splitting of H_2 in the inner-sphere mechanism (**$TS_{I,J}$**). The color codes for the atoms are: ruthenium (orange), nitrogen (blue), carbon (grey) and hydrogen (white). Selected bond distances (Å): Ru–C1, 2.05; Ru–O, 2.10; Ru–H1, 1.73; Ru–H2, 1.73; O–H2, 1.59; H1–H2, 0.90.

Section 8

Complete citation for reference 26:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. J. Montgomery, S. R. E., J. Burant, S. C.; Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. G. Johnson, W. Chen, M. W. Wong, J. L. Andres, M. Head-Gordon, E. S. Replogle and J. A. Pople, *Gaussian 03, Revision C.02 ed; Gaussian Inc.: Wallingford, CT*, 2004.

Complete citation for reference 27:

M. J. T. Frisch, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., *Gaussian 09, Revision A.1; Gaussian Inc.: Wallingford, CT*, 2009.

Section 9 Cartesian coordinates and energies for all of the computed structures

1. Hydrogen

H	0.32157	-0.18575	0.00000
H	-0.32157	0.18575	0.00000

Sum of electronic and thermal Enthalpies= -1.160215
Sum of electronic and thermal Free Energies= -1.175007

2. Acetone

C	0.37008	0.15088	-0.49747
O	1.07498	0.43813	-1.44344
C	-0.80362	1.01137	-0.09292
C	0.62388	-1.08463	0.33401
H	-0.84433	1.90436	-0.71544
H	-0.72810	1.29512	0.96138
H	-1.73504	0.44641	-0.20318
H	0.87436	-0.79773	1.36067
H	1.44453	-1.65994	-0.09272
H	-0.27673	-1.70398	0.38910

Sum of electronic and thermal Enthalpies= -193.030215
Sum of electronic and thermal Free Energies= -193.065104

3. 2-Propanol

O	0.84093	-0.97286	1.01106
C	0.35455	0.13183	0.25214
H	1.02679	0.99199	0.39598
C	-1.00603	0.47677	0.82585
C	0.29400	-0.20406	-1.23143
H	1.28538	-0.45783	-1.62179
H	-0.36842	-1.05801	-1.40002
H	-0.07984	0.64597	-1.80982
H	-1.69442	-0.36323	0.69656
H	-1.42635	1.35286	0.32531
H	-0.92483	0.69104	1.89367
H	1.69825	-1.23446	0.66249

Sum of electronic and thermal Enthalpies= -194.213443
Sum of electronic and thermal Free Energies= -194.247206

4. Acetophenone

C	0.00000	-1.40604	-1.16938
O	0.00000	-1.42224	-2.38286
C	0.00000	-2.66638	-0.34370
H	0.00000	-3.54300	-0.99124
H	-0.87648	-2.68101	0.31204
H	0.87648	-2.68101	0.31204
C	0.00000	-0.10409	-0.41034
C	-1.20712	0.50551	-0.06280
C	1.20712	0.50551	-0.06280
C	-1.20536	1.71851	0.62157
C	1.20536	1.71851	0.62157
C	0.00000	2.32610	0.96602
H	-2.14829	0.03933	-0.33754
H	2.14829	0.03933	-0.33754
H	-2.14687	2.18995	0.88311
H	2.14687	2.18995	0.88311
H	0.00000	3.27106	1.49872

Sum of electronic and thermal Enthalpies= -384.669648
Sum of electronic and thermal Free Energies= -384.709879

5. 1-Phenylethanol

O	1.11030	1.66192	1.60889
H	0.34359	2.24166	1.55969
C	1.25344	0.99521	0.36079
H	1.48456	1.72941	-0.42563
C	2.44154	0.05781	0.51126
H	3.33203	0.62572	0.79082
H	2.24087	-0.68183	1.29043
H	2.63545	-0.46924	-0.42560
C	-0.00956	0.25946	-0.03992
C	-0.44143	0.26198	-1.36769
C	-0.74721	-0.45614	0.90834
C	-1.58164	-0.44376	-1.74738
C	-1.88957	-1.15753	0.53298
C	-2.30897	-1.15577	-0.79679
H	0.11818	0.82290	-2.11174
H	-0.42222	-0.45182	1.94396
H	-1.90508	-0.43103	-2.78317
H	-2.45429	-1.70711	1.27923
H	-3.19998	-1.70185	-1.08847

Sum of electronic and thermal Enthalpies= -385.858938
Sum of electronic and thermal Free Energies= -385.901685

6. A_6

C	1.97422	-1.33173	-1.59631
C	0.79637	2.98203	-1.14168
C	1.93510	2.27701	-1.34115
C	-1.49350	2.50327	-0.32713
H	-3.01093	-1.90808	-0.36150
C	-2.37038	-1.66344	0.47753
C	-1.52417	-2.66100	1.04514
C	-2.42373	-0.36493	1.04871
C	-0.62060	-2.29890	2.05766
C	-1.53405	-0.01835	2.08633
C	-0.58388	-0.95699	2.54900
H	0.14940	-0.67019	3.29219
H	2.74020	-2.10853	-1.69140
H	1.61059	-1.10730	-2.60899
H	-1.65922	3.49389	-0.74785
H	0.56222	4.01373	-1.34633
H	2.88866	2.57414	-1.74595
H	-2.18244	1.80494	-0.79964
H	-1.67999	2.54813	0.74642
H	-1.50553	-3.66026	0.62635
H	-3.11386	0.36485	0.64920
H	0.10572	-3.01802	2.41838
H	-1.50936	0.99284	2.47232
N	-0.12522	2.10811	-0.60395
N	1.67207	0.99289	-0.92413
Ru	-0.33163	-0.90094	0.36332
C	0.40720	0.86428	-0.44788
N	0.89292	-1.81333	-0.75652
H	0.84629	-2.82730	-0.78380
C	2.62567	-0.10576	-0.99821
H	3.46266	0.22205	-1.61658
H	2.99921	-0.32713	0.00646

Sum of electronic and thermal Enthalpies= -725.523183
Sum of electronic and thermal Free Energies= -725.579871

7. B_6

C	2.20796	-1.28782	-1.26913
C	0.88576	2.99820	-0.99450

C	2.05237	2.32239	-1.12057
C	-1.42440	2.47480	-0.26950
H	-2.83280	-1.93765	-0.23596
C	-2.22814	-1.66935	0.62215
C	-1.38605	-2.64352	1.23558
C	-2.32454	-0.36402	1.17112
C	-0.52696	-2.25112	2.27464
C	-1.47722	0.01491	2.23257
C	-0.52803	-0.90022	2.74288
H	0.17431	-0.58909	3.50593
H	2.99920	-2.04400	-1.30462
H	1.88902	-1.10137	-2.30431
H	-1.59674	3.45102	-0.72020
H	0.63147	4.01586	-1.24115
H	3.01459	2.63626	-1.49076
H	-2.07114	1.74757	-0.75797
H	-1.66212	2.53815	0.79285
H	-1.33572	-3.64860	0.83362
H	-3.01246	0.34707	0.73572
H	0.19710	-2.95219	2.67345
H	-1.48211	1.03292	2.60134
N	-0.03408	2.11300	-0.47250
N	1.80753	1.04379	-0.67644
Ru	-0.19856	-0.87321	0.56997
C	0.52625	0.89106	-0.25437
N	1.10032	-1.77839	-0.46985
H	1.08334	-2.79362	-0.47021
C	2.79429	-0.02779	-0.67427
H	3.65105	0.30833	-1.26016
H	3.12376	-0.21208	0.35300
H	-2.25050	-0.40126	-3.45991
H	-1.76674	-0.46000	-2.89845

Sum of electronic and thermal Enthalpies= -726.682454
Sum of electronic and thermal Free Energies= -726.748067

8. $TS_{B,C(6)}$

C	1.96144	-1.23198	-1.57921
C	0.57130	3.00210	-1.21549
C	1.76448	2.37509	-1.34031
C	-1.72134	2.37507	-0.50706
H	-3.34638	-1.53912	0.83702
C	-2.38002	-1.39152	1.30534
C	-1.50003	-2.51087	1.47341
C	-2.02005	-0.11751	1.78131
C	-0.22596	-2.31588	2.01537
C	-0.69810	0.09514	2.23710
C	0.22602	-0.99329	2.32253
H	1.23429	-0.82490	2.67890
H	2.76040	-1.95145	-1.78781
H	1.50561	-0.97318	-2.54481
H	-2.04114	3.10512	-1.25063
H	0.27728	4.01300	-1.44583
H	2.71566	2.73214	-1.69997
H	-2.31632	1.47219	-0.62584
H	-1.88065	2.79427	0.48891
H	-1.80011	-3.49139	1.12449
H	-2.71457	0.70805	1.70176
H	0.46264	-3.15047	2.08752
H	-0.36459	1.09451	2.49009
N	-0.31900	2.06715	-0.72473
N	1.57143	1.07726	-0.92184
Ru	-0.42644	-0.88551	0.30837

C	0.29327	0.86831	-0.52766
N	0.97716	-1.83288	-0.70635
H	1.40398	-2.59310	-0.18938
C	2.58502	0.02770	-0.99915
H	3.38897	0.40018	-1.63719
H	2.99095	-0.16062	-0.00049
H	-1.39948	-1.49607	-1.56249
H	-1.53573	-0.74754	-1.58590

Sum of electronic and thermal Enthalpies= -726.666128
Sum of electronic and thermal Free Energies= -726.724959

9. C_6

C	1.88083	-1.29460	-1.64349
C	0.63468	3.00003	-1.16503
C	1.80072	2.33783	-1.34262
C	-1.66278	2.42402	-0.43163
H	-3.34979	-1.75544	0.80443
C	-2.39957	-1.51165	1.26616
C	-1.44204	-2.54898	1.48235
C	-2.15605	-0.18857	1.70116
C	-0.18790	-2.21334	2.00900
C	-0.86496	0.14169	2.16088
C	0.14117	-0.86034	2.30039
H	1.12480	-0.59923	2.66832
H	2.66427	-2.01290	-1.91889
H	1.34899	-1.04107	-2.56970
H	-1.95350	3.22855	-1.10685
H	0.37137	4.02919	-1.34614
H	2.75629	2.67530	-1.70924
H	-2.29787	1.56136	-0.62138
H	-1.80029	2.76394	0.59735
H	-1.65972	-3.56644	1.18398
H	-2.92286	0.56880	1.60452
H	0.56937	-2.98285	2.11193
H	-0.62298	1.16992	2.40484
N	-0.27644	2.07753	-0.68943
N	1.57510	1.03071	-0.96909
Ru	-0.53357	-0.87074	0.20324
C	0.30064	0.85156	-0.55251
N	0.97927	-1.92608	-0.71449
H	1.54853	-2.34321	0.01608
H	-1.16090	-1.51425	-1.29511
C	2.56142	-0.03600	-1.12062
H	3.32197	0.32736	-1.81574
H	3.04211	-0.22709	-0.15550
H	-1.33031	-0.69502	-1.34716

Sum of electronic and thermal Enthalpies= -726.668317
Sum of electronic and thermal Free Energies= -726.726649

10. $TS_{C,D(6)}$

C	2.18790	-0.97930	-1.42257
C	0.20129	2.97020	-1.42187
C	1.47350	2.51518	-1.32680
C	-2.06813	2.05197	-0.96368
H	-2.58748	-2.92449	0.98878
C	-1.90884	-2.18801	1.40335
C	-0.60944	-2.56559	1.77600
C	-2.33295	-0.83039	1.52427
C	0.29973	-1.58016	2.26069
C	-1.42545	0.13720	1.99422
C	-0.09874	-0.23946	2.38578
H	0.59636	0.51028	2.73782

