Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Mechanistic Study of Allopurinol Oxidation Using Aldehyde Oxidase, Xanthine Oxidase and Cytochrome P450 Enzymes

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Figure S1. The 2D sketch of all 10 tautomers of allopurinol.

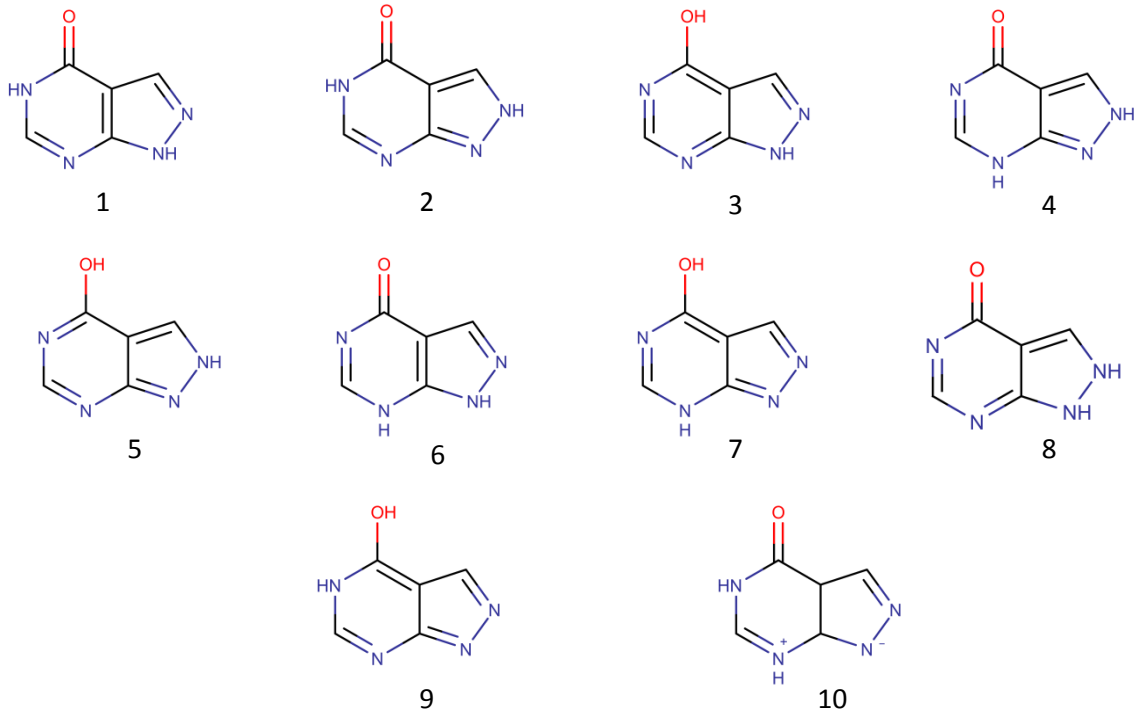


Table S1. Relative free energies of allopurinol tautomers (ΔG in kcal.mol^{-1}).

	Vacuo		Water	
structure	B3LYP[a]	G3MP2	SM8[a]	SMD[a]
1	0.00 (0.00)	0.00	0.00	0.00 (0.00)
2	3.64 (3.66)	3.28	0.55	0.92 (0.53)
3	6.75 (7.02)	4.34	8.32	10.12 (11.63)
4	12.61 (14.45)	11.85	4.67	5.95 (5.84)
5	13.83 (14.11)	11.25	10.54	12.70 (13.83)
6	17.74 (17.22)	16.45	8.28	7.71 (7.53)
7	26.09 (26.26)	23.26	17.38	20.62 (19.42)
8	32.28 (32.81)	34.1	14.44	15.41 (15.21)
9	40.83 (40.74)	36.58	22.37	24.01 (25.65)
10	27.82 (27.81)	27.86	10.40	13.98 (10.07)

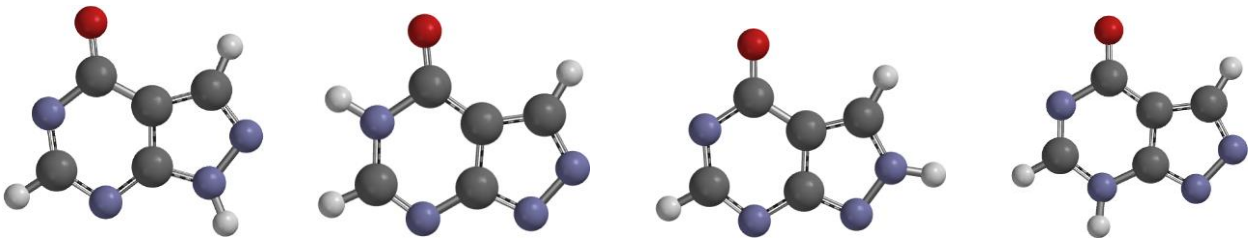
[a] These data are calculated at B3LYP/6-31+G* level. The numbers in parentheses are calculated using the B3LYP-D3BJ/6-31+G* method.

Table S2. Effect of basis set on the relative free energies of tautomer 1 and tautomer 2.

	Tauto-1	Tauto-2
6-31+G*	0.00	3.64
6-311++G(3df,3pd)	0.00	3.52
Aug-CC-pVTZ	0.00	3.51

All calculations were done using the B3LYP functional.

Figure S2. Structures of deprotonated allopurinol.



I II III IV

Table S3. Allopurinol deprotonation free energy (ΔG in kcal.mol^{-1}) in comparison to the most stable tautomer (tauto-1). The values in parentheses are calculated using SM8 solvation model.

	Relative Energy		Deprotonation Energy	
structure	B3LYP	G3MP2	B3LYP	G3MP2
I	0.00 (0.09)	0.00	331.64 (277.93)	333.95
II	3.89 (0.00)	3.23	335.53 (277.83)	337.18
III	8.41 (1.99)	8.10	340.05 (279.83)	342.05
IV	10.37 (4.57)	9.34	342.01 (282.40)	343.29

Figure S3. The 3D representation of the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) plots of the tautomer 1, 2 and 10 of allopurinol.

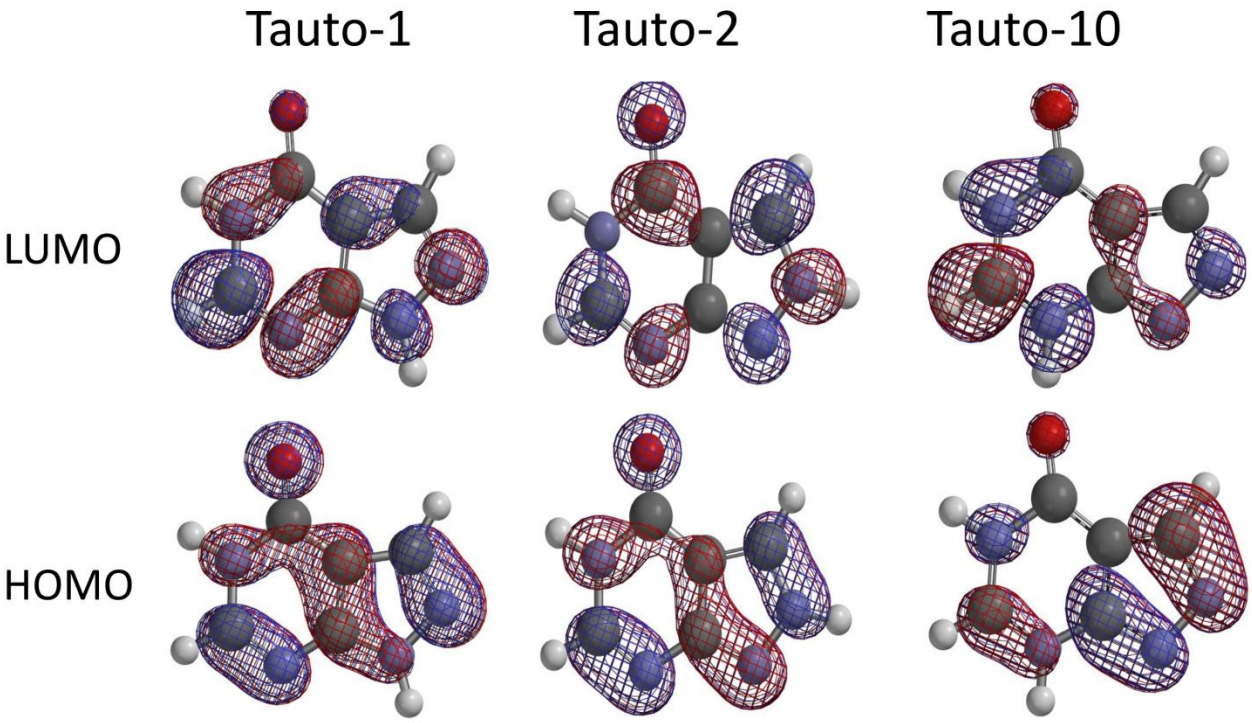


Table S4. The orbital contribution analysis (for C3, see scheme 1) of HOMO and LUMO of the tautomer 1, 2 and 10 of allopurinol using the Hirshfeld method.