H	3.09057	-1.60114	-1.46196
H	1.95345	-0.70627	-2.45632
H	-2.41610	2.38558	-1.94235
H	-0.18774	3.91124	-1.77499
H	2.41094	2.98267	-1.58020
H	-2.47685	1.06287	-0.76154
H	-2.40423	2.75640	-0.20393
H	-0.28863	-3.59333	1.65851
H	-3.33167	-0.54158	1.22678
H	1.32002	-1.85847	2.49829
H	-1.72579	1.17608	2.05626
N	-0.61953	1.95479	-0.96893
N	1.39788	1.23836	-0.81214
Ru	-0.45586	-0.88730	0.25925
C	0.10974	0.87941	-0.58681
N	1.10757	-1.76254	-0.85725
H	1.42487	-2.57923	-0.34550
H	-0.13930	-1.65653	-1.26612
C	2.51431	0.30941	-0.67404
H	3.39814	0.79151	-1.09655
H	2.69960	0.12280	0.38693
H	-1.10911	-1.26216	-1.23336

Sum of electronic and thermal Enthalpies= -726.666694
Sum of electronic and thermal Free Energies= -726.724550

11. D_6

C	1.75330	-1.24465	-1.84772
C	0.75296	3.02257	-1.16826
C	1.86710	2.27845	-1.35325
C	-1.56966	2.60558	-0.36601
H	-3.14331	-2.28191	0.77147
C	-2.29968	-1.80540	1.25489
C	-1.14396	-2.54334	1.55116
C	-2.33046	-0.40656	1.54595
C	-0.02443	-1.91977	2.19329
C	-1.20880	0.20528	2.15243
C	-0.06243	-0.56273	2.52624
H	0.78045	-0.08877	3.01400
H	2.49341	-1.98825	-2.15978
H	1.31551	-0.80517	-2.74626
H	-1.90158	3.27481	-1.16045
H	0.56016	4.06334	-1.37083
H	2.83571	2.54120	-1.74622
H	-2.20574	1.72298	-0.35438
H	-1.63620	3.12937	0.59028
H	-1.09762	-3.59462	1.29033
H	-3.20776	0.18006	1.30483
H	0.85831	-2.50727	2.42139
H	-1.22821	1.26834	2.35925
N	-0.20800	2.18258	-0.63559
N	1.55862	1.00306	-0.91736
Ru	-0.58392	-0.74449	0.27042
C	0.27830	0.92555	-0.46641
N	0.67091	-1.89318	-1.07466
H	0.03522	-2.35039	-1.72078
H	1.07556	-2.63760	-0.51401
H	-1.45240	-0.52649	-1.03365
C	2.42752	-0.15240	-1.03627
H	3.34431	0.16569	-1.53496
H	2.69680	-0.51588	-0.03908

Sum of electronic and thermal Enthalpies= -726.727561
Sum of electronic and thermal Free Energies= -726.785712

12. E_6

C	2.22574	-0.03340	-0.64841
C	1.05283	4.15770	0.28362
C	2.19813	3.44659	0.17709
C	-1.34529	3.63963	0.70641
H	-2.99966	-1.26788	0.96125
C	-2.25861	-0.87227	1.64443
C	-1.17726	-1.66877	2.05062
C	-2.34414	0.48144	2.09343
C	-0.19083	-1.14589	2.94883
C	-1.34510	0.99358	2.95450
C	-0.28690	0.16155	3.43465
H	0.45477	0.55458	4.11896
H	3.02241	-0.72610	-0.93975
H	1.86435	0.46315	-1.55159
H	-1.56961	4.41103	-0.03116
H	0.86529	5.21249	0.16730
H	3.20504	3.75758	-0.04870
H	-1.96027	2.76483	0.50591
H	-1.56245	4.02982	1.70344
H	-1.07913	-2.67849	1.66971
H	-3.16705	1.10944	1.77670
H	0.64031	-1.77339	3.25246
H	-1.39971	2.02511	3.28071
N	0.04832	3.25671	0.58623
N	1.86293	2.12937	0.42721
Ru	-0.39684	0.24845	1.11153
C	0.53533	1.99057	0.68731
N	1.10337	-0.77392	-0.04653
H	0.62763	-1.30269	-0.78340
H	1.49324	-1.48617	0.56465
H	-1.00534	0.56607	-0.31338
C	2.77480	1.00603	0.31176
H	3.72861	1.38791	-0.05551
H	2.94759	0.56878	1.30108
C	-0.36816	-3.23457	-2.92026
O	0.19587	-2.79460	-1.92806
C	-1.20477	-2.35351	-3.80630
C	-0.24858	-4.68311	-3.30115
H	-1.36289	-1.37936	-3.34460
H	0.50152	-5.17994	-2.68745
H	-2.16571	-2.82523	-4.02967
H	-0.69325	-2.21932	-4.76562
H	-0.00013	-4.78817	-4.36104
H	-1.21639	-5.17564	-3.15723

Sum of electronic and thermal Enthalpies= -919.771411
Sum of electronic and thermal Free Energies= -919.851099

13. $TS_{E,F(6)}$

C	2.26942	-1.28669	-1.11583
C	1.87888	2.99845	0.02586
C	2.88084	2.10485	-0.15250
C	-0.55417	2.88380	0.54291
H	-2.69817	-2.35956	1.04466
C	-1.90702	-1.86493	1.59441
C	-0.72249	-2.55060	1.88528
C	-2.04850	-0.48884	1.96424
C	0.36252	-1.86748	2.52006
C	-1.02117	0.16252	2.66981
C	0.20270	-0.52210	2.92500
H	1.02579	-0.00118	3.39930
H	2.87434	-2.17150	-1.33599

H	2.15462	-0.73366	-2.05471
H	-0.76419	3.59656	-0.25559
H	1.87355	4.07434	-0.03845
H	3.91989	2.24960	-0.39969
H	-1.31112	2.10285	0.53184
H	-0.57139	3.40612	1.50208
H	-0.60147	-3.57831	1.56203
H	-2.95532	0.04593	1.70834
H	1.29865	-2.38098	2.70252
H	-1.13258	1.19927	2.96068
N	0.74164	2.26968	0.31858
N	2.32917	0.85583	0.04005
Ru	-0.16706	-0.66725	0.76361
C	1.01026	0.93950	0.33210
N	0.93718	-1.69391	-0.64308
H	0.14706	-1.61093	-1.69431
H	0.98410	-2.67119	-0.37094
H	-1.06485	-0.23683	-0.75854
C	3.02376	-0.41370	-0.12952
H	4.02692	-0.19652	-0.50063
H	3.11708	-0.90523	0.84322
C	-1.41702	-0.41826	-1.95958
O	-0.60121	-1.31408	-2.50328
C	-2.85951	-0.88590	-1.82612
C	-1.27565	0.98528	-2.53515
H	-0.23537	1.31348	-2.50476
H	-1.58441	0.94940	-3.58421
H	-1.90823	1.71073	-2.01779
H	-3.29687	-0.93022	-2.82828
H	-3.46453	-0.20598	-1.22043
H	-2.89608	-1.89237	-1.40723

Sum of electronic and thermal Enthalpies= -919.731909
Sum of electronic and thermal Free Energies= -919.801138

14. F_6

C	2.95223	-0.23000	-0.28888
C	0.63620	3.43800	-1.10752
C	1.91025	3.12865	-0.76495
C	-1.60055	2.36179	-0.83339
H	-2.94470	0.03669	1.58784
C	-1.96304	-0.18110	1.98945
C	-1.48309	-1.52791	2.02578
C	-1.14507	0.85640	2.46830
C	-0.21498	-1.83124	2.53764
C	0.16533	0.57388	2.95994
C	0.63351	-0.75980	2.95715
H	1.64597	-0.97058	3.28080
H	3.86312	-0.76788	-0.00492
H	3.00147	-0.07851	-1.37514
H	-1.82762	2.53943	-1.88532
H	0.23559	4.28115	-1.64626
H	2.83633	3.64922	-0.94648
H	-1.94535	1.36728	-0.56050
H	-2.10378	3.11589	-0.22409
H	-2.09940	-2.32160	1.61902
H	-1.48789	1.88305	2.41640
H	0.14663	-2.85226	2.54152
H	0.80984	1.37842	3.29099
N	-0.16444	2.41732	-0.63073
N	1.85201	1.93104	-0.08293
Ru	0.03583	-0.24092	0.93240
C	0.58023	1.48308	0.00523

N	1.76604	-1.01642	0.05136
H	2.05815	-1.82891	0.58202
C	2.99341	1.14321	0.36605
H	3.90051	1.68179	0.08510
H	2.96462	1.06176	1.45596
O	-0.37688	-0.91701	-1.08715
H	0.62737	-1.18778	-0.99469
C	-1.20485	-2.03377	-1.46532
H	-1.14522	-2.79500	-0.67420
C	-0.66487	-2.61857	-2.76046
C	-2.63610	-1.55400	-1.60625
H	-3.01249	-1.12182	-0.67567
H	-2.70812	-0.79773	-2.39254
H	-3.28996	-2.38690	-1.87599
H	-0.69202	-1.87148	-3.55808
H	-1.27013	-3.47449	-3.06999
H	0.36586	-2.96235	-2.64151

Sum of electronic and thermal Enthalpies= -919.746138
Sum of electronic and thermal Free Energies= -919.816691

15. E_6'

C	2.28924	0.73703	0.17040
C	0.90067	4.95886	0.39481
C	2.07461	4.29191	0.47581
C	-1.50492	4.39605	0.72548
H	-3.10124	-0.31155	1.62596
C	-2.36673	0.13490	2.28476
C	-1.31780	-0.64427	2.79960
C	-2.43536	1.52643	2.59546
C	-0.33923	-0.04819	3.65805
C	-1.43808	2.10366	3.41783
C	-0.41310	1.30422	4.01049
H	0.32070	1.74771	4.67172
H	3.12694	0.04130	0.05495
H	2.00543	1.08519	-0.82513
H	-1.68495	5.12172	-0.06802
H	0.68697	5.97649	0.11200
H	3.08461	4.61227	0.27875
H	-2.06728	3.48818	0.51581
H	-1.83037	4.82451	1.67623
H	-1.23785	-1.69068	2.53080
H	-3.23591	2.13589	2.19654
H	0.47296	-0.65766	4.04063
H	-1.47255	3.16573	3.63011
N	-0.09290	4.06652	0.75409
N	1.76622	3.01094	0.89252
Ru	-0.46733	1.15051	1.69012
C	0.42834	2.85201	1.07451
N	1.13257	0.04454	0.76534
H	0.72637	-0.57552	0.05384
H	1.48014	-0.58207	1.48563
H	-1.01503	1.24435	0.20814
C	2.72005	1.92340	1.01383
H	3.68990	2.29108	0.67502
H	2.81834	1.63725	2.06645
C	-0.23689	-2.32267	-2.09785
O	0.41827	-2.01480	-1.10293
C	-1.21891	-1.34484	-2.68834
H	-1.24985	-0.44675	-2.07242
H	-2.22036	-1.78039	-2.74394
H	-0.92653	-1.07507	-3.70763
C	-0.06420	-3.65443	-2.72540

C	-0.77689	-4.03194	-3.87213
C	0.84255	-4.55830	-2.15274
C	-0.58534	-5.28958	-4.43428
C	1.03123	-5.81349	-2.71411
C	0.31721	-6.18043	-3.85615
H	-1.48166	-3.34990	-4.33420
H	1.38856	-4.25541	-1.26673
H	-1.13872	-5.57497	-5.32201
H	1.73303	-6.50851	-2.26627
H	0.46504	-7.16124	-4.29537

Sum of electronic and thermal Enthalpies= -1111.418174
Sum of electronic and thermal Free Energies= -1111.504128

16. $TS_{E,F'(6)}$

C	2.55604	-1.90475	-0.35126
C	2.23399	2.45874	0.46147
C	3.20631	1.51565	0.44633
C	-0.23971	2.48538	0.72433
H	-2.71307	-2.52658	1.39585
C	-1.91419	-2.08678	1.98010
C	-0.81457	-2.86618	2.35648
C	-1.95492	-0.69232	2.30494
C	0.28739	-2.25974	3.03774
C	-0.91256	-0.11168	3.04895
C	0.22615	-0.89458	3.40123
H	1.06298	-0.43337	3.91179
H	3.11271	-2.84570	-0.39454
H	2.64159	-1.43343	-1.33718
H	-0.38846	3.03603	-0.20559
H	2.28415	3.52616	0.32166
H	4.27071	1.59992	0.29949
H	-1.02670	1.74124	0.81423
H	-0.27490	3.17374	1.57169
H	-0.76774	-3.91047	2.06966
H	-2.79436	-0.08790	1.98287
H	1.16357	-2.84679	3.28528
H	-0.94062	0.94209	3.29602
N	1.04091	1.80126	0.68825
N	2.57922	0.30752	0.66585
Ru	-0.03322	-1.06631	1.22756
C	1.24366	0.46772	0.81557
N	1.13424	-2.16832	-0.07012
H	0.50072	-1.94353	-1.23332
H	1.03874	-3.15251	0.16015
H	-0.82025	-0.62802	-0.36473
C	3.22116	-0.99882	0.66914
H	4.27444	-0.85457	0.42182
H	3.16069	-1.42440	1.67482
C	-1.07711	-0.82297	-1.59068
O	-0.05975	-1.50765	-2.10781
C	-2.38362	-1.60995	-1.55610
H	-2.76705	-1.68398	-2.57752
H	-3.15319	-1.15267	-0.93095
H	-2.18270	-2.62093	-1.19863
C	-1.18550	0.60485	-2.08369
C	-2.35106	1.36140	-1.91400
C	-0.09500	1.18297	-2.74082
C	-2.42339	2.66917	-2.38864
C	-0.16458	2.49174	-3.21082
C	-1.32813	3.24087	-3.03440
H	-3.21965	0.93390	-1.42495
H	0.79114	0.58065	-2.90364

H	-3.33966	3.23693	-2.26533
H	0.68315	2.92164	-3.73442
H	-1.38799	4.25532	-3.41416

Sum of electronic and thermal Enthalpies= -1111.377086
Sum of electronic and thermal Free Energies= -1111.453891

17. F_6'

C	2.97389	0.53743	-0.11566
C	0.78657	4.37375	-0.44451
C	2.05526	4.00306	-0.15143
C	-1.44834	3.29352	-0.39979
H	-2.90547	-0.09616	1.21740
C	-1.97757	-0.03963	1.77573
C	-1.18367	-1.22264	1.94623
C	-1.58043	1.17633	2.35581
C	0.02423	-1.15886	2.64189
C	-0.30917	1.25948	2.99167
C	0.50684	0.10508	3.11531
H	1.47340	0.17644	3.59858
H	3.91878	-0.01473	-0.04692
H	2.82179	0.76972	-1.17908
H	-1.63497	3.51054	-1.45307
H	0.39347	5.29473	-0.84309
H	2.98633	4.53811	-0.24321
H	-1.84088	2.30848	-0.16138
H	-1.94841	4.04425	0.21600
H	-1.49480	-2.15181	1.48388
H	-2.19479	2.06172	2.25124
H	0.64455	-2.04363	2.72653
H	0.05275	2.21275	3.35814
N	-0.02127	3.29352	-0.14322
N	1.98770	2.71071	0.32312
Ru	0.11332	0.43056	1.03731
C	0.71334	2.25574	0.33698
N	1.88754	-0.28808	0.37508
H	2.27162	-0.91181	1.07792
C	3.14177	1.86533	0.61408
H	4.03081	2.39857	0.27022
H	3.22478	1.71662	1.69496
O	-0.49740	0.04137	-1.14639
H	-1.45926	0.03727	-1.20564
C	-0.00583	-1.11914	-1.88683
H	1.04104	-1.16720	-1.58499
C	-0.13695	-0.84364	-3.37391
H	-1.18155	-0.74251	-3.68364
H	0.29563	-1.66989	-3.94337
H	0.39241	0.07434	-3.63805
C	-0.70356	-2.37349	-1.41833
C	0.01962	-3.36514	-0.75065
C	-2.07478	-2.56535	-1.62612
C	-0.61108	-4.52195	-0.29526
C	-2.71222	-3.71231	-1.15818
C	-1.98032	-4.69417	-0.49076
H	1.08402	-3.22457	-0.58883
H	-2.65722	-1.82931	-2.17637
H	-0.03415	-5.28990	0.20950
H	-3.77443	-3.84967	-1.33078
H	-2.47293	-5.59381	-0.13808

Sum of electronic and thermal Enthalpies= -1111.377034
Sum of electronic and thermal Free Energies= -1111.457317

18. A_7

C	1.41594	-1.85918	-0.53783
C	0.36933	2.03614	-2.62397
C	1.44399	1.88809	-1.81769
C	2.24121	-0.88075	0.25723
C	3.20561	-1.30196	1.17356
C	-1.90120	1.04568	-2.79320
C	2.00751	0.49532	0.13389
C	3.92510	-0.38442	1.93489
C	2.71688	1.42192	0.89370
C	3.67864	0.97939	1.79712
H	-3.39847	-2.79395	0.68742
C	-3.11879	-1.77342	0.92204
C	-2.31747	-1.50266	2.04091
C	-3.50839	-0.71278	0.04350
C	-1.83563	-0.17465	2.25703
C	-3.15734	0.61865	0.35301
C	-2.30091	0.89044	1.44250
H	-1.94030	1.89664	1.61502
H	1.90566	-2.83673	-0.54767
H	1.32465	-1.53014	-1.57662
H	-1.73898	0.94183	-3.86687
H	0.23163	2.63329	-3.51072
H	2.43121	2.31680	-1.86357
H	3.40430	-2.36406	1.27978
H	-2.37305	0.14066	-2.41737
H	4.67844	-0.73368	2.63212
H	-2.54660	1.90814	-2.61302
H	2.51266	2.48166	0.78108
H	4.23150	1.69908	2.39008
H	-1.97405	-2.31167	2.67507
H	-4.10792	-0.93125	-0.83203
H	-1.13699	0.02690	3.05994
H	-3.45895	1.42336	-0.30496
N	-0.62018	1.20989	-2.12930
N	1.08473	0.96852	-0.84663
Ru	-1.28883	-0.69412	0.22914
C	-0.20428	0.54897	-1.01709
N	0.08399	-1.97819	0.05695
H	0.03534	-2.80776	0.64255

Sum of electronic and thermal Enthalpies= -917.169689
Sum of electronic and thermal Free Energies= -917.233316

19. D_7

C	0.69691	-1.16840	-2.07238
C	-0.08017	3.25282	-1.15785
C	1.11629	2.63176	-1.07343
C	1.82968	-0.84957	-1.14356
C	2.87401	-1.75720	-0.95353
C	-2.45636	2.66287	-0.73798
C	1.87393	0.36455	-0.44672
C	3.93823	-1.46530	-0.10424
C	2.93775	0.66929	0.39929
C	3.97102	-0.24767	0.57047
H	-3.89816	-1.92690	1.14067
C	-2.95562	-1.52820	1.49438
C	-1.82242	-2.35266	1.57045
C	-2.83923	-0.14470	1.83379
C	-0.57063	-1.83630	2.04106
C	-1.59289	0.36302	2.26524
C	-0.45850	-0.49612	2.41765
H	0.48662	-0.10018	2.76794

H	1.02264	-1.90249	-2.81628
H	0.36502	-0.27562	-2.60570
H	-2.74755	3.15584	-1.66673
H	-0.33122	4.25731	-1.45748
H	2.11328	2.97208	-1.29897
H	2.86557	-2.69596	-1.49996
H	-3.02139	1.74101	-0.62426
H	4.74424	-2.17975	0.01932
H	-2.66096	3.33022	0.10229
H	2.95032	1.61899	0.92379
H	4.79897	-0.00836	1.22831
H	-1.89602	-3.39139	1.26842
H	-3.69664	0.51154	1.75526
H	0.29452	-2.48760	2.09489
H	-1.50028	1.41740	2.49756
N	-1.04274	2.33173	-0.78760
N	0.85409	1.33753	-0.64854
Ru	-1.35451	-0.54313	0.27442
C	-0.48728	1.13465	-0.46066
N	-0.47379	-1.69468	-1.32466
H	-1.22330	-1.87801	-1.98594
H	-0.21874	-2.59983	-0.93776
H	-2.40470	-0.22258	-0.86095

Sum of electronic and thermal Enthalpies= -918.377427
Sum of electronic and thermal Free Energies= -918.443876

20. E_7

C	0.74008	-0.91255	-1.42606
C	1.96726	3.33547	-0.21024
C	2.81373	2.30692	-0.43412
C	2.07406	-1.15392	-0.78472
C	2.69398	-2.40270	-0.86977
C	-0.31264	3.62255	0.73543
C	2.73459	-0.13835	-0.08260
C	3.93689	-2.63456	-0.28594
C	3.98136	-0.35673	0.49952
C	4.58349	-1.60747	0.39687
H	-2.99781	-0.21156	2.78355
C	-1.92330	-0.28462	2.89653
C	-1.26759	-1.49839	2.63613
C	-1.15839	0.86628	3.26137
C	0.15502	-1.60164	2.77781
C	0.24677	0.75774	3.36984
C	0.90980	-0.49493	3.17613
H	1.98524	-0.56958	3.27736
H	0.58363	-1.62259	-2.24382
H	0.68575	0.09265	-1.84830
H	-0.62926	4.23751	-0.10895
H	2.07502	4.39003	-0.40524
H	3.79595	2.27542	-0.87561
H	2.20387	-3.19808	-1.42390
H	-1.12431	2.96080	1.02806
H	4.40374	-3.60913	-0.37459
H	-0.03992	4.27117	1.57094
H	4.47137	0.44936	1.03570
H	5.55418	-1.77643	0.84949
H	-1.84151	-2.35947	2.31346
H	-1.64826	1.81372	3.44636
H	0.64991	-2.54223	2.56320
H	0.82936	1.63769	3.61677
N	0.81913	2.80154	0.34562
N	2.15850	1.16215	-0.00542

Ru	-0.36822	0.14016	1.34605
C	0.91393	1.45227	0.48737
N	-0.36454	-1.03909	-0.44587
H	-1.23873	-0.87990	-0.95425
H	-0.40304	-2.01256	-0.15460
H	-1.42275	0.97084	0.51295
C	-3.57541	-0.82151	-2.93157
O	-2.51271	-1.13345	-2.41395
C	-4.07839	-1.52889	-4.15853
H	-3.31177	-2.19011	-4.56000
H	-4.96296	-2.11994	-3.89752
H	-4.39566	-0.81102	-4.92011
C	-4.43172	0.28026	-2.36952
H	-5.46563	-0.05603	-2.24982
H	-4.03616	0.62635	-1.41513
H	-4.45591	1.11651	-3.07636

Sum of electronic and thermal Enthalpies= -1111.419983
Sum of electronic and thermal Free Energies= -1111.507872