	Tauto-1	**Tauto-2**	**Tauto-3**
LUMO	30.741%	11.118%	36.731%
HOMO	8.518%	10.161%	5.798%

Table S5. Highest Occupied Molecular Orbital (HOMO) energy- Lowest Unoccupied Molecular Orbital (LUMO) energy - Hardness ɳ- Electronegativity X- Global electrophilicity ω, and Nucelophilicity Index N. All data calculated at G3MP2**.**

structure	**HOMO (au)**	**LUMO (au)**	***η* (eV)**	***X* (eV)**	***ω* (eV)**	***N* (eV)**
Tauto-1	-0.33826	0.02641	9.923	8.486	3.628	0.276
Tauto-2	-0.33852	0.03257	10.098	8.325	3.432	0.291
Tauto-10	-0.31383	0.00112	8.570	8.509	4.224	0.237
Deprotonated-I	-0.15335	0.13948	7.968	0.377	0.009	111.112

Reactivity and electrophilicity of table S4 species were considered using the following standard equations:

$$\eta = -E_{LUMO} - E_{HOMO}$$

$$X = -(E_{LUMO} + E_{HOMO})/2$$

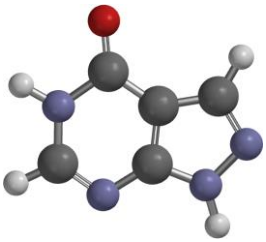
$$\omega = X^2/2\eta$$

$$N = 1/\omega$$

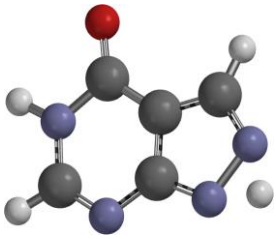
This method for calculating reactivity has been used by several groups: [1-5]

1. P. A. Krieter, , A. E. Colletti, G. A. Doss, , R. R. Miller. Drug Metab. Dispos. 1994, **22**, 625.
2. (a) H. Toufar, K. Nulens, G. O. A. Janssens, W. J. Mortier, , R. A. Schoonheydt, F. De Proft, P. Geerlings. J. Phys. Chem. B. 1996, **100**, 15383. (b) F. De Proft, P. Geerlings. Chem. Rev. 2001, **101**, 1451. (c) P. Geerlings, F. De Proft, W. Langenaeker. Chem. Rev. 2003, **103**, 1793. (d) T. Fievez, N. Sablon, F. DeProft, P. W. Ayers, P. J. Geerlings. Chem. Theory Comput. 2008, **4**, 1065. (e) G. Roos, P. Geerlings, J. Messens. J. Phys. Chem. B. 2009, **113**, 13465. (f) J. T. Muya, F. De Proft, P. Geerlings, M. T. Nguyen, A. Ceulemans. J. Phys. Chem. A. 2011, **115**, 9069.
3. (a) N. T. Brown, N. Mora-Diez. Phys. Chem. B 2006, **110**, 9270. (b) L. A. M. M. Barbosa, R. A. van Santen. J. Mol. Struct. THEOCHEM. 2000, **497**, 173.
4. P. K. Chattaraj, U. Sarkar, D. R. Roy. Chem. Rev. 2006, **106**, 2065.
5. P. K. Chattaraj, A. Chakraborty, S. Giri. J. Phys. Chem. A. 2009, **113**, 10068.

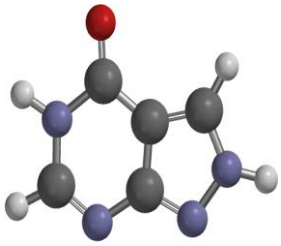
Figure S4. The gas and water-assisted interconversion between the tautomer 1 and tautomer 2 of allopurinol. The values are calculated at B3LYP/6-31+G* (ΔE in kcal.mol^{-1}) and the numbers in bolds and in parentheses are calculated using the B3LYP-D3BJ/6-31+G* and SMD solvation models, respectively.



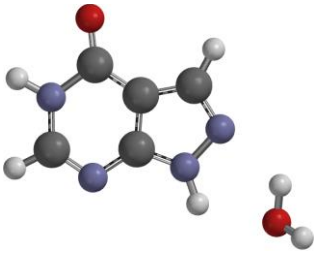
Tauto-1 = 0.00, **0.00** (0.00, **0.00**)



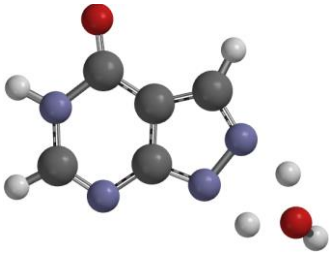
TS = 53.32, **58.86** (52.77, **52.86**)



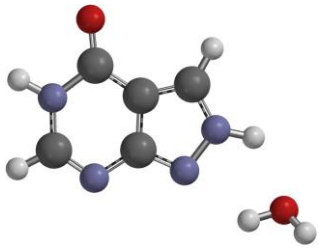
Tauto-2 = 3.61, **3.64** (0.87, **0.51**)



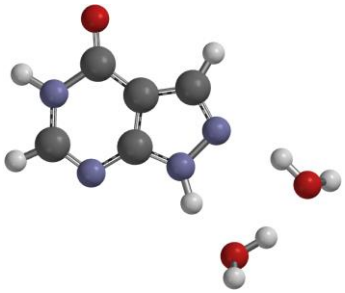
Tauto-1+1w = 0.00 (0.00)



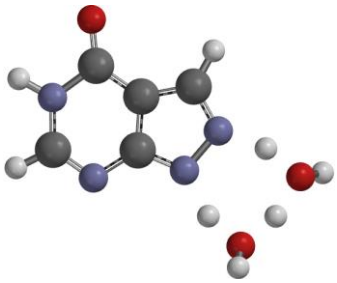
TS+1w = 29.08 (28.40)



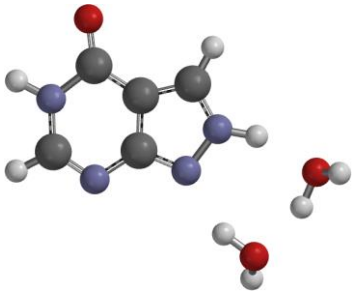
Tauto-2+1w = 2.45 (0.67)



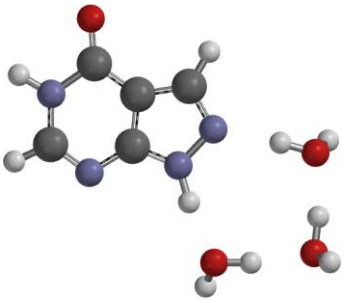
Tauto-1+2w= 0.00, **0.00** (0.00, **0.00**)



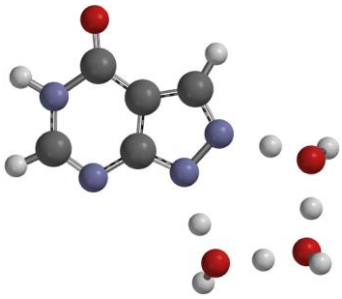
TS+2w= 17.77, **15.27** (16.38, **16.27**)



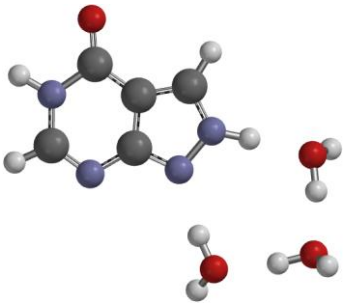
Tauto-2+2w= 1.52, **1.44** (0.49, **0.37**)



Tauto-1+3w = 0.00 (0.00)



TS+3w = 17.82 (17.02)



Tauto-2+3w = 0.92 (0.40)

Figure S5. The stepwise mechanism for O-up orientation of allopurinol tautomer 1.