21. $TS_{E,F(7)}$

C	1.20906	-1.43115	-1.44050
C	1.30651	3.15437	-0.74011
C	2.35562	2.30840	-0.64644
C	2.41206	-1.26323	-0.55869
C	3.27949	-2.32559	-0.29374
C	-1.13021	3.05647	-0.27940
C	2.67663	-0.03521	0.05656
C	4.37790	-2.17029	0.54820
C	3.77257	0.13475	0.90067
C	4.62564	-0.93717	1.14682
H	-3.21025	-1.80593	1.68217
C	-2.33202	-1.26195	2.00660
C	-1.12561	-1.94011	2.21484
C	-2.38549	0.16164	2.15416
C	0.06210	-1.21601	2.54795
C	-1.24975	0.87388	2.57903
C	-0.01361	0.18330	2.74297
H	0.88683	0.73728	2.97979
H	1.35461	-2.28961	-2.10500
H	1.06924	-0.55601	-2.07991
H	-1.37944	3.53620	-1.22656
H	1.25764	4.18589	-1.04912
H	3.40125	2.44378	-0.86776
H	3.09997	-3.28333	-0.77338
H	-1.86184	2.28235	-0.06131
H	5.04393	-3.00672	0.72854
H	-1.13920	3.80563	0.51547
H	3.95370	1.09968	1.36325
H	5.47988	-0.80642	1.80145
H	-1.07694	-3.01046	2.04779
H	-3.31162	0.68681	1.95309
H	1.01032	-1.72863	2.65180
H	-1.29371	1.94829	2.70533
N	0.18207	2.44181	-0.36835
N	1.84597	1.09363	-0.21735
Ru	-0.72452	-0.29358	0.72481
C	0.49295	1.15952	-0.04631
N	-0.02368	-1.63194	-0.66206
H	-1.00334	-1.68622	-1.51704
H	0.04214	-2.55197	-0.23174
H	-1.85453	-0.01144	-0.70351
C	-2.47843	-0.37763	-1.74604

O	-1.93784	-1.51240	-2.17043
C	-2.26347	0.79946	-2.69140
H	-1.20049	0.95972	-2.88158
H	-2.73653	0.54428	-3.64419
H	-2.71743	1.72195	-2.32343
C	-3.91333	-0.51267	-1.25624
H	-4.26516	0.38657	-0.74316
H	-4.01280	-1.37891	-0.60130
H	-4.55683	-0.68110	-2.12524

Sum of electronic and thermal Enthalpies= -1111.379232
Sum of electronic and thermal Free Energies= -1111.455690

22. F_7

C	0.75563	-0.86058	-1.87684
C	1.53206	3.22831	0.04763
C	2.49501	2.35015	-0.30886
C	2.14603	-1.04398	-1.32743
C	2.91527	-2.17257	-1.62060
C	-0.78818	3.09963	0.92497
C	2.68214	-0.10711	-0.43711
C	4.17571	-2.35721	-1.05764
C	3.94174	-0.27747	0.13492
C	4.69132	-1.40806	-0.17733
H	-2.69619	-2.31152	1.95528
C	-1.75371	-1.83111	2.18967
C	-0.54906	-2.45789	1.85675
C	-1.74466	-0.52764	2.79140
C	0.69171	-1.77048	2.04576
C	-0.53271	0.09911	3.11779
C	0.68498	-0.50428	2.69574
H	1.62268	0.01882	2.84129
H	0.64687	-1.46935	-2.78308
H	0.60704	0.18136	-2.17972
H	-0.96379	4.03441	0.39136
H	1.52888	4.30606	0.05760
H	3.49128	2.50111	-0.68980
H	2.52329	-2.90845	-2.31671
H	-1.62322	2.42777	0.74973
H	4.75863	-3.23567	-1.31188
H	-0.68649	3.31526	1.99107
H	4.33049	0.46895	0.82049
H	5.67234	-1.54351	0.26385
H	-0.56275	-3.42141	1.35937
H	-2.68322	-0.03793	3.02760
H	1.62703	-2.21362	1.72850
H	-0.52679	1.07144	3.59399
N	0.42513	2.48537	0.41229
N	1.95278	1.08600	-0.14825
Ru	-0.50218	-0.42871	0.89352
C	0.66469	1.15358	0.29814
N	-0.28039	-1.23977	-0.92389
H	-0.23569	-2.25274	-0.83937
O	-2.38365	0.57672	-0.15027
C	-2.84015	0.33254	-1.51132
H	-1.92487	0.06634	-2.04028
C	-3.44750	1.60736	-2.06771
C	-3.78643	-0.85137	-1.53799
H	-3.29594	-1.74408	-1.14476
H	-4.69403	-0.65110	-0.95531
H	-4.10203	-1.06171	-2.56284
H	-4.35427	1.89007	-1.52290
H	-3.72208	1.46590	-3.11642

H	-2.73802	2.43610	-2.01398
H	-3.14477	0.48690	0.43362

Sum of electronic and thermal Enthalpies= -1111.380131
Sum of electronic and thermal Free Energies= -1111.459908

23. D_7'

C	1.41004	-0.71362	-0.66934
C	2.43323	3.62452	0.38409
C	3.32641	2.62242	0.23372
C	2.73144	-0.87592	0.02172
C	3.39997	-2.10209	0.01164
C	0.11793	3.86313	1.25305
C	3.33126	0.19399	0.69736
C	4.63183	-2.26015	0.64189
C	4.56654	0.04978	1.32511
C	5.21803	-1.18000	1.29687
H	-2.46200	0.01692	3.41620
C	-1.38837	-0.01299	3.55440
C	-0.68506	-1.21168	3.35492
C	-0.67269	1.17768	3.89070
C	0.73688	-1.25820	3.52964
C	0.73288	1.12337	4.03238
C	1.44371	-0.11120	3.90158
H	2.51862	-0.14341	4.02765
H	1.30719	-1.46418	-1.45903
H	1.33299	0.26863	-1.13930
H	-0.19390	4.43083	0.37450
H	2.50455	4.67230	0.14158
H	4.32191	2.61078	-0.17796
H	2.95735	-2.93948	-0.52021
H	-0.67832	3.18434	1.54880
H	5.13705	-3.21901	0.61109
H	0.34043	4.55488	2.06862
H	5.00889	0.89737	1.83828
H	6.17969	-1.29118	1.78522
H	-1.22117	-2.10420	3.05342
H	-1.19918	2.11345	4.02840
H	1.26900	-2.18768	3.36070
H	1.27843	2.03286	4.25575
N	1.29082	3.07041	0.93206
N	2.70434	1.47300	0.69774
Ru	0.18481	0.40727	2.02271
C	1.43502	1.73419	1.14036
N	0.27691	-0.83737	0.27828
H	-0.58379	-0.72211	-0.26805
H	0.25583	-1.80004	0.60502
H	-0.87912	1.16467	1.13427
C	-2.92061	-0.63223	-2.10981
O	-1.79580	-0.94996	-1.72860
C	-3.77180	0.28530	-1.27077
H	-4.69716	-0.21477	-0.96996
H	-3.21439	0.57981	-0.38227
H	-4.05465	1.17907	-1.83403
C	-3.45193	-1.14868	-3.39468
C	-2.64598	-1.99857	-4.16587
C	-4.73140	-0.81135	-3.85726
C	-3.10976	-2.50025	-5.37399
C	-5.19484	-1.31502	-5.06819
C	-4.38528	-2.15855	-5.82668
H	-1.65842	-2.25227	-3.79822
H	-5.37298	-0.15666	-3.27831
H	-2.48182	-3.15708	-5.96600

H	-6.18572	-1.05045	-5.42021
H	-4.74788	-2.55058	-6.77094

Sum of electronic and thermal Enthalpies= -1303.066429
Sum of electronic and thermal Free Energies= -1303.159745

24. $TS_{E,F'(7)}$

C	1.62326	-1.82883	-0.83832
C	1.80568	2.74047	-0.29349
C	2.81494	1.87390	-0.05627
C	2.73669	-1.68514	0.15795
C	3.53337	-2.76869	0.53407
C	-0.66769	2.72579	-0.09817
C	2.98664	-0.44854	0.76255
C	4.55160	-2.62541	1.47374
C	4.00302	-0.29029	1.70286
C	4.78793	-1.38352	2.05882
H	-3.08492	-1.88840	2.00348
C	-2.18192	-1.40588	2.35550
C	-1.04181	-2.16967	2.62981
C	-2.13628	0.02154	2.47066
C	0.18052	-1.52528	3.00059
C	-0.96900	0.65660	2.92815
C	0.20244	-0.12085	3.16762
H	1.13119	0.36904	3.43377
H	1.79985	-2.70989	-1.46462
H	1.59208	-0.96499	-1.50695
H	-0.85115	3.04724	-1.12398
H	1.81763	3.75621	-0.65384
H	3.88111	1.97139	-0.17588
H	3.36514	-3.73376	0.06515
H	-1.43453	2.01150	0.18863
H	5.16589	-3.47828	1.74030
H	-0.69640	3.58885	0.57061
H	4.17713	0.68229	2.15214
H	5.58146	-1.26244	2.78758
H	-1.06679	-3.24448	2.48906
H	-3.01048	0.60974	2.21842
H	1.08427	-2.10230	3.15341
H	-0.93376	1.73490	3.02057
N	0.62914	2.07789	-0.00338
N	2.22753	0.69535	0.37367
Ru	-0.45055	-0.58577	1.13050
C	0.86620	0.80667	0.40314
N	0.30464	-1.95479	-0.19551
H	-0.57197	-1.91643	-1.18656
H	0.26363	-2.88266	0.22102
H	-1.52180	-0.30303	-0.36942
C	-2.10268	-0.69186	-1.43327
O	-1.33517	-1.63052	-1.97981
C	-3.44484	-1.21956	-0.93531
H	-3.96130	-0.53334	-0.26045
H	-3.28495	-2.17293	-0.43070
H	-4.08761	-1.40296	-1.80077
C	-2.16621	0.59514	-2.23069
C	-3.21090	1.51459	-2.08280
C	-1.15663	0.86544	-3.15974
C	-3.23916	2.68403	-2.84051
C	-1.18030	2.03560	-3.91292
C	-2.22052	2.95197	-3.75332
H	-4.02086	1.32243	-1.38751
H	-0.37381	0.12976	-3.30371
H	-4.06379	3.37972	-2.72583

H	-0.39775	2.22455	-4.64057
H	-2.24746	3.85791	-4.34949

Sum of electronic and thermal Enthalpies= -1303.024893
Sum of electronic and thermal Free Energies= -1303.108256

25. F_7'

C	1.68837	-0.25213	-1.77657
C	2.05506	3.64043	0.60601
C	3.09951	2.85431	0.26449
C	3.04173	-0.41382	-1.13588
C	3.90259	-1.45709	-1.48546
C	-0.33037	3.30116	1.21455
C	3.44420	0.43964	-0.10217
C	5.12241	-1.63945	-0.83869
C	4.66129	0.26981	0.55545
C	5.50347	-0.77503	0.18553
H	-2.04935	-2.18687	1.55911
C	-1.14209	-1.72834	1.93443
C	0.10082	-2.30132	1.64978
C	-1.21440	-0.49237	2.66102
C	1.30462	-1.61681	2.01347
C	-0.04887	0.12073	3.14518
C	1.21578	-0.41929	2.77535
H	2.12574	0.10220	3.04697
H	1.69294	-0.75591	-2.75142
H	1.48169	0.80499	-1.97022
H	-0.47079	4.30834	0.82150
H	1.98460	4.70996	0.71870
H	4.11567	3.09462	-0.00017
H	3.61550	-2.12597	-2.29171
H	-1.10349	2.65325	0.81273
H	5.77832	-2.44943	-1.13843
H	-0.38777	3.33572	2.30484
H	4.94532	0.95059	1.35179
H	6.45164	-0.90923	0.69381
H	0.15253	-3.20955	1.05976
H	-2.18176	-0.04467	2.86201
H	2.27363	-2.01231	1.73624
H	-0.10667	1.04291	3.70961
N	0.96670	2.80760	0.78454
N	2.62332	1.55388	0.24778
Ru	0.17736	-0.18571	0.89637
C	1.29731	1.50825	0.56872
N	0.61840	-0.80910	-0.95699
H	0.76087	-1.81708	-0.94862
O	-1.65434	0.81021	-0.23963
C	-2.14838	0.33008	-1.53399
H	-1.29382	-0.21631	-1.93956
C	-2.48083	1.52845	-2.40349
H	-3.28978	2.13275	-1.98462
H	-2.79066	1.19251	-3.39634
H	-1.60084	2.16565	-2.51703
H	-2.38871	0.73096	0.37991
C	-3.28867	-0.63059	-1.30051
C	-3.10156	-2.00092	-1.50642
C	-4.53448	-0.18277	-0.84202
C	-4.13314	-2.90519	-1.26206
C	-5.56362	-1.08613	-0.58493
C	-5.36487	-2.44961	-0.79540
H	-2.14160	-2.35534	-1.86989
H	-4.71715	0.87961	-0.70232
H	-3.97834	-3.96411	-1.44103

H	-6.52527	-0.72434	-0.23685
H	-6.16978	-3.15182	-0.60719

Sum of electronic and thermal Enthalpies= -1303.023734
Sum of electronic and thermal Free Energies= -1303.112750

26. G_6

C	3.10877	-0.14016	-0.13939
C	0.59457	3.33354	-1.29782
C	1.86427	3.09302	-0.89056
C	-1.62207	2.19424	-1.02010
H	-2.85766	0.19723	1.50987
C	-1.90918	-0.11497	1.92628
C	-1.54437	-1.49561	1.94176
C	-1.02034	0.83971	2.47048
C	-0.30348	-1.90412	2.44274
C	0.23727	0.44541	3.00390
C	0.61460	-0.91193	2.91587
H	1.60157	-1.21277	3.24945
H	3.92702	-0.64525	0.37921
H	3.39053	-0.05396	-1.19215
H	-1.85849	2.62971	-1.99062
H	0.18935	4.12556	-1.90605
H	2.77961	3.63238	-1.07156
H	-1.86187	1.13271	-1.03344
H	-2.18919	2.71718	-0.24675
H	-2.21195	-2.22749	1.50279
H	-1.28348	1.89080	2.44535
H	-0.01720	-2.94839	2.41320
H	0.92008	1.18404	3.40436
N	-0.19361	2.32266	-0.78254
N	1.81279	1.94170	-0.12766
Ru	0.04580	-0.26291	0.89066
C	0.54807	1.46160	-0.05561
N	1.87428	-0.95086	-0.02889
H	2.10240	-1.88380	0.29681
C	2.94286	1.24728	0.46239
H	3.84237	1.83921	0.28539
H	2.78841	1.17893	1.54166
O	-0.46055	-0.77977	-1.02834
H	1.38137	-1.05755	-0.92937
C	-1.26098	-1.90120	-1.33514
H	-1.13464	-2.68394	-0.56552
C	-0.77335	-2.47714	-2.66235
C	-2.74308	-1.54360	-1.42214
H	-3.11146	-1.09902	-0.49320
H	-2.91059	-0.82465	-2.23011
H	-3.35207	-2.42822	-1.63085
H	-0.84932	-1.72197	-3.44989
H	-1.36875	-3.34531	-2.95952
H	0.27172	-2.79230	-2.59257

Sum of electronic and thermal Enthalpies= -919.756421
Sum of electronic and thermal Free Energies= -919.826458

27. H_6

C	3.28004	0.23494	-1.08386
C	0.36818	3.36289	-1.20567
C	1.62397	2.92033	-0.96230
C	-1.93825	2.57014	-0.68072
H	-3.09313	0.61838	2.30377
C	-2.13528	0.14141	2.47435
C	-2.01735	-1.28097	2.35080
C	-1.02306	0.92328	2.88530

C	-0.75996	-1.87841	2.46261
C	0.24343	0.32112	3.00194
C	0.38973	-1.05816	2.70168
H	1.37650	-1.50648	2.70885
H	3.68798	1.00254	-1.74768
H	2.50245	-0.29553	-1.65129
H	-2.24580	2.81702	-1.69743
H	0.01616	4.23620	-1.73029
H	2.58117	3.33289	-1.23637
H	-2.37832	1.61403	-0.40492
H	-2.28449	3.34991	0.00127
H	-2.88208	-1.87140	2.07119
H	-1.12950	1.99511	2.99668
H	-0.63684	-2.93809	2.27240
H	1.11822	0.92552	3.20742
N	-0.49163	2.44968	-0.62882
N	1.50043	1.75040	-0.23786
Ru	-0.60108	-0.17326	0.98512
C	0.19691	1.45474	-0.02212
N	4.36774	-0.60580	-0.61886
H	5.11397	-0.67621	-1.29704
C	2.63560	0.91237	0.12862
H	3.37882	1.51824	0.65241
H	2.26309	0.15645	0.82115
O	-0.83508	-0.85848	-0.76106
H	4.06095	-1.54506	-0.40086
C	-1.44249	-2.09730	-1.10320
H	-1.64873	-2.67216	-0.18768
C	-0.46886	-2.88030	-1.97249
C	-2.75630	-1.81204	-1.81767
H	-3.43813	-1.25062	-1.17290
H	-2.57638	-1.22767	-2.72380
H	-3.24777	-2.74608	-2.10256
H	-0.24496	-2.32468	-2.88676
H	-0.89764	-3.84639	-2.25170
H	0.46777	-3.06248	-1.43966

Sum of electronic and thermal Enthalpies= -919.727798
Sum of electronic and thermal Free Energies= -919.804680

28. I_6

C	2.42720	-1.56662	-2.26692
C	0.75209	-3.10061	1.40654
C	1.14937	-3.28537	0.12746
C	-0.54675	-1.39888	2.66779
C	0.99170	-2.03318	-2.00922
H	-2.85991	2.29872	1.10933
C	-2.78688	1.58293	0.29902
C	-2.42276	2.01570	-0.98391
C	-2.97305	0.19853	0.57020
C	-2.19689	1.04224	-2.00353
C	-2.84371	-0.74049	-0.48372
C	-2.47732	-0.32869	-1.78422
H	-2.36185	-1.05116	-2.58221
H	3.11687	-2.31206	-1.86107
H	2.61847	-0.63582	-1.70954
H	0.10920	-1.62813	3.50784
H	0.88955	-3.71022	2.28461
H	1.70295	-4.08762	-0.33243
H	-0.64629	-0.31775	2.58187
H	-1.50982	-1.89001	2.82731
H	-2.24537	3.06554	-1.18163
H	-3.22672	-0.12996	1.56915

H	-1.84563	1.36474	-2.97746
H	-2.97417	-1.79643	-0.27500
N	0.07273	-1.90108	1.44745
N	0.69870	-2.19438	-0.58967
Ru	-0.91942	0.42362	-0.29792
C	0.03243	-1.32920	0.22098
N	2.63568	-1.47062	-3.69776
H	2.34270	-0.57905	-4.07633
H	3.60361	-1.61116	-3.95352
C	0.38342	2.48381	1.45747
H	-0.37143	3.12419	0.96625
C	1.74164	2.77316	0.82274
C	0.39675	2.83648	2.94330
H	-0.58166	2.65024	3.39324
H	1.13659	2.22528	3.46781
H	0.65190	3.88904	3.09445
H	2.50921	2.13876	1.27464
H	2.02726	3.81875	0.96881
H	1.74656	2.59359	-0.25845
O	0.01972	1.12449	1.36332
H	0.39564	1.29041	-0.94093
H	0.53392	0.47230	-1.17422
H	0.27391	-1.32350	-2.42278
H	0.82985	-2.99056	-2.50915

Sum of electronic and thermal Enthalpies= -920.880618
Sum of electronic and thermal Free Energies= -920.957554

29. $TS_{I,J(6)}$

C	2.55027	-1.62559	-2.20738
C	0.60018	-3.25001	1.27432
C	1.07019	-3.38046	0.01228
C	-0.71618	-1.54261	2.53064
C	1.07258	-1.99659	-2.05868
H	-2.44267	2.98725	0.18349
C	-2.47124	2.01961	-0.30170
C	-2.01718	1.88102	-1.61648
C	-2.91429	0.86907	0.42572
C	-1.97976	0.58719	-2.22729
C	-2.93424	-0.39272	-0.18972
C	-2.45604	-0.53888	-1.52919
H	-2.42158	-1.51861	-1.98934
H	3.16286	-2.45694	-1.84717
H	2.77690	-0.76716	-1.55654
H	-0.16846	-1.89263	3.40552
H	0.66958	-3.90757	2.12541
H	1.62979	-4.17483	-0.45392
H	-0.68953	-0.45483	2.50540
H	-1.74074	-1.91874	2.57985
H	-1.63471	2.74145	-2.15274
H	-3.21106	0.96946	1.46285
H	-1.58564	0.47423	-3.23011
H	-3.25698	-1.26402	0.36645
N	-0.04946	-2.03469	1.33479
N	0.69241	-2.24171	-0.67271
Ru	-0.85141	0.40666	-0.32265
C	-0.00150	-1.40361	0.13839
N	2.83628	-1.41329	-3.61266
H	2.63677	-0.46701	-3.91083
H	3.80125	-1.61082	-3.84032
C	0.18787	2.33197	1.83392
H	-0.87564	2.55105	2.02392
C	0.74952	3.39541	0.89694

C	0.91913	2.33610	3.17108
H	0.50054	1.58696	3.84686
H	1.97868	2.11069	3.02337
H	0.83698	3.31487	3.65202
H	1.81267	3.21185	0.71093
H	0.65384	4.39209	1.33605
H	0.22979	3.40758	-0.06617
O	0.31437	1.01731	1.30961
H	0.77505	0.97974	-0.21001
H	0.66000	0.76728	-1.07228
H	0.86209	-2.89252	-2.64702
H	0.43873	-1.19301	-2.43490

Sum of electronic and thermal Enthalpies= -920.878018
Sum of electronic and thermal Free Energies= -920.952702

30. J_6

C	2.59341	-1.46354	-2.17382
C	0.56131	-3.33945	1.14529
C	1.09192	-3.39515	-0.09751
C	-0.87389	-1.75471	2.41043
C	1.14007	-1.93339	-2.10810
H	-2.37783	3.04865	-0.02139
C	-2.45619	2.04824	-0.43058
C	-1.96770	1.78835	-1.71746
C	-3.06689	1.01096	0.35104
C	-1.98723	0.44643	-2.20975
C	-3.15988	-0.28643	-0.15219
C	-2.55567	-0.58172	-1.41612
H	-2.55464	-1.59971	-1.78703
H	3.24475	-2.25694	-1.79489
H	2.71715	-0.59970	-1.50139
H	-0.19903	-1.65363	3.26233
H	0.60618	-4.03756	1.96540
H	1.69032	-4.15440	-0.57427
H	-1.35227	-0.79790	2.21805
H	-1.63144	-2.50725	2.63868
H	-1.52275	2.58137	-2.30542
H	-3.44983	1.24119	1.33884
H	-1.57744	0.21445	-3.18457
H	-3.62136	-1.07463	0.43032
N	-0.12967	-2.14670	1.22647
N	0.71520	-2.23658	-0.74708
Ru	-0.92756	0.35264	-0.33528
C	-0.04611	-1.44741	0.05934
N	2.93816	-1.20813	-3.55806
H	2.61676	-0.30092	-3.87191
H	3.93539	-1.25595	-3.71793
C	0.29238	2.41833	1.86503
H	-0.76352	2.67178	1.98460
C	0.94549	3.33539	0.85026
C	0.97732	2.42904	3.21840
H	0.48360	1.75008	3.91634
H	2.02954	2.13869	3.13052
H	0.95043	3.43542	3.64322
H	2.00978	3.10277	0.73898
H	0.86929	4.37508	1.17807
H	0.46831	3.24158	-0.12730
O	0.25449	1.04532	1.37323
H	1.16066	0.76569	1.19519
H	0.43590	0.57747	-1.09548
H	1.01662	-2.82817	-2.72224
H	0.47648	-1.15893	-2.49029