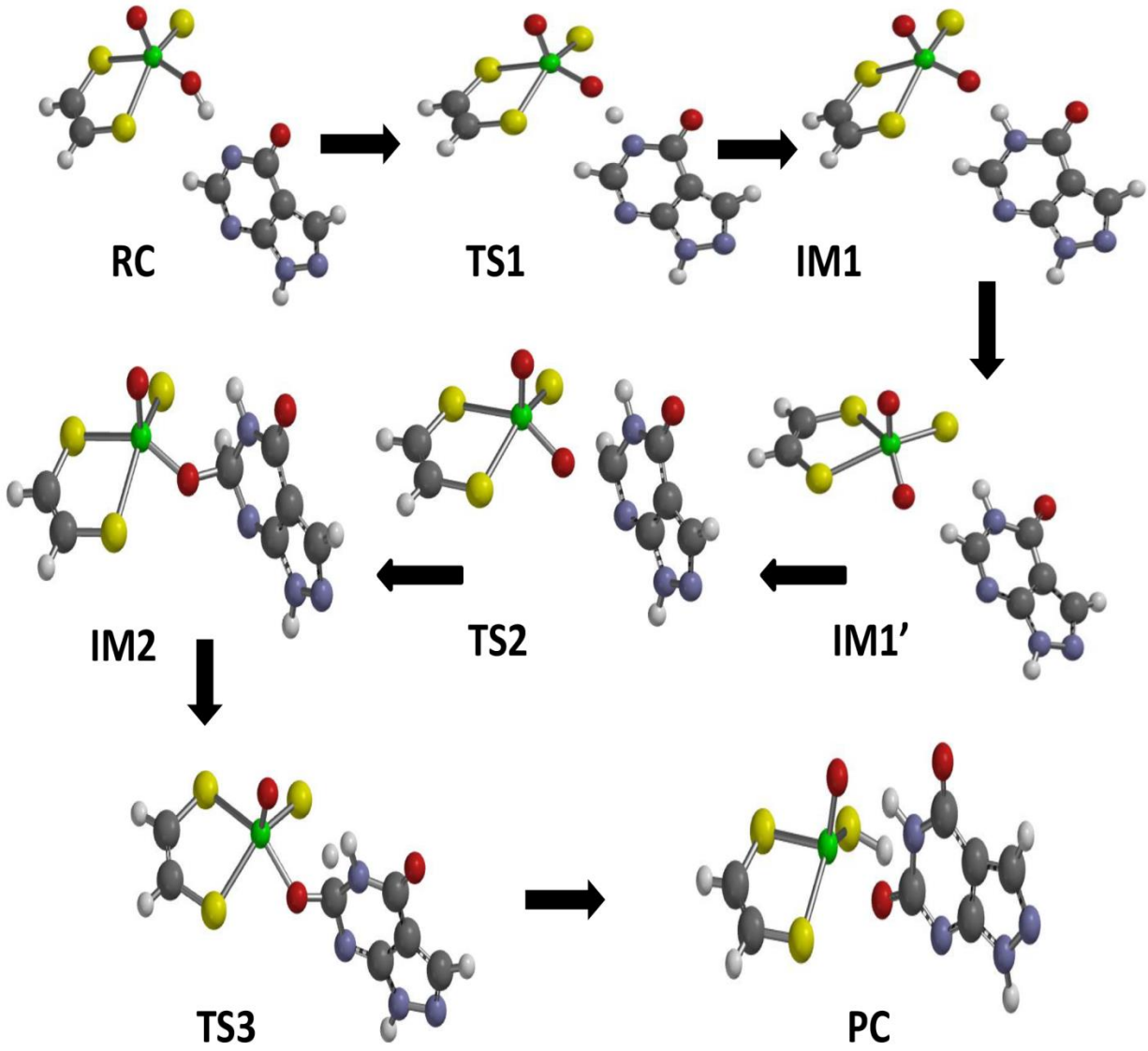


Figure S6. The stepwise mechanism for the O-up of allopurinol tautomer 10.

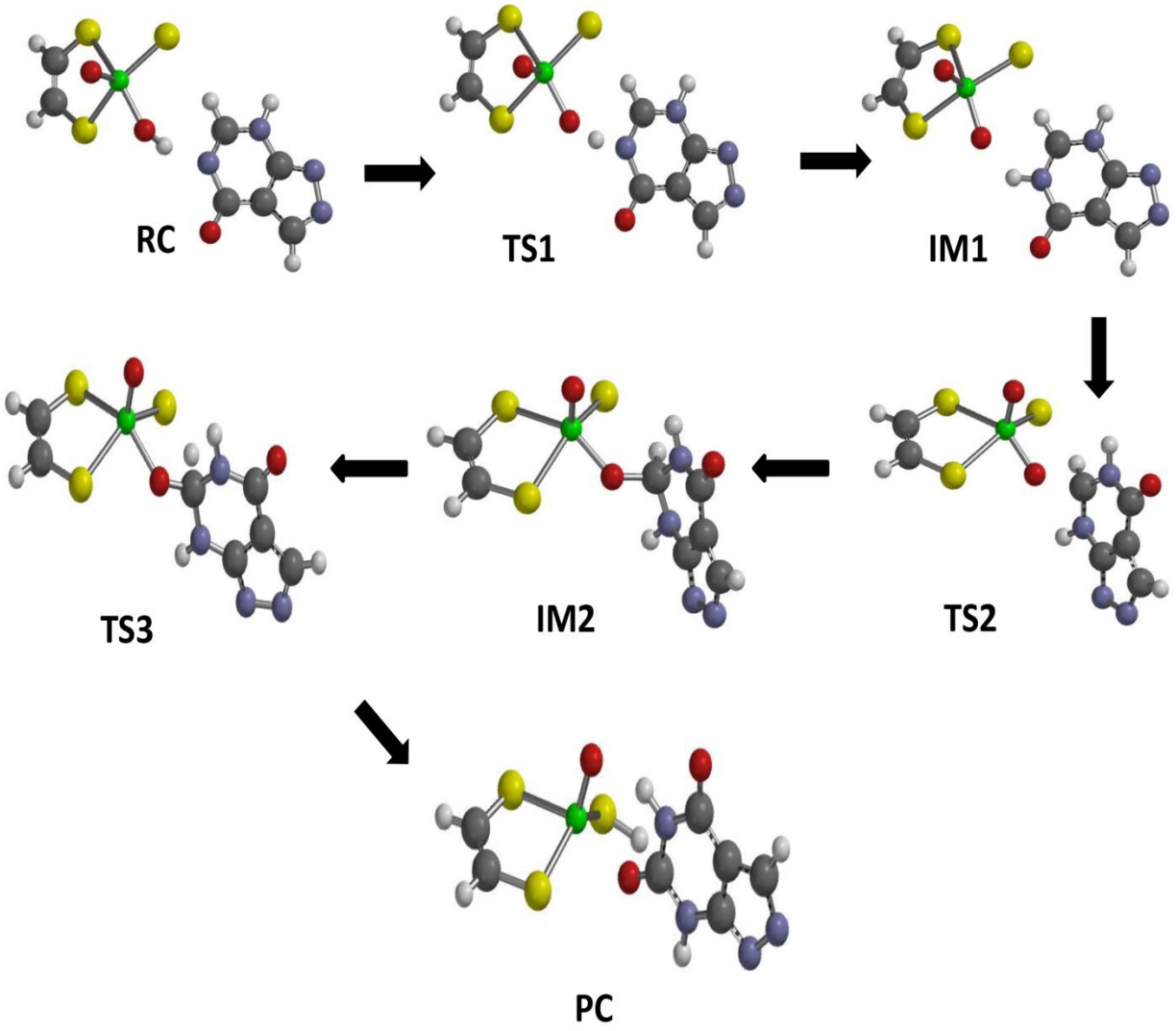


Figure S7. The stepwise mechanism for the O-down of allopurinol tautomer 10.

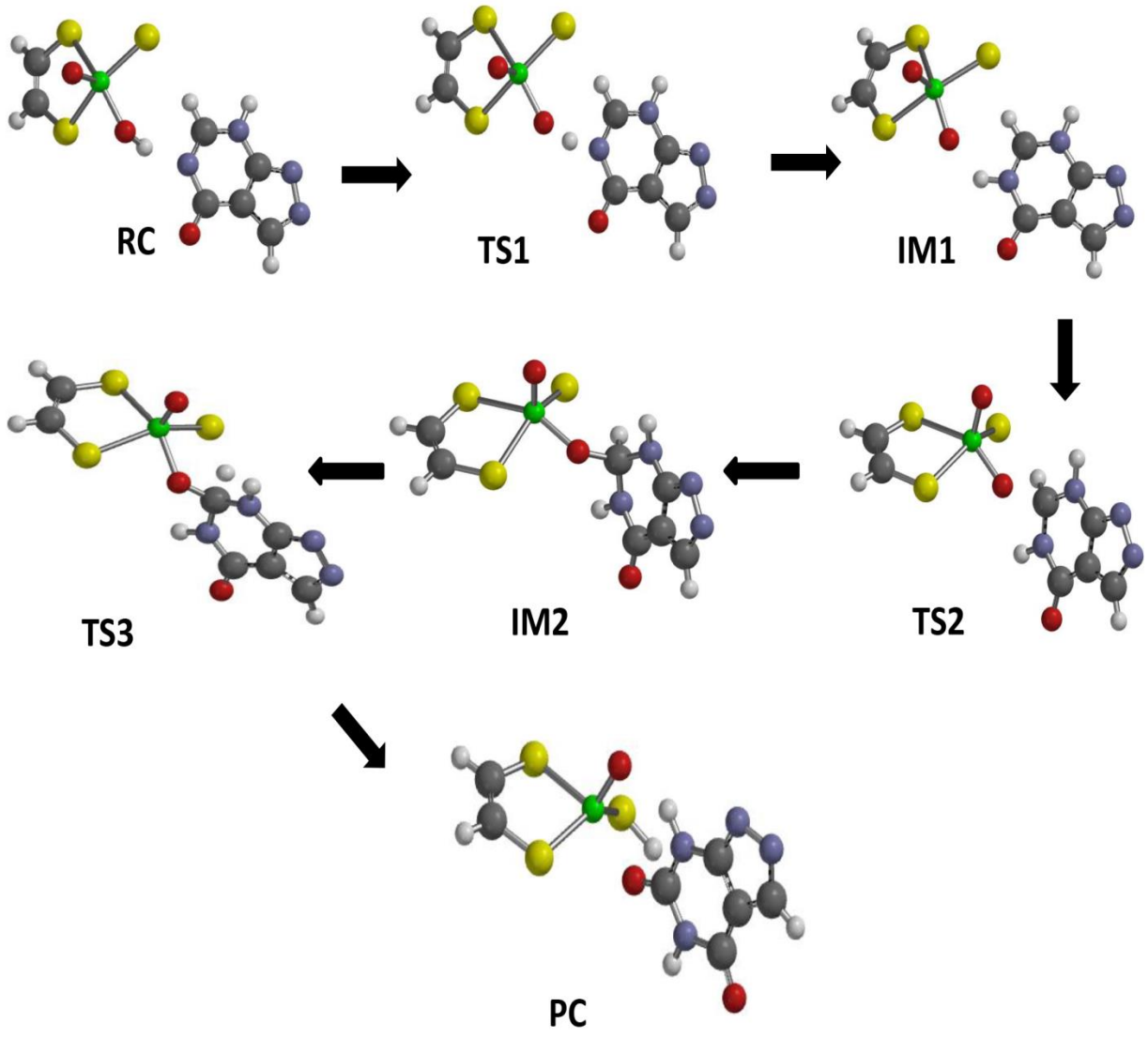


Figure S8. The concerted mechanism of neutral allopurinol (tautomer1-O-Up, ΔE in kcal.mol^{-1}). The numbers in bold are calculated using the B3LYP-D3BJ method.