Sum of electronic and thermal Enthalpies= -920.920660
Sum of electronic and thermal Free Energies= -920.997893

31. K_6

C	2.54986	-1.36649	-1.97671
C	0.46591	-3.17596	1.34409
C	1.01800	-3.25682	0.11254
C	-0.98379	-1.56414	2.55472
C	1.09680	-1.83853	-1.92675
H	-2.45206	3.16230	0.08390
C	-2.51791	2.17260	-0.35303
C	-1.98835	1.94155	-1.62976
C	-3.15248	1.11927	0.38633
C	-1.98659	0.60843	-2.14769
C	-3.21570	-0.16920	-0.14375
C	-2.57492	-0.43828	-1.39603
H	-2.55876	-1.44872	-1.78643
H	3.19577	-2.15164	-1.57221
H	2.66025	-0.49099	-1.31817
H	-0.31051	-1.38999	3.39598
H	0.49710	-3.85686	2.17909
H	1.62460	-4.02506	-0.33864
H	-1.50558	-0.64035	2.31977
H	-1.70617	-2.33697	2.82504
H	-1.53239	2.74831	-2.18991
H	-3.56544	1.32818	1.36643
H	-1.54364	0.39812	-3.11307
H	-3.68725	-0.97202	0.41028
N	-0.22982	-1.98371	1.38760
N	0.64879	-2.11302	-0.56787
Ru	-0.98664	0.48708	-0.23597
C	-0.12468	-1.30834	0.21014
N	2.91815	-1.13752	-3.36063
H	2.59700	-0.23875	-3.69832
H	3.91867	-1.18074	-3.50047
C	0.78566	2.15883	1.71611
C	1.18217	3.13144	0.65619
C	1.32767	2.35502	3.09641
H	0.83240	1.69701	3.80856
H	2.40154	2.13742	3.09069
H	1.22319	3.39808	3.40761
H	2.24704	3.36697	0.72785
H	0.64344	4.07126	0.82478
H	0.93485	2.74515	-0.33184
O	0.02845	1.20682	1.50477
H	0.40029	0.67100	-0.95932
H	0.98621	-2.74650	-2.52393
H	0.43888	-1.07422	-2.33840

Sum of electronic and thermal Enthalpies= -919.742507
Sum of electronic and thermal Free Energies= -919.820685

32. $TS_{K,H(6)}$

C	1.92757	-2.12468	-1.95999
C	0.62752	-2.59967	2.09764
C	0.84789	-2.97882	0.81757
C	-0.37452	-0.62516	3.23966
C	0.49497	-1.98274	-1.44158
H	-2.56663	3.35330	0.71856
C	-2.62863	2.37009	0.26727
C	-2.29314	2.19631	-1.08252
C	-3.00346	1.25072	1.07373
C	-2.25673	0.88141	-1.63652

C	-3.02428	-0.03413	0.51189
C	-2.63190	-0.22926	-0.84943
H	-2.60626	-1.22723	-1.26864
H	2.34530	-3.07744	-1.62280
H	2.55324	-1.33341	-1.52085
H	0.29151	-0.87723	4.06490
H	0.81996	-3.10933	3.02769
H	1.26795	-3.88652	0.41705
H	-0.31830	0.44338	3.05011
H	-1.39294	-0.91858	3.50461
H	-1.99232	3.04548	-1.68422
H	-3.23636	1.39370	2.12168
H	-1.94642	0.73369	-2.66404
H	-3.27604	-0.89095	1.12522
N	0.06415	-1.34138	2.04995
N	0.41376	-1.94205	0.01418
Ru	-0.97478	0.81644	0.15962
C	-0.08090	-0.92289	0.76679
N	1.88869	-2.13287	-3.40987
H	1.87509	-1.19930	-3.80069
H	2.67755	-2.62281	-3.80980
C	1.03937	1.93561	0.40592
C	2.38836	1.23907	0.41733
C	1.03678	3.28564	-0.28804
H	0.06029	3.76142	-0.21273
H	1.76592	3.92116	0.22567
H	1.33542	3.21318	-1.33560
H	3.04417	1.82936	1.06563
H	2.84289	1.19884	-0.57456
H	2.31218	0.23641	0.83544
O	0.30396	1.80455	1.47855
H	0.42903	1.01744	-0.67328
H	-0.10583	-2.81643	-1.81493
H	0.05595	-1.05433	-1.80656

Sum of electronic and thermal Enthalpies= -919.727387
Sum of electronic and thermal Free Energies= -919.799867

33. G_6'

C	3.76055	-0.28469	0.12860
C	1.76427	3.53693	-0.99305
C	2.97110	3.11057	-0.54927
C	-0.59266	2.70590	-0.85210
H	-2.30868	-0.18007	1.29804
C	-1.37983	-0.22145	1.85391
C	-0.75009	-1.48744	2.07968
C	-0.78847	0.96084	2.33153
C	0.49608	-1.53594	2.71133
C	0.48424	0.90344	2.98028
C	1.13459	-0.33378	3.15368
H	2.10726	-0.37769	3.62843
H	4.44562	-0.91719	0.69785
H	4.15188	-0.20773	-0.88952
H	-0.72786	2.93625	-1.90946
H	1.49453	4.40266	-1.57559
H	3.95667	3.53094	-0.66564
H	-1.03435	1.73468	-0.64245
H	-1.05989	3.48809	-0.24955
H	-1.21358	-2.38973	1.70380
H	-1.27086	1.91557	2.16399
H	1.00316	-2.48734	2.83045
H	0.96941	1.81849	3.29898
N	0.82683	2.61945	-0.55798

N	2.73346	1.94402	0.15257
Ru	0.66309	-0.05506	0.99600
C	1.41373	1.63395	0.15233
N	2.42084	-0.91392	0.09422
H	2.49813	-1.89733	0.33019
C	3.72858	1.09163	0.77648
H	4.70430	1.57115	0.68232
H	3.49314	1.00411	1.83961
O	0.13971	-0.41342	-0.96804
H	1.97968	-0.86363	-0.83610
C	-0.57101	-1.57448	-1.32813
H	-0.24683	-2.43572	-0.71392
C	-0.23711	-1.89382	-2.78756
H	-0.52345	-1.05694	-3.42961
H	-0.77141	-2.78532	-3.12654
H	0.83667	-2.06578	-2.90766
C	-2.07563	-1.44778	-1.15034
C	-2.82242	-2.47929	-0.57572
C	-2.75183	-0.30933	-1.60059
C	-4.20469	-2.36815	-0.42216
C	-4.13112	-0.19025	-1.44841
C	-4.86233	-1.21718	-0.85029
H	-2.32075	-3.38991	-0.25479
H	-2.18844	0.48035	-2.08608
H	-4.76673	-3.18070	0.02657
H	-4.64082	0.69824	-1.80748
H	-5.93672	-1.12616	-0.73279

Sum of electronic and thermal Enthalpies= -1111.401466
Sum of electronic and thermal Free Energies= -1111.479340

34. H_6'

C	3.90992	0.21089	-0.78235
C	1.41756	3.70146	-0.58644
C	2.60726	3.08543	-0.39266
C	-0.97640	3.13185	-0.16558
H	-2.67163	0.82561	1.95908
C	-1.76647	0.36388	2.33562
C	-1.61084	-1.05728	2.24880
C	-0.77261	1.16124	2.96527
C	-0.39666	-1.63580	2.62523
C	0.44904	0.57741	3.34887
C	0.66920	-0.80040	3.09369
H	1.64021	-1.23504	3.30116
H	4.40754	0.97449	-1.38729
H	3.07345	-0.17724	-1.37975
H	-1.22207	3.57632	-1.13064
H	1.18097	4.66365	-1.01066
H	3.61152	3.40829	-0.61385
H	-1.52924	2.20033	-0.05737
H	-1.25710	3.82699	0.62905
H	-2.38549	-1.65345	1.78121
H	-0.91175	2.23205	3.04667
H	-0.22118	-2.69343	2.46751
H	1.25641	1.19398	3.72374
N	0.44521	2.83950	-0.11736
N	2.33278	1.86514	0.19316
Ru	0.04229	0.06380	1.20465
C	1.00114	1.70639	0.37214
N	4.89127	-0.78514	-0.39285
H	5.60357	-0.91513	-1.09837
C	3.35176	0.86349	0.48422
H	4.16206	1.32781	1.05113

H	2.88542	0.10838	1.12050
O	0.14704	-0.63028	-0.56033
H	4.46942	-1.68713	-0.21187
C	-0.44466	-1.84984	-0.99081
H	-0.32001	-2.61289	-0.20845
C	0.29056	-2.30828	-2.24606
H	0.19087	-1.56026	-3.03618
H	-0.12482	-3.25088	-2.61073
H	1.35262	-2.45503	-2.03382
C	-1.93017	-1.67178	-1.23789
C	-2.41858	-0.52578	-1.87264
C	-2.83011	-2.67453	-0.86878
C	-3.78143	-0.38286	-2.12208
C	-4.19466	-2.53564	-1.12144
C	-4.67404	-1.38613	-1.74516
H	-1.72331	0.24997	-2.17736
H	-2.46212	-3.57968	-0.39126
H	-4.14874	0.50719	-2.62291
H	-4.88058	-3.32563	-0.83407
H	-5.73440	-1.27601	-1.94470

Sum of electronic and thermal Enthalpies= -1111.371298
Sum of electronic and thermal Free Energies= -1111.457062

35. K_6'

C	2.10762	-1.40447	-3.08911
C	0.46147	-3.50343	0.31414
C	0.89542	-3.48298	-0.96623
C	-0.94473	-2.04306	1.75027
C	0.69247	-1.95576	-2.91624
H	-2.82750	2.75366	-0.31482
C	-2.90593	1.78825	-0.80086
C	-2.47040	1.64119	-2.12485
C	-3.44965	0.67730	-0.07431
C	-2.46793	0.33713	-2.71298
C	-3.51202	-0.58486	-0.66380
C	-2.95922	-0.76678	-1.97287
H	-2.93927	-1.75532	-2.41590
H	2.83050	-2.17542	-2.80573
H	2.24721	-0.56383	-2.39201
H	-0.20884	-1.75995	2.50541
H	0.60824	-4.22698	1.09937
H	1.49336	-4.18901	-1.51911
H	-1.62498	-1.21118	1.58519
H	-1.50527	-2.91272	2.09806
H	-2.08124	2.49079	-2.67165
H	-3.78934	0.82237	0.94467
H	-2.09824	0.19219	-3.72029
H	-3.91522	-1.43092	-0.12020
N	-0.28911	-2.35824	0.49479
N	0.40300	-2.32589	-1.53754
Ru	-1.31670	0.15993	-0.89393
C	-0.33270	-1.61112	-0.64279
N	2.31162	-1.07527	-4.48676
H	1.91333	-0.17694	-4.73018
H	3.29158	-1.05709	-4.73517
C	0.68315	1.58534	1.09474
C	1.52294	2.17793	0.00803
H	2.51896	1.72328	0.01465
H	1.65368	3.25190	0.16085
H	1.05508	1.98830	-0.95627
O	-0.29604	0.86194	0.84479
H	-0.00433	0.44970	-1.70759

H	0.56217	-2.83467	-3.55173
H	-0.04070	-1.20664	-3.21194
C	1.00366	1.86178	2.50764
C	2.18567	2.52615	2.86902
C	0.11171	1.45470	3.51319
C	2.47303	2.76787	4.20746
C	0.39678	1.70593	4.84733
C	1.57983	2.36037	5.19656
H	2.89037	2.85011	2.11200
H	-0.80676	0.95482	3.22936
H	3.39136	3.27616	4.47885
H	-0.30058	1.39788	5.61851
H	1.80248	2.55555	6.24000

Sum of electronic and thermal Enthalpies= -1111.389594
Sum of electronic and thermal Free Energies= -1111.474186

36. $TS_{K,H'(6)}$

C	1.94843	-2.79035	-1.74971
C	0.37315	-3.45244	2.18685
C	0.68527	-3.78220	0.91206
C	-0.72125	-1.52280	3.32585
C	0.48049	-2.70439	-1.32716
H	-2.72413	2.53265	0.86209
C	-2.75585	1.58499	0.33850
C	-2.29669	1.50693	-0.98348
C	-3.20306	0.41339	1.02456
C	-2.21681	0.23627	-1.62735
C	-3.17285	-0.82768	0.36901
C	-2.66705	-0.92645	-0.96403
H	-2.60736	-1.89133	-1.45159
H	2.37049	-3.74033	-1.41000
H	2.51892	-1.99506	-1.24711
H	-0.19518	-1.89828	4.20318
H	0.50411	-3.99594	3.10832
H	1.13928	-4.67188	0.50812
H	-0.54934	-0.45358	3.23218
H	-1.78755	-1.73192	3.43673
H	-1.91344	2.39227	-1.47656
H	-3.53065	0.47959	2.05467
H	-1.80983	0.16163	-2.62885
H	-3.47466	-1.72566	0.89500
N	-0.19429	-2.19586	2.14676
N	0.30004	-2.71789	0.11986
Ru	-1.10557	0.03422	0.27164
C	-0.25267	-1.72996	0.87342
N	2.00976	-2.75811	-3.19863
H	1.98701	-1.81484	-3.56499
H	2.84292	-3.20679	-3.55485
C	0.86132	1.16141	0.67767
C	2.24532	0.53431	0.75224
H	2.82057	1.12891	1.46832
H	2.77227	0.55918	-0.20238
H	2.18253	-0.48968	1.11980
O	0.08197	0.94830	1.71358
H	0.38232	0.27703	-0.41589
H	-0.06954	-3.54013	-1.76796
H	0.03924	-1.77616	-1.69061
C	0.81220	2.53422	0.04691
C	1.33615	2.77918	-1.22610
C	0.27416	3.59303	0.78265
C	1.30691	4.06261	-1.76337
C	0.25329	4.87921	0.24712

C	0.76485	5.11632	-1.02710
H	1.75873	1.96640	-1.81043
H	-0.11098	3.39814	1.77755
H	1.71141	4.24310	-2.75354
H	-0.15398	5.69861	0.82994
H	0.74966	6.11786	-1.44288

Sum of electronic and thermal Enthalpies= -1111.373096
Sum of electronic and thermal Free Energies= -1111.454168

37. G_7

C	0.67046	-0.55958	-2.32526
C	2.79467	2.28672	0.52664
C	3.33825	1.17183	-0.01095
C	1.71075	-1.47074	-1.74526
C	1.94311	-2.74052	-2.27677
C	0.54528	2.97623	1.35973
C	2.48775	-1.05953	-0.65450
C	2.92539	-3.57526	-1.74878
C	3.47874	-1.88243	-0.12417
C	3.69719	-3.14348	-0.67309
H	-3.47049	-0.69942	1.65507
C	-2.43018	-0.97673	1.77124
C	-1.91612	-2.06857	1.07016
C	-1.56501	-0.16948	2.58133
C	-0.51772	-2.37626	1.14838
C	-0.21426	-0.52786	2.73177
C	0.31701	-1.64295	2.01332
H	1.37018	-1.88351	2.08008
H	0.45634	-0.84647	-3.35918
H	1.03020	0.47129	-2.33917
H	0.78765	3.97767	1.00316
H	3.23524	3.24197	0.76149
H	4.33602	0.96025	-0.35788
H	1.36230	-3.06979	-3.13349
H	-0.46375	2.71127	1.04668
H	3.09607	-4.55330	-2.18444
H	0.65234	2.94715	2.44659
H	4.07317	-1.53576	0.71503
H	4.46948	-3.78319	-0.26103
H	-2.56274	-2.64365	0.41666
H	-1.95289	0.71127	3.07781
H	-0.10236	-3.18611	0.56061
H	0.44040	0.08213	3.34250
N	1.45538	2.02382	0.73970
N	2.30986	0.24668	-0.11065
Ru	-0.62600	-0.24809	0.57265
C	1.13519	0.76789	0.35555
N	-0.58237	-0.56906	-1.53568
H	-1.13157	-1.38725	-1.78097
O	-1.47924	1.43772	-0.24823
C	-2.84088	1.75530	-0.06465
H	-3.12741	1.61667	0.99222
C	-3.75596	0.88762	-0.93021
C	-3.03261	3.23087	-0.40527
H	-2.43092	3.86764	0.24772
H	-2.72716	3.41929	-1.43863
H	-4.08001	3.52708	-0.29630
H	-3.56809	1.08457	-1.99133
H	-4.81158	1.10044	-0.73687
H	-3.59283	-0.17927	-0.74610
H	-1.13626	0.27488	-1.73725

Sum of electronic and thermal Enthalpies= -1111.407640

Sum of electronic and thermal Free Energies= -1111.484363

38. H_7

C	2.55489	-0.55262	-0.87983
C	0.41270	-3.00351	2.00661
C	0.76706	-3.20394	0.71607
C	1.58211	-1.19016	-1.85393
C	1.77051	-1.08700	-3.23475
C	-0.84646	-1.26106	3.26971
C	0.49903	-1.95973	-1.40964
C	0.92850	-1.73944	-4.13218
C	-0.32956	-2.64455	-2.29609
C	-0.11978	-2.53092	-3.66719
H	-2.92873	3.06699	0.77734
C	-2.85513	2.15869	0.19107
C	-2.13319	2.14553	-1.00539
C	-3.37297	0.93067	0.71383
C	-1.94111	0.90839	-1.70174
C	-3.32838	-0.25729	-0.06393
C	-2.61983	-0.26265	-1.27922
H	-2.47725	-1.18381	-1.82721
H	3.15183	-1.35787	-0.43533
H	1.99443	-0.09866	-0.05136
H	-0.13780	-1.39945	4.08661
H	0.59079	-3.59750	2.88824
H	1.32373	-3.99607	0.24300
H	2.61493	-0.50223	-3.58248
H	-1.01540	-0.19626	3.12938
H	1.10661	-1.64804	-5.19834
H	-1.78470	-1.76277	3.51666
H	-1.12352	-3.27321	-1.90440
H	-0.75974	-3.06448	-4.36122
H	-1.63864	3.04435	-1.35491
H	-3.84943	0.91824	1.68708
H	-1.30757	0.86984	-2.57998
H	-3.74409	-1.17606	0.33071
N	-0.28080	-1.81021	2.04824
N	0.27108	-2.12887	-0.00055
Ru	-1.28382	0.54457	0.33090
C	-0.38389	-1.26206	0.81572
N	3.46872	0.36520	-1.53717
H	3.07411	1.29366	-1.62247
H	4.33823	0.44746	-1.02799
C	0.39601	2.65876	1.56404
H	-0.45024	3.25068	1.18520
C	1.66041	3.08866	0.83306
C	0.50379	2.85740	3.06948
H	-0.41449	2.54183	3.57164
H	1.33703	2.27472	3.47115
H	0.67491	3.91085	3.30642
H	2.51757	2.50457	1.17860
H	1.86840	4.14636	1.01521
H	1.55029	2.94321	-0.24504
O	0.16884	1.27980	1.30635

Sum of electronic and thermal Enthalpies= -1111.375080
Sum of electronic and thermal Free Energies= -1111.459703

39. K_7

C	2.84318	-0.70636	-0.82448
C	0.22505	-3.01720	1.79672
C	0.72428	-3.12145	0.54500
C	1.85619	-1.16771	-1.87623

C	2.13628	-1.03180	-3.23790
C	-1.18260	-1.38556	3.03665
C	0.64455	-1.77315	-1.52174
C	1.24779	-1.48907	-4.20792
C	-0.23961	-2.25526	-2.48328
C	0.05719	-2.10823	-3.83496
H	-2.53158	3.42873	0.26673
C	-2.66190	2.40795	-0.07240
C	-2.14066	2.01385	-1.31331
C	-3.36591	1.47357	0.75765
C	-2.23175	0.64276	-1.70733
C	-3.52823	0.14914	0.35186
C	-2.89442	-0.27922	-0.85916
H	-2.94585	-1.32140	-1.14882
H	3.35948	-1.58773	-0.42553
H	2.27940	-0.27756	0.01749
H	-0.47776	-1.10482	3.82115
H	0.29369	-3.68242	2.64210
H	1.31032	-3.89286	0.07329
H	3.07712	-0.57129	-3.51759
H	-1.79122	-0.52259	2.77777
H	1.49465	-1.37590	-5.25812
H	-1.82278	-2.19281	3.39720
H	-1.14636	-2.75911	-2.16521
H	-0.62757	-2.48657	-4.58604
H	-1.62097	2.72820	-1.93990
H	-3.75889	1.80208	1.71322
H	-1.78166	0.30180	-2.63051
H	-4.06589	-0.55916	0.97043
N	-0.47181	-1.82429	1.84934
N	0.32425	-1.98575	-0.13790
Ru	-1.24913	0.63734	0.21371
C	-0.41886	-1.16515	0.66106
N	3.85246	0.17947	-1.37494
H	3.49329	1.11307	-1.53323
H	4.65890	0.24783	-0.76894
C	0.51956	2.30752	2.17237
C	0.95183	3.25196	1.10017
C	1.02785	2.53143	3.56149
H	0.51130	1.89184	4.27533
H	2.10093	2.31171	3.58927
H	0.91846	3.58162	3.84655
H	2.00218	3.52647	1.22409
H	0.37312	4.17810	1.19786
H	0.77069	2.82197	0.11530
O	-0.24150	1.35888	1.96183
H	0.14289	0.75713	-0.51017

Sum of electronic and thermal Enthalpies= -1111.387229
Sum of electronic and thermal Free Energies= -1111.474124

40. $TS_{K,H(7)}$

C	2.16984	-0.93367	-1.69488
C	0.78296	-2.44420	2.41540
C	0.79244	-2.85132	1.12657
C	0.82456	-1.54520	-2.01642
C	0.44745	-1.75751	-3.34663
C	-0.00436	-0.46002	3.67955
C	-0.05204	-1.98266	-1.01747
C	-0.73794	-2.41040	-3.67059
C	-1.22265	-2.67425	-1.33270
C	-1.57312	-2.88691	-2.66144
H	-2.03750	3.85454	0.09949

C	-2.26020	2.79540	0.08715
C	-1.96960	2.01775	-1.05642
C	-2.76854	2.16494	1.24966
C	-2.25457	0.62535	-1.07816
C	-3.06259	0.78422	1.25575
C	-2.78310	0.02341	0.08629
H	-2.94543	-1.04655	0.09738
H	2.88889	-1.75380	-1.57865
H	2.11211	-0.44214	-0.71685
H	0.89967	0.05283	4.00707
H	1.10516	-2.94210	3.31545
H	1.11678	-3.77263	0.67164
H	1.12084	-1.40703	-4.12100
H	-0.78353	0.27978	3.52462
H	-0.99833	-2.56819	-4.71168
H	-0.31915	-1.18056	4.43543
H	-1.84523	-3.05557	-0.52937
H	-2.48242	-3.42563	-2.90401
H	-1.51762	2.48501	-1.92385
H	-2.89691	2.74527	2.15630
H	-2.02989	0.02446	-1.95007
H	-3.45307	0.30473	2.14401
N	0.23139	-1.17771	2.43348
N	0.25254	-1.81843	0.38015
Ru	-0.90427	1.04289	0.64261
C	-0.09361	-0.76507	1.18179
N	2.65225	-0.08204	-2.76665
H	2.19155	0.81953	-2.77742
H	3.65032	0.06931	-2.70720
C	1.12032	2.09555	1.10713
C	2.46040	1.38644	1.18299
C	1.19598	3.48128	0.49262
H	0.24047	3.99623	0.56219
H	1.93383	4.05425	1.06478
H	1.52966	3.45554	-0.54646
H	3.04306	1.90764	1.95006
H	3.01596	1.44379	0.24521
H	2.35071	0.34745	1.49108
O	0.30561	1.90421	2.10650
H	0.56093	1.22179	-0.08444