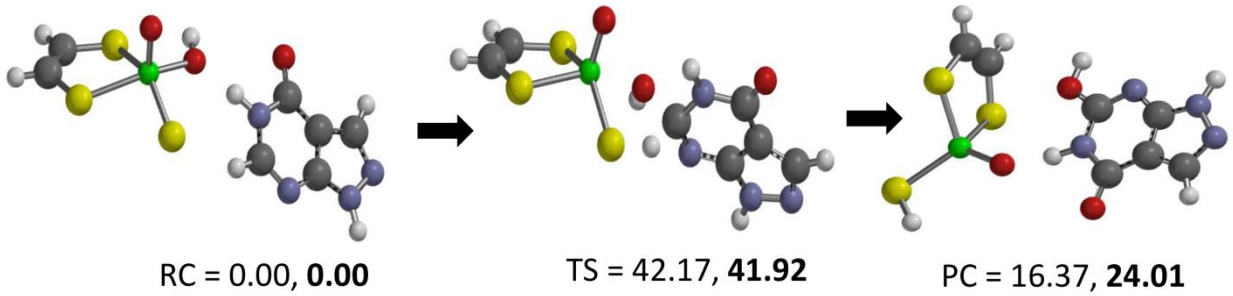


Figure S9. The concerted mechanism of neutral allopurinol (tautomer2-O-Up, ΔE in kcal.mol^{-1}). The numbers in bold are calculated using the B3LYP-D3BJ method.

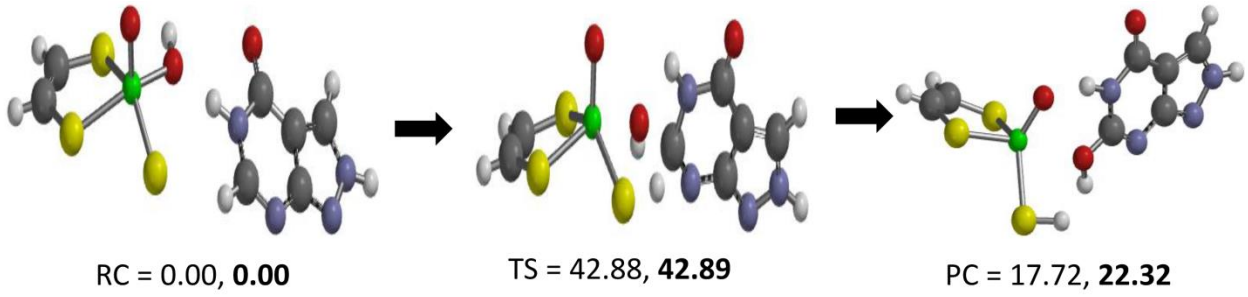


Figure S10. The concerted mechanism of neutral allopurinol (tautomer2-O-Down, ΔE in kcal.mol^{-1}). The numbers in bold are calculated using the B3LYP-D3BJ method.

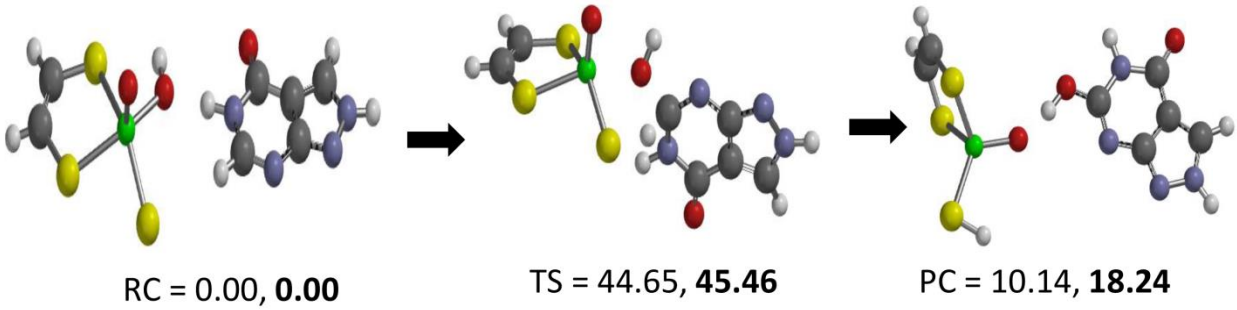


Figure S11. The concerted mechanism of neutral allopurinol (tautomer10-O-Down, ΔE in kcal.mol^{-1}). The numbers in bold are calculated using the B3LYP-D3BJ method.

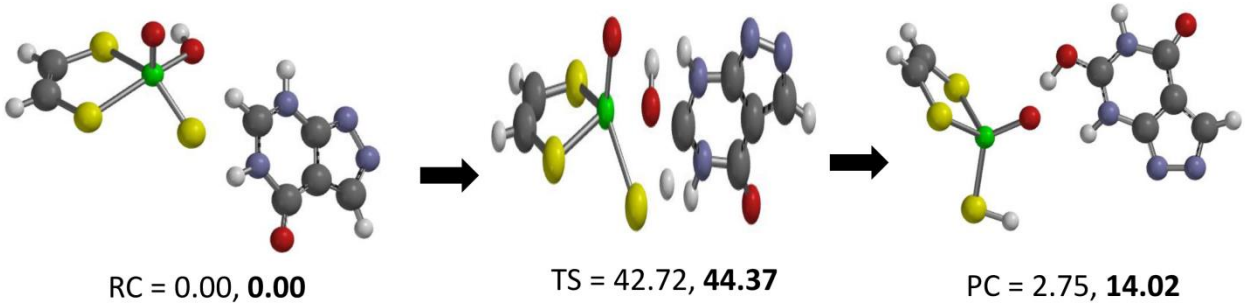


Figure S12. The concerted mechanism of deprotonated allopurinol (structure I, ΔE in kcal.mol^{-1}). The numbers in bold are calculated using the B3LYP-D3BJ method.

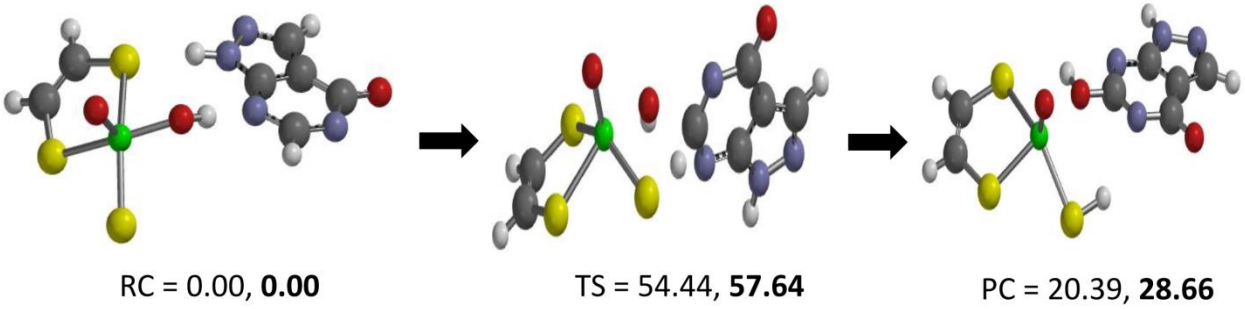


Figure S13. The concerted mechanism of deprotonated allopurinol (structure III, ΔE in kcal.mol^{-1}).

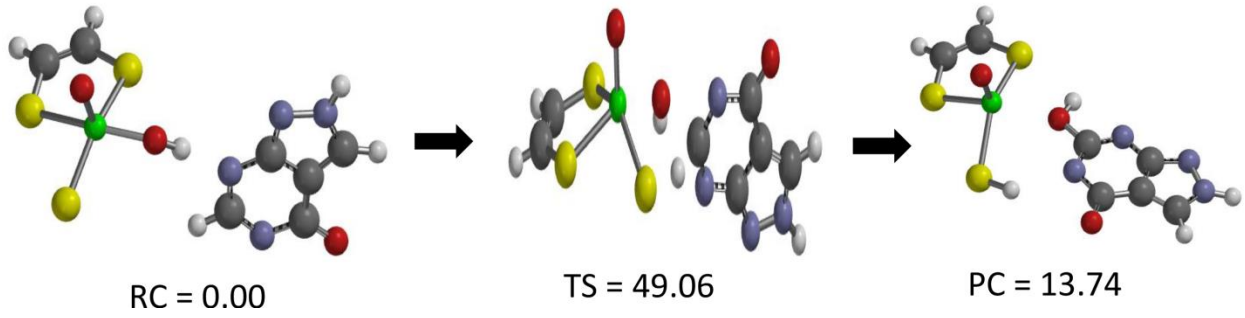


Table S6. Transition state bond lengths (in Å) of the concerted mechanism for different structures (figure S7-S12)

	Mo-OH	**OH-C**	**C-H**	**H-S**	**S-Mo**
T1 (O-up)	2.19	1.47	1.40	1.58	2.29
T2 (O-up)	2.18	1.49	1.37	1.60	2.28
T2 (O-down)	2.22	1.48	1.39	1.59	2.29
T10 (O-down)	2.24	1.43	1.59	1.48	2.32
Deprotonated-I	2.08	1.78	1.37	1.58	2.29
Deprotonated-III	2.07	1.80	1.38	1.58	2.29

Table S7. The bond lengths (in Å) of the P450 mechanism for some selected structures (figure 13). The numbers in bold are for quartet spin states.