Sum of electronic and thermal Enthalpies= -1111.369212
Sum of electronic and thermal Free Energies= -1111.449208

41. G_7'

C	1.05225	-1.25618	-2.28635
C	3.12672	1.65951	0.54057
C	3.69619	0.56221	-0.00634
C	2.12759	-2.13256	-1.71658
C	2.39196	-3.39630	-2.24772
C	0.87742	2.28411	1.41734
C	2.90491	-1.69444	-0.63664
C	3.40579	-4.19901	-1.73002
C	3.92698	-2.48544	-0.11658
C	4.17727	-3.74063	-0.66514
H	-3.04689	-1.47278	1.72693
C	-2.00029	-1.72879	1.83686
C	-1.46962	-2.81288	1.13629
C	-1.14453	-0.90229	2.63857
C	-0.06437	-3.09079	1.20429
C	0.21442	-1.23184	2.77983
C	0.76348	-2.33644	2.05836
H	1.82205	-2.55463	2.11625

H	0.83724	-1.55023	-3.31813
H	1.37716	-0.21387	-2.30288
H	1.10509	3.29588	1.08223
H	3.54155	2.62741	0.77049
H	4.69470	0.38111	-0.36805
H	1.81106	-3.74556	-3.09643
H	-0.13085	2.02293	1.10395
H	3.60103	-5.17256	-2.16540
H	0.98896	2.23153	2.50283
H	4.52052	-2.11835	0.71449
H	4.97401	-4.35509	-0.26126
H	-2.10898	-3.40310	0.48921
H	-1.54519	-0.02740	3.13548
H	0.36294	-3.89300	0.61455
H	0.86076	-0.60594	3.38323
N	1.79928	1.35708	0.77361
N	2.69460	-0.39310	-0.09289
Ru	-0.21968	-0.96895	0.62376
C	1.51203	0.09259	0.39112
N	-0.19066	-1.30872	-1.48313
H	-0.70748	-2.15207	-1.71364
O	-1.10526	0.69098	-0.20896
C	-2.43331	1.06068	0.06816
H	-2.68506	0.86227	1.12299
C	-3.42349	0.28941	-0.81202
H	-3.24339	0.52404	-1.86560
H	-4.45855	0.55953	-0.58520
H	-3.31461	-0.79186	-0.67075
H	-0.78256	-0.49202	-1.68748
C	-2.60317	2.55814	-0.13785
C	-1.90662	3.22682	-1.14806
C	-3.49146	3.28385	0.65959
C	-2.09786	4.59069	-1.35768
C	-3.68743	4.64790	0.45093
C	-2.99012	5.30572	-0.55992
H	-1.20511	2.67187	-1.76206
H	-4.03835	2.77970	1.45290
H	-1.55189	5.09722	-2.14731
H	-4.38121	5.19626	1.07966
H	-3.13996	6.36735	-0.72440

Sum of electronic and thermal Enthalpies= -1303.050662
Sum of electronic and thermal Free Energies= -1303.136008

42. H_7'

C	2.49252	-0.81334	-1.66630
C	0.59428	-3.30262	1.36794
C	0.90925	-3.52528	0.07021
C	1.51988	-1.53096	-2.58318
C	1.64437	-1.45166	-3.97276
C	-0.69956	-1.57217	2.62730
C	0.50140	-2.34843	-2.07599
C	0.80230	-2.17007	-4.81813
C	-0.32754	-3.09553	-2.91021
C	-0.18217	-3.00363	-4.29119
H	-3.08810	2.52800	0.23720
C	-3.00175	1.62084	-0.34886
C	-2.37917	1.64286	-1.59945
C	-3.39154	0.36709	0.22258
C	-2.16094	0.41288	-2.30184
C	-3.32927	-0.82393	-0.55103
C	-2.72404	-0.79596	-1.82168
H	-2.56287	-1.71195	-2.37352

H	3.16151	-1.56926	-1.23786
H	1.94150	-0.38017	-0.82054
H	-0.08740	-1.89275	3.46963
H	0.83050	-3.86345	2.25751
H	1.48194	-4.30626	-0.40217
H	2.43891	-0.82964	-4.36979
H	-0.67022	-0.48600	2.56644
H	0.93023	-2.09526	-5.89276
H	-1.72429	-1.91734	2.78049
H	-1.07039	-3.75407	-2.47039
H	-0.82200	-3.58561	-4.94530
H	-1.97390	2.56808	-1.99240
H	-3.78053	0.33417	1.23334
H	-1.59550	0.40713	-3.22619
H	-3.64672	-1.76431	-0.11796
N	-0.14729	-2.13844	1.40505
N	0.34061	-2.49278	-0.65514
Ru	-1.32509	0.11053	-0.32461
C	-0.31882	-1.63281	0.16271
N	3.31164	0.14965	-2.38150
H	2.84811	1.04542	-2.47052
H	4.19255	0.30593	-1.91063
C	0.25951	2.31889	0.87586
H	-0.62155	2.86535	0.51107
C	1.49791	2.86853	0.17626
H	2.39232	2.33197	0.50109
H	1.62925	3.92709	0.41342
H	1.39942	2.76450	-0.90794
O	0.13729	0.93703	0.56558
C	0.32004	2.47961	2.38099
C	-0.55732	3.34370	3.03801
C	1.26429	1.77309	3.13404
C	-0.49200	3.50928	4.42141
C	1.32807	1.93200	4.51524
C	0.45012	2.80162	5.16294
H	-1.29094	3.90530	2.46520
H	1.95113	1.09683	2.63449
H	-1.17440	4.19166	4.91699
H	2.06941	1.38462	5.08833
H	0.50505	2.93001	6.23854

Sum of electronic and thermal Enthalpies= -1303.018122
Sum of electronic and thermal Free Energies= -1303.110416

43. K_7'

C	2.60763	-1.03942	-1.66367
C	0.07718	-3.37165	1.02784
C	0.52926	-3.46342	-0.24248
C	1.58038	-1.48656	-2.68232
C	1.81093	-1.33870	-4.05201
C	-1.27172	-1.74434	2.33709
C	0.38101	-2.09238	-2.28890
C	0.88671	-1.78568	-4.99301
C	-0.53844	-2.56446	-3.22201
C	-0.29061	-2.40635	-4.58230
H	-2.64662	3.12564	-0.39425
C	-2.81023	2.10887	-0.73083
C	-2.31454	1.69809	-1.97704
C	-3.52390	1.19289	0.11093
C	-2.44081	0.32803	-2.36491
C	-3.72018	-0.12973	-0.28482
C	-3.10774	-0.57665	-1.50049
H	-3.18339	-1.61923	-1.78389

H	3.14271	-1.92556	-1.30164
H	2.07774	-0.62737	-0.79211
H	-0.53801	-1.41655	3.07583
H	0.17255	-4.04733	1.86219
H	1.09212	-4.23263	-0.74496
H	2.74170	-0.87700	-4.36184
H	-1.93247	-0.91503	2.09500
H	1.09521	-1.66327	-6.05048
H	-1.85487	-2.57143	2.74582
H	-1.43451	-3.06854	-2.87534
H	-1.00320	-2.77655	-5.31122
H	-1.78686	2.39856	-2.61254
H	-3.89501	1.53453	1.07063
H	-2.01232	-0.02578	-3.29346
H	-4.26779	-0.82265	0.34238
N	-0.61069	-2.17605	1.11970
N	0.11123	-2.31714	-0.89648
Ru	-1.42846	0.31297	-0.46028
C	-0.59702	-1.50094	-0.06083
N	3.59103	-0.14071	-2.23991
H	3.22141	0.79261	-2.37407
H	4.42024	-0.07631	-1.66504
C	0.46297	1.84959	1.53241
C	1.24177	2.49493	0.42953
H	2.27557	2.13448	0.44005
H	1.27439	3.57926	0.56166
H	0.78933	2.24277	-0.52823
O	-0.45935	1.05123	1.29741
H	-0.04906	0.42614	-1.20151
C	0.77645	2.16542	2.93860
C	1.92559	2.89346	3.28269
C	-0.09058	1.73332	3.95523
C	2.20697	3.17090	4.61547
C	0.18750	2.02094	5.28363
C	1.33911	2.73705	5.61595
H	2.60997	3.23938	2.51663
H	-0.98602	1.18676	3.68443
H	3.10072	3.72756	4.87380
H	-0.49165	1.69374	6.06316
H	1.55669	2.96029	6.65483

Sum of electronic and thermal Enthalpies= -1303.034291
Sum of electronic and thermal Free Energies= -1303.127071

44. $TS_{K,H'}$ (7)

C	1.95218	-1.72201	-1.68820
C	0.60430	-3.17167	2.43050
C	0.57173	-3.57657	1.14158
C	0.58616	-2.29437	-1.99630
C	0.18512	-2.51197	-3.31784
C	-0.09992	-1.17295	3.71723
C	-0.29438	-2.68275	-0.98023
C	-1.03243	-3.11730	-3.61675
C	-1.49778	-3.32595	-1.26938
C	-1.87532	-3.54031	-2.59098
H	-1.91230	3.21604	0.03486
C	-2.24029	2.18529	0.07477
C	-2.01850	1.32466	-1.02685
C	-2.77331	1.65473	1.27140
C	-2.40832	-0.03986	-0.97421
C	-3.16524	0.29609	1.35625
C	-2.96664	-0.53995	0.22638
H	-3.20723	-1.59335	0.29786

H	2.61653	-2.55582	-1.43059
H	1.87866	-1.10621	-0.78287
H	0.81908	-0.67477	4.02434
H	0.93079	-3.68108	3.32250
H	0.85529	-4.50706	0.67817
H	0.86670	-2.21226	-4.10606
H	-0.87279	-0.42193	3.58568
H	-1.31213	-3.28002	-4.65205
H	-0.40714	-1.89288	4.47683
H	-2.12564	-3.66749	-0.45243
H	-2.81101	-4.04075	-2.81443
H	-1.53341	1.70998	-1.91617
H	-2.84413	2.28745	2.14879
H	-2.23865	-0.69978	-1.81488
H	-3.57485	-0.10643	2.27367
N	0.09340	-1.88871	2.46269
N	0.04734	-2.52556	0.40916
Ru	-1.00470	0.37818	0.70419
C	-0.24697	-1.46301	1.21915
N	2.53226	-1.03976	-2.82929
H	2.12983	-0.12227	-2.97564
H	3.53403	-0.93846	-2.73731
C	1.02411	1.39417	1.12766
C	2.38336	0.71349	1.13972
H	2.98530	1.24247	1.88546
H	2.90286	0.78607	0.18362
H	2.29422	-0.33024	1.44163
O	0.26040	1.16070	2.16321
H	0.46749	0.52697	-0.02563
C	1.02558	2.79286	0.55978
C	1.49143	3.06971	-0.72856
C	0.61707	3.84624	1.38254
C	1.53028	4.37978	-1.19673
C	0.66624	5.15836	0.91669
C	1.11774	5.42794	-0.37387
H	1.81539	2.26025	-1.37694
H	0.27431	3.62557	2.38752
H	1.88751	4.58506	-2.20022
H	0.35960	5.97175	1.56578
H	1.15679	6.44972	-0.73524

Sum of electronic and thermal Enthalpies= -1303.015465
Sum of electronic and thermal Free Energies= -1303.103378