	Tauto-1			Tauto-2		
	TS1	Int1	TS2	TS1	Int1	TS2
Fe-O	1.72/**1.71**	1.83/**1.84**	1.94/**2.12**	1.72/**1.71**	1.87/**1.87**	1.93/**2.11**
O-C	1.82/**1.85**	1.40/**1.40**	1.34/**1.31**	1.82/**1.85**	1.39/**1.39**	1.34/**1.32**
C-H	1.08/**1.08**	1.09/**1.09**	1.19/**1.21**	1.08/**1.08**	1.10/**1.10**	1.18/**1.20**
H-N	2.65/**2.66**	2.54/**2.72**	1.79/**1.72**	2.60/**2.56**	2.67/**2.69**	1.80/**1.76**

Figure S14. The structure of allopurinol oxidation using P450.

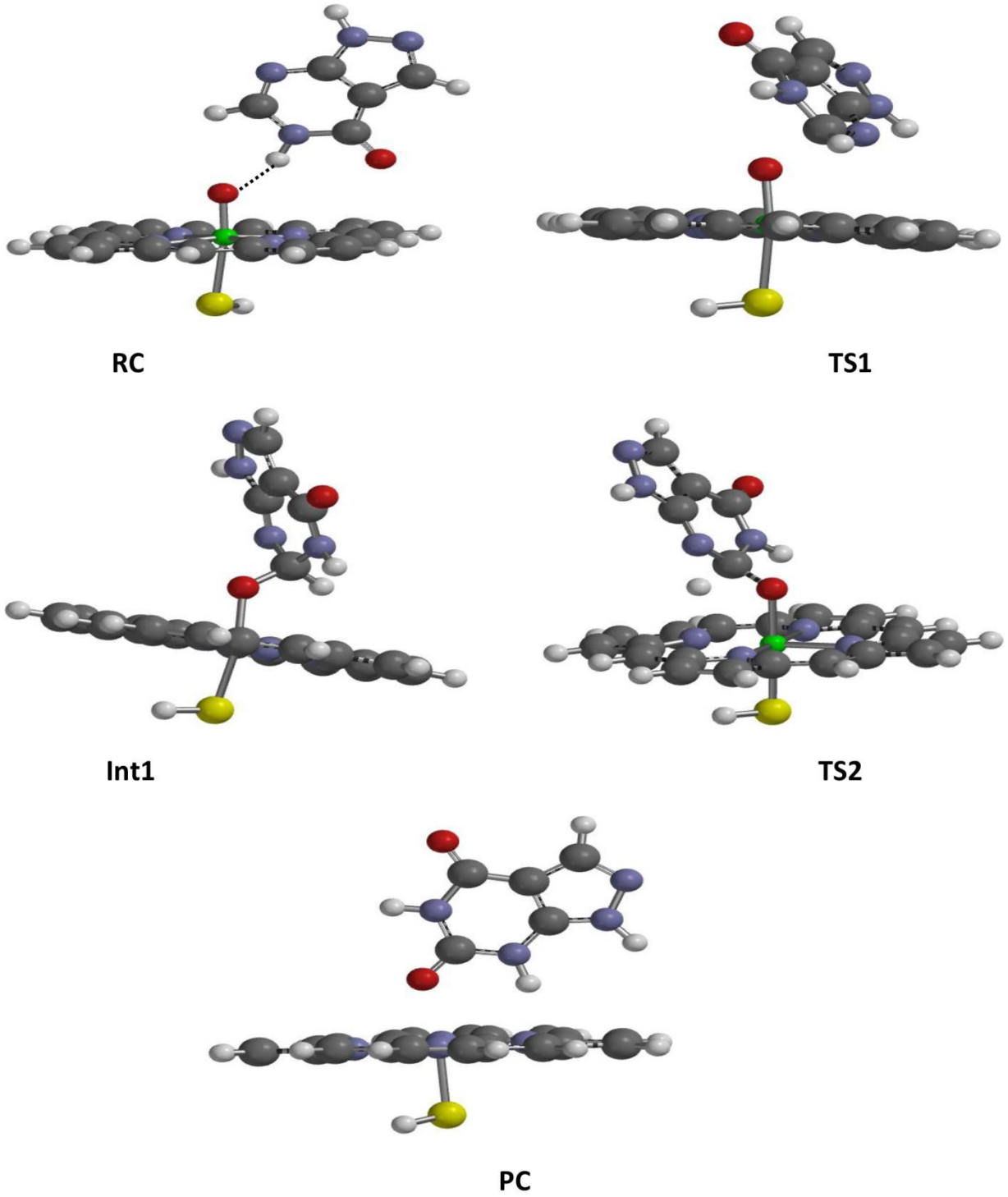


Figure S15. Relative energy profile (ΔE in kcal.mol^{-1}) for allopurinol tautomer 2 metabolism using the active site of P450 (Cpd I). The numbers are calculated using the B3LYP/B1+ZPE(B1) and B3LYP(SMD)/B2//B1+ZPE(B1), respectively.

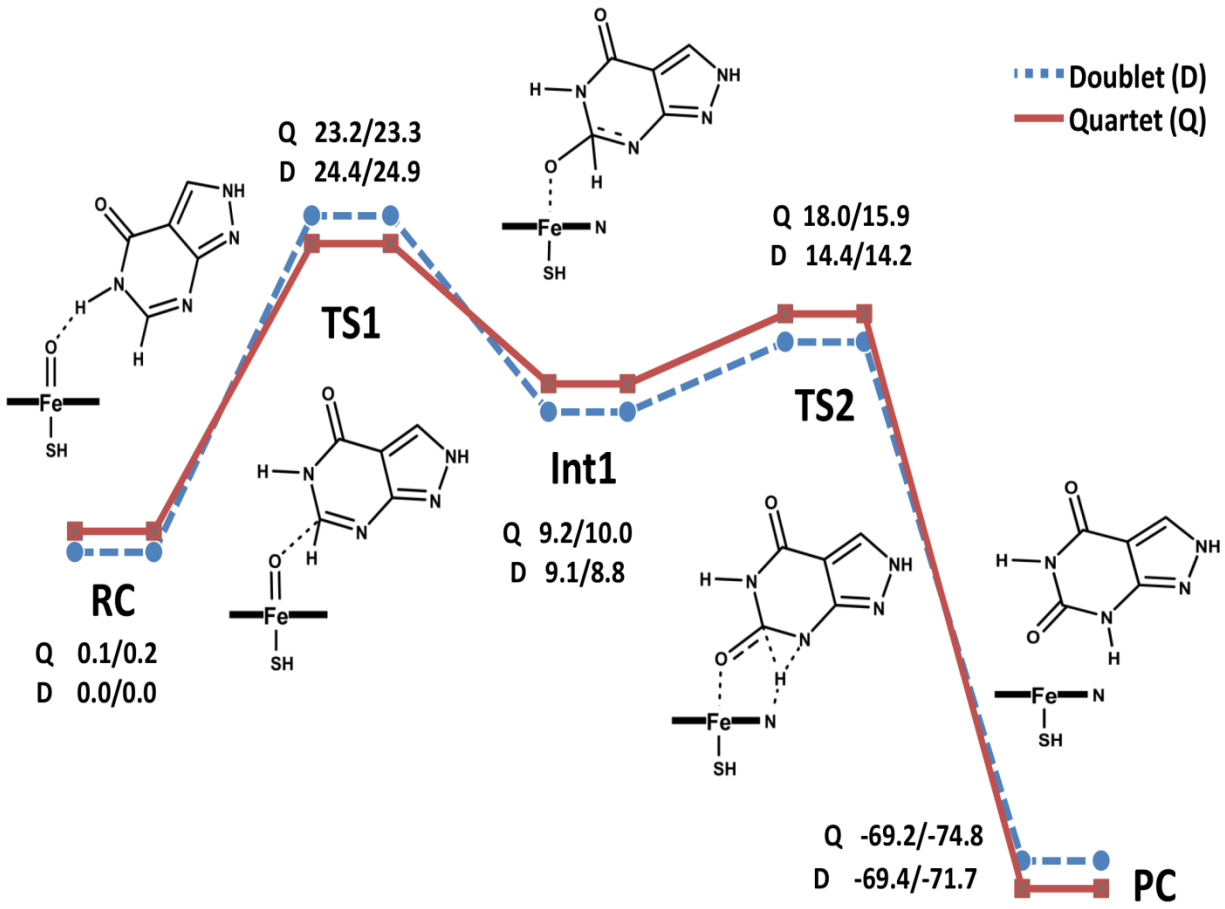
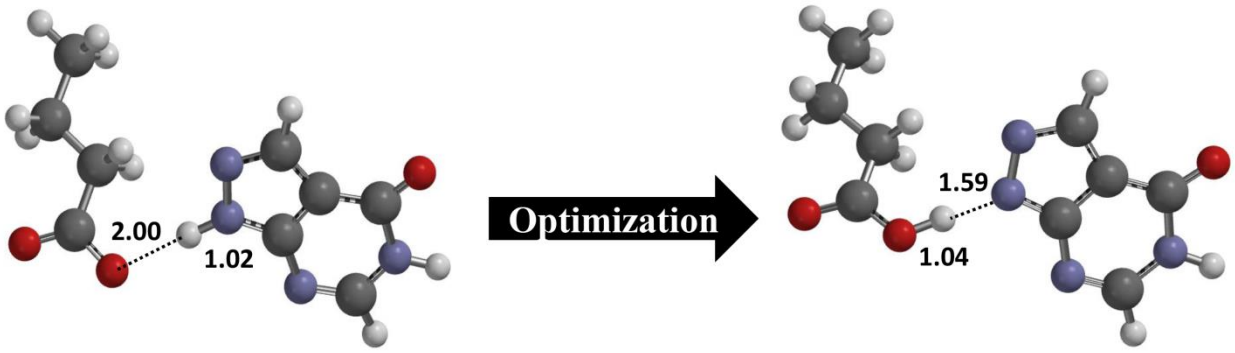


Figure S16. The 3D representation and Cartesian coordinate of glutamate model compound (butanoic acid) and allopurinol tautomer 1 complex input and output structures (B3LYP/6-31+G(d,p)).



Input Structure

C	-3.66197100	0.70700700	0.00322900
N	-1.96658500	-1.64037200	0.57757300
N	-4.05368900	-0.51198000	0.63016500
C	-2.27251100	0.65741800	-0.33476400
C	-1.49250000	-0.49631700	-0.03972400
C	-3.22213700	-1.58445800	0.87821600
N	-0.22879500	-0.31017200	-0.44661800
N	-0.14039400	0.93745000	-1.00790900
C	-1.34143600	1.51979900	-0.94648800
O	-4.50187600	1.59418000	-0.16157900
H	-5.02835000	-0.55424900	0.90011900
H	-3.70032900	-2.43239800	1.36848600
H	0.60305051	-0.89990552	-0.47206244
H	-1.49502500	2.51945600	-1.33626100
C	4.10489100	2.33700900	0.99575400
H	3.48770200	2.96036600	0.33690500
H	3.61333000	2.31841700	1.97730800
H	5.07509100	2.83610800	1.11885300
C	4.26785000	0.92255500	0.42965200
H	4.79479500	0.96465100	-0.53223900
H	4.90664700	0.32130600	1.08775500
C	2.92946700	0.20868600	0.23561800
H	2.37613200	0.16260200	1.18550200
H	2.26770900	0.76612500	-0.44026700
C	3.07956700	-1.22375100	-0.27988500
O	1.95312300	-1.85450400	-0.58717700
O	4.16959900	-1.76618800	-0.38881700

Output Structure

C	-3.66945600	0.67814300	0.02608600
N	-1.91472200	-1.61401500	0.60857100
N	-4.02247400	-0.52642600	0.69260000
C	-2.29074100	0.65195200	-0.35258400
C	-1.47984900	-0.47966600	-0.05064700
C	-3.16339000	-1.57753100	0.94504900
N	-0.23141600	-0.27790900	-0.49881900
N	-0.18484200	0.95619200	-1.09207300
C	-1.39545800	1.51912100	-1.01391300
O	-4.53298600	1.54996700	-0.13867600
H	-4.98741200	-0.58249200	0.99202300
H	-3.60836700	-2.42140400	1.46928400
H	1.07447200	-1.18581300	-0.55545600
H	-1.57857100	2.50404200	-1.42392900
C	4.14684900	2.30449900	1.05969400
H	3.56036600	2.95012500	0.39497000
H	3.63126100	2.28192000	2.02823800
H	5.12379600	2.77960400	1.21373900
C	4.29667400	0.89398600	0.47621300
H	4.84803600	0.94025200	-0.47095400
H	4.90508400	0.27176200	1.14264200
C	2.94686100	0.21481600	0.23792600
H	2.37319100	0.16164300	1.17432800
H	2.31822700	0.80414000	-0.44098000
C	3.05669900	-1.20942400	-0.30818900
O	1.91712600	-1.78950300	-0.65451000
O	4.13148000	-1.79096900	-0.40852100

S1. Cartesian coordinates of gas and water-assisted interconversion between the tautomer 1 and tautomer 2 of allopurinol (figure S3)**.**

T1

Zero-point correction= 0.100394 (Hartree/Particle)
Thermal correction to Energy= 0.107163
Thermal correction to Enthalpy= 0.108107
Thermal correction to Gibbs Free Energy= 0.068916
Sum of electronic and zero-point Energies= -487.091597
Sum of electronic and thermal Energies= -487.084829
Sum of electronic and thermal Enthalpies= -487.083885
Sum of electronic and thermal Free Energies= -487.123075

C	1.42312800	0.39880900	0.00000000
N	-0.53929500	-1.80059900	0.00000000
N	1.69027000	-1.00467700	0.00000000
C	0.00000000	0.62813300	0.00000000
C	-0.86805100	-0.47452800	0.00000000
C	0.74791800	-1.99615700	0.00000000
N	-2.12083200	0.03643600	0.00000000
N	-2.12963200	1.39903300	0.00000000
C	-0.85309200	1.76200700	0.00000000
O	2.34650500	1.20059300	0.00000000
H	2.67490100	-1.25128000	0.00000000
H	1.13160400	-3.01336000	0.00000000
H	-2.99490900	-0.47100800	0.00000000
H	-0.58663000	2.80997300	0.00000000

T2

Zero-point correction= 0.100422 (Hartree/Particle)
Thermal correction to Energy= 0.107143
Thermal correction to Enthalpy= 0.108087
Thermal correction to Gibbs Free Energy= 0.068992
Sum of electronic and zero-point Energies= -487.085884
Sum of electronic and thermal Energies= -487.079163
Sum of electronic and thermal Enthalpies= -487.078218
Sum of electronic and thermal Free Energies= -487.117314

C	1.42903100	0.37796700	0.00000000
C	-0.91698600	-0.48988400	0.00000000
C	0.73371500	-2.00375400	0.00000000
N	-0.54549800	-1.81811400	0.00000000
N	1.69295300	-1.00958000	0.00000000
C	0.00000000	0.60741800	0.00000000
C	-0.79704300	1.74268500	0.00000000
N	-2.06737800	1.27978100	0.00000000
N	-2.18545400	-0.07018700	0.00000000
O	2.33948700	1.19711200	0.00000000
H	1.12689300	-3.01799100	0.00000000
H	2.67487300	-1.26474600	0.00000000
H	-0.55681600	2.79623500	0.00000000
H	-2.91551900	1.82971200	0.00000000

TS

Zero-point correction= 0.093810 (Hartree/Particle)
Thermal correction to Energy= 0.100513
Thermal correction to Enthalpy= 0.101457
Thermal correction to Gibbs Free Energy= 0.062339
Sum of electronic and zero-point Energies= -487.006617
Sum of electronic and thermal Energies= -486.999914
Sum of electronic and thermal Enthalpies= -486.998970
Sum of electronic and thermal Free Energies= -487.038088

C	-0.23935700	0.55960400	-0.00502000
C	-0.64974700	-0.79336100	-0.01331900
N	-1.99631800	-0.88304900	-0.09556500
N	-2.48148700	0.49711200	-0.06220800
C	-1.41394700	1.31122600	0.03476100
C	1.44598700	-1.56953000	0.01914200
C	1.17527900	0.89437100	-0.00861600
H	-2.75228100	-0.36323000	0.78022000
H	-1.54508200	2.38362800	0.10096400
H	2.19300900	-2.35959800	0.03923600
H	2.95650100	-0.14887100	0.00818100
O	1.70072300	1.99711200	-0.01087800
N	0.18883400	-1.88265600	0.01149300
N	1.95079500	-0.28893500	0.00295600

T1+1w

Zero-point correction= 0.124621 (Hartree/Particle)
Thermal correction to Energy= 0.134700
Thermal correction to Enthalpy= 0.135644
Thermal correction to Gibbs Free Energy= 0.088352
Sum of electronic and zero-point Energies= -563.502388
Sum of electronic and thermal Energies= -563.492308
Sum of electronic and thermal Enthalpies= -563.491364
Sum of electronic and thermal Free Energies= -563.538656

C	1.93697800	-0.69756100	-0.00455000
C	1.73310900	1.78154400	-0.00089100
C	-0.14797600	0.60111800	0.01073400
C	0.49617800	-0.64849000	0.00536900
C	-0.55453400	-1.59870800	0.00889800
N	-1.73614900	-0.99194300	0.01756600
N	-1.47303200	0.34501800	0.01989500
H	2.30602300	2.70548100	-0.00396100
H	3.48242000	0.68036500	-0.01495100
H	-0.49413900	-2.67829300	0.00516400
H	-2.26357500	0.98529100	0.01853800
H	-5.04129200	0.27835000	0.50596800
O	-4.28353100	0.31715100	-0.09525900
H	-3.85264900	-0.55842600	-0.05615100
N	0.43327700	1.83858300	0.00871600
N	2.46871100	0.62696000	-0.00722100
O	2.68741000	-1.66346600	-0.01032400

TS+1w

Zero-point correction= 0.119169 (Hartree/Particle)
Thermal correction to Energy= 0.127495
Thermal correction to Enthalpy= 0.128439
Thermal correction to Gibbs Free Energy= 0.085413
Sum of electronic and zero-point Energies= -563.458551
Sum of electronic and thermal Energies= -563.450225
Sum of electronic and thermal Enthalpies= -563.449281
Sum of electronic and thermal Free Energies= -563.492307

C	-1.85363800	-0.73785100	-0.00129000
C	-1.73885000	1.74335700	-0.00180600
C	0.20532400	0.64516000	0.00793700
C	-0.41522200	-0.63206300	0.00575900
C	0.64575600	-1.55348900	0.00664800
N	1.79035000	-0.86831300	0.01451300
N	1.53541400	0.48212600	0.01609600
H	-2.35211300	2.64159400	-0.00545800
H	-3.45003300	0.57505000	-0.01203400
H	0.62882100	-2.63461900	0.00152800
H	2.88619300	0.82367600	-0.04769100
H	4.38958100	0.33697100	0.71079900
O	3.88311500	0.23216600	-0.11204000
H	3.16364000	-0.68544500	-0.03888200
N	-2.43544700	0.55846800	-0.00559400
N	-0.44694600	1.85570000	0.00576600
O	-2.56185300	-1.73763900	-0.00386300

T1+2w

Zero-point correction= 0.150633 (Hartree/Particle)
Thermal correction to Energy= 0.162920
Thermal correction to Enthalpy= 0.163865
Thermal correction to Gibbs Free Energy= 0.111525
Sum of electronic and zero-point Energies= -639.921884
Sum of electronic and thermal Energies= -639.909597
Sum of electronic and thermal Enthalpies= -639.908653
Sum of electronic and thermal Free Energies= -639.960992

C	-0.97138500	-0.66366300	-0.01248600
C	-0.33391700	0.59067900	0.00353500
N	0.99310400	0.35269200	-0.00837500
N	1.25920800	-0.98361200	-0.03296500
C	0.08371000	-1.60461300	-0.03547800
C	-2.22741000	1.75354700	0.03096800
C	-2.41205200	-0.72558100	-0.00461400
H	3.14733600	-1.31226400	-0.02742700
H	0.03313100	-2.68463600	-0.05476500
H	-2.80918200	2.67193000	0.04777300
H	-3.96865400	0.63810500	0.02603000
H	1.78578700	1.01296200	-0.00445500
O	3.53718900	1.55842900	0.03958400
H	3.93149300	2.08016100	-0.67449300
H	3.97611000	0.67277900	0.01917100
O	4.11666800	-1.12144200	-0.02314200
H	4.48206000	-1.57306000	0.75205300
N	-2.95461800	0.59256400	0.01908400
N	-0.92897600	1.82259900	0.02421900
O	-3.15295400	-1.69922200	-0.01509000

T2-1w

Zero-point correction= 0.124721 (Hartree/Particle)
Thermal correction to Energy= 0.134739
Thermal correction to Enthalpy= 0.135683
Thermal correction to Gibbs Free Energy= 0.088563
Sum of electronic and zero-point Energies= -563.498593
Sum of electronic and thermal Energies= -563.488575
Sum of electronic and thermal Enthalpies= -563.487630
Sum of electronic and thermal Free Energies= -563.534751

C	1.79076400	1.74926700	-0.00272300
C	0.47816800	-0.62581900	0.00565200
C	-0.16039900	0.65191500	0.00979300
C	1.92088100	-0.72943300	-0.00405600
N	-1.49145900	0.52745400	0.01814300
N	-1.69151400	-0.81398100	0.01946000
C	-0.56220500	-1.54801700	0.01118500
H	2.40506800	2.64683800	-0.00659000
H	3.51021500	0.58579300	-0.01551800
H	-2.66218900	-1.12179400	0.02321600
H	-0.56887900	-2.62858500	0.00929500
H	-3.62864900	0.84084500	-0.06475300
O	-4.31426700	0.14501000	-0.09331200
H	-5.02463400	0.43480700	0.49714100
O	2.62193800	-1.73327500	-0.00824600
N	2.49576600	0.56289500	-0.00817500
N	0.50212700	1.86088000	0.00636700

2w-TS

Zero-point correction= 0.141729 (Hartree/Particle)
Thermal correction to Energy= 0.152107
Thermal correction to Enthalpy= 0.153051
Thermal correction to Gibbs Free Energy= 0.105191
Sum of electronic and zero-point Energies= -639.896130
Sum of electronic and thermal Energies= -639.885753
Sum of electronic and thermal Enthalpies= -639.884809
Sum of electronic and thermal Free Energies= -639.932669

C	0.89587300	-0.65443800	0.00794700
C	0.25030000	0.60762200	-0.01157300
N	-1.07782700	0.42372200	-0.01022300
N	-1.30875600	-0.92485600	0.01257300
C	-0.15059300	-1.58940700	0.02331600
H	-2.23606800	1.13082700	-0.01562600
H	-0.11926000	-2.67026000	0.04303000
H	3.90510000	0.61412400	-0.01085600
H	-3.76226700	0.21757400	0.00676200
O	-3.37355800	1.36503100	-0.03907100
H	-3.63027200	1.85921400	0.75595500
H	-2.62298800	-1.17549700	0.01009200
O	-3.78669400	-1.00957200	0.04258700
H	-4.20869400	-1.37282400	-0.75237300
N	0.87623800	1.83208700	-0.02644100
C	2.33593100	-0.73163200	0.00928700
C	2.17033800	1.74686100	-0.02531700
H	2.76484600	2.65753100	-0.03701900
N	2.89104200	0.57656400	-0.01018700
O	3.06445500	-1.71637700	0.02373700

T2+2w

Zero-point correction= 0.150735 (Hartree/Particle)
Thermal correction to Energy= 0.162958
Thermal correction to Enthalpy= 0.163902
Thermal correction to Gibbs Free Energy= 0.111758
Sum of electronic and zero-point Energies= -639.919584
Sum of electronic and thermal Energies= -639.907362
Sum of electronic and thermal Enthalpies= -639.906418
Sum of electronic and thermal Free Energies= -639.958561

C	-0.96900300	-0.65140700	0.00407100
C	-0.30207100	0.60890200	-0.02146500
N	1.02553000	0.44770100	-0.02976100
N	1.20112200	-0.89799500	-0.00814200
C	0.05266600	-1.59682300	0.01233300
C	-2.22319800	1.75585300	-0.02273100
C	-2.41290300	-0.71911100	0.01569500
H	2.17341800	-1.24551300	-0.01019200
H	0.03290000	-2.67714400	0.03224400
H	-2.81396900	2.66903000	-0.03118000
H	-3.96976400	0.63593100	0.00598000
H	2.68514000	1.39071700	-0.03913100
O	3.66734500	1.50140500	-0.02458400
H	3.86440500	2.10012400	0.71080000
H	4.10315100	-0.22510800	0.05322600
O	3.98872100	-1.20918300	0.05240900
H	4.55379700	-1.54992900	-0.65639600
O	-3.14046500	-1.70366400	0.03612300
N	-2.95621600	0.58837900	-0.00048200
N	-0.93141100	1.83462200	-0.03366500

T1+3w

Zero-point correction= 0.175718 (Hartree/Particle)
Thermal correction to Energy= 0.190726
Thermal correction to Enthalpy= 0.191671
Thermal correction to Gibbs Free Energy= 0.132312
Sum of electronic and zero-point Energies= -716.338455
Sum of electronic and thermal Energies= -716.323447
Sum of electronic and thermal Enthalpies= -716.322503
Sum of electronic and thermal Free Energies= -716.381861

C	1.45987500	-0.66622400	0.01216700
C	0.82172500	0.58739500	-0.03039600
N	-0.50559500	0.35144200	-0.05607300
N	-0.76971000	-0.98377500	-0.02987200
C	0.40509400	-1.60621800	0.01108300
C	2.71619800	1.75012000	-0.01461600
C	2.89994200	-0.72841000	0.04711700
H	-1.28710400	1.03158500	-0.06780300
H	0.45404900	-2.68617600	0.04038800
H	3.29798600	2.66861100	-0.02268600
H	4.45699100	0.63538400	0.05458500
H	-2.50076500	-1.66004200	-0.06631900
O	-3.44937500	-1.94789700	-0.09115400
H	-3.56528500	-2.42254800	-0.92773300
H	-4.44658100	-0.52884200	0.08108600
O	-4.88306900	0.35837700	0.16607800
H	-5.36521600	0.34349900	1.00605200
H	-2.89975000	2.69575900	-0.71215600
O	-2.74331300	2.03711100	-0.01981500
H	-3.57736100	1.50401800	0.05586900
N	1.41829900	1.81910900	-0.04729800
N	3.44320100	0.58958400	0.03065400
O	3.63983900	-1.70206000	0.08547900

3w-TS

Zero-point correction= 0.165563 (Hartree/Particle)
Thermal correction to Energy= 0.178312
Thermal correction to Enthalpy= 0.179256
Thermal correction to Gibbs Free Energy= 0.125261
Sum of electronic and zero-point Energies= -716.313162
Sum of electronic and thermal Energies= -716.300413
Sum of electronic and thermal Enthalpies= -716.299469
Sum of electronic and thermal Free Energies= -716.353464

C	1.37321300	-0.67064500	0.01714200
C	0.69251800	0.57160100	-0.02874200
N	-0.63186100	0.35983000	-0.04301800
N	-0.83031300	-0.99143200	-0.00576100
C	0.34612400	-1.62639600	0.03003400
C	2.58225200	1.76453500	-0.03831100
C	2.81309700	-0.70887400	0.03829900
H	-1.73578100	1.27470500	0.01426600
H	0.40195900	-2.70625600	0.06536100
H	3.15314700	2.69020600	-0.05839100
H	4.34620300	0.67792500	0.02171400
H	-2.65139500	2.51297900	-0.66932500
O	-2.65301800	1.88993000	0.07457300
H	-3.65260300	1.11668600	0.06326700
H	-4.97749700	0.34702200	0.90703100
O	-4.48481800	0.30242900	0.07145500
H	-3.94534100	-0.71048100	-0.00035100
H	-2.13838100	-1.47639900	-0.04826600
O	-3.22699500	-1.77265200	-0.07289500
H	-3.40101000	-2.25728200	-0.89524600
O	3.57085300	-1.67225500	0.07563700
N	3.33376300	0.61361700	0.00806600
N	1.28688200	1.81369100	-0.05939500

T2-3w

Zero-point correction= 0.175705 (Hartree/Particle)
Thermal correction to Energy= 0.190703
Thermal correction to Enthalpy= 0.191647
Thermal correction to Gibbs Free Energy= 0.132253
Sum of electronic and zero-point Energies= -716.336943
Sum of electronic and thermal Energies= -716.321945
Sum of electronic and thermal Enthalpies= -716.321001
Sum of electronic and thermal Free Energies= -716.380395

C	1.45992300	-0.66773500	0.01510000
C	0.76117800	0.57167400	-0.06622800
N	-0.56115900	0.37387300	-0.10840600
N	-0.70405400	-0.97373500	-0.05397900
C	0.46196500	-1.63857500	0.02031300
C	2.64881000	1.77252400	-0.04714900
C	2.90367100	-0.69441200	0.07338500
H	-1.65880500	-1.37632400	-0.08756500
H	0.50741900	-2.71705800	0.07208100
H	3.21441400	2.70130500	-0.06714200
H	4.42279300	0.70344100	0.07288900
H	-5.29878000	0.37748700	1.01342100
O	-4.83514700	0.25575100	0.17167800
H	-4.17210600	0.99341200	0.11303200
H	-2.78259400	2.76101400	-0.62587200
O	-2.83078100	2.08458000	0.06560400
H	-1.98945200	1.56493500	0.00105000
H	-3.93821500	-1.20772300	0.00624800
O	-3.31615700	-1.97276200	-0.12832400
H	-3.64028200	-2.44250300	-0.91098200
O	3.65768700	-1.65638000	0.14498900
N	1.35609400	1.81407100	-0.10043700
N	3.41162000	0.62745400	0.03549800

S2. Cartesian coordinates of stepwise mechanisms.

T1-RC

Zero-point correction= 0.140844 (Hartree/Particle)
Thermal correction to Energy= 0.159527
Thermal correction to Enthalpy= 0.160471
Thermal correction to Gibbs Free Energy= 0.088058
Sum of electronic and zero-point Energies= -1977.940154
Sum of electronic and thermal Energies= -1977.921471
Sum of electronic and thermal Enthalpies= -1977.920526
Sum of electronic and thermal Free Energies= -1977.992939

Mo	-2.17767100	-0.70302800	-0.17150200
S	-3.84047900	0.85120100	0.93453500
S	-1.44077500	1.53371800	-1.10693900
S	-2.33954100	-1.87307500	1.70389700
C	-3.66875500	2.42771800	0.17761800
H	-4.39248300	3.18450900	0.48146000
C	-2.65327400	2.72197600	-0.65863900
H	-2.52246400	3.72557600	-1.06336700
O	-3.19702000	-1.43597800	-1.34041800
O	-0.43563800	-1.11073100	-0.76675100
H	0.51187500	-0.79828300	-0.58937400
C	4.43357200	0.90262100	0.49139500
C	4.52573500	-0.35478400	-0.12352800
C	3.29522700	-1.00629500	-0.55520800
C	2.22438400	0.93184000	0.31174500
N	5.71651700	1.27243100	0.78707300
H	6.40808500	-1.52425200	-0.53867900
O	3.26072200	-2.11464100	-1.11750900
N	2.14069900	-0.26336600	-0.28087100
N	3.30999000	1.60559200	0.73765200
H	1.27100200	1.43637700	0.46541500
C	5.91395700	-0.64468000	-0.14600200
N	6.64029400	0.33011800	0.40161800
H	6.01680300	2.12074700	1.23854900

T1-TS1

Zero-point correction= 0.137511 (Hartree/Particle)
Thermal correction to Energy= 0.155739
Thermal correction to Enthalpy= 0.156683
Thermal correction to Gibbs Free Energy= 0.085963
Sum of electronic and zero-point Energies= -1977.939836
Sum of electronic and thermal Energies= -1977.921608
Sum of electronic and thermal Enthalpies= -1977.920664
Sum of electronic and thermal Free Energies= -1977.991385

Mo	-2.06179300	-0.70171500	-0.21053500
S	-3.83349700	0.75614800	0.95337400
S	-1.42158400	1.66039600	-1.01869200
S	-2.33071400	-2.02732800	1.56865800
C	-3.70817300	2.37645600	0.28271400
H	-4.46355200	3.09206300	0.61189300
C	-2.69942700	2.76203700	-0.52757800
H	-2.61908400	3.79215300	-0.87719600
O	-2.98328900	-1.37675500	-1.49991800
O	-0.30878500	-0.95171000	-0.65008400
H	0.90175100	-0.68449600	-0.47614100
C	4.30809600	0.92540100	0.44942800
C	4.41771000	-0.36248100	-0.09138600
C	3.20412100	-1.05860600	-0.48993000
C	2.09911000	0.94806800	0.27797300
N	5.58207600	1.32746700	0.72535100
H	6.31565400	-1.53063800	-0.43442200
O	3.16299700	-2.18884900	-0.98778800
N	2.05175100	-0.29085200	-0.24800800
N	3.17544500	1.63548100	0.65626700
H	1.12844000	1.42906900	0.38549800
C	5.80907000	-0.63681500	-0.09477100
N	6.51715700	0.37861400	0.39736900
H	5.86939800	2.20561300	1.1261820

T1-IM1

Zero-point correction= 0.141323 (Hartree/Particle)
Thermal correction to Energy= 0.159903
Thermal correction to Enthalpy= 0.160848
Thermal correction to Gibbs Free Energy= 0.088546
Sum of electronic and zero-point Energies= -1977.936782
Sum of electronic and thermal Energies= -1977.918201
Sum of electronic and thermal Enthalpies= -1977.917257
Sum of electronic and thermal Free Energies= -1977.989558

Mo	2.12864300	-0.67783300	0.26202300
S	3.72222200	0.85460900	-1.04496600
S	1.30558400	1.72994700	0.96398000
S	2.75143600	-2.18412300	-1.28500800
C	3.47002100	2.51138300	-0.49903700
H	4.14941800	3.25738100	-0.91575000
C	2.46704600	2.88165700	0.32610900
H	2.32283300	3.92942000	0.59532400
O	2.94753100	-1.11608700	1.71845100
O	0.37923700	-1.01155000	0.48223500
H	-1.10645500	-0.81487900	0.33834600
C	-4.33316500	0.91363000	-0.31525200
C	-4.46095900	-0.44851500	-0.01409800
C	-3.26256200	-1.21887600	0.26738700
C	-2.12377800	0.90811900	-0.11980400
N	-5.59839900	1.37063000	-0.52968200
H	-6.37314200	-1.63931000	0.09412400
O	-3.21888600	-2.41619100	0.55364900
N	-2.11016600	-0.41353500	0.17693000
N	-3.19355100	1.64393700	-0.37974200
H	-1.14061600	1.37971800	-0.11971700
C	-5.85426200	-0.70523300	-0.07501200
N	-6.54466000	0.38994700	-0.38615100
H	-5.87260500	2.31047100	-0.76732800

T1-IM1' (O-Up)

Zero-point correction= 0.142189 (Hartree/Particle)
Thermal correction to Energy= 0.160817
Thermal correction to Enthalpy= 0.161761
Thermal correction to Gibbs Free Energy= 0.089620
Sum of electronic and zero-point Energies= -1977.933300
Sum of electronic and thermal Energies= -1977.914672
Sum of electronic and thermal Enthalpies= -1977.913728
Sum of electronic and thermal Free Energies= -1977.985869

Mo	-1.95622200	0.01638100	0.67370300
S	-3.31731900	1.28364200	-1.11440300
S	-3.35482800	-1.90342400	-0.41224400
S	-0.60541500	1.87102400	0.52588600
C	-4.53952200	0.17427900	-1.73236200
H	-5.26826100	0.60046200	-2.42462800
C	-4.56135600	-1.14406600	-1.43740100
H	-5.31338100	-1.80130600	-1.87829400
O	-2.80436500	0.16562400	2.17405500
O	-0.76892600	-1.27539300	0.81738500
C	4.36171800	-1.03795000	-0.08767000
C	4.64582800	0.31554000	-0.31262800
C	3.55930300	1.27334800	-0.25736600
C	2.18399400	-0.71281300	0.22795700
N	5.55062100	-1.69227200	-0.19831700
H	6.66105500	1.22218200	-0.76568800
O	3.64201900	2.49046500	-0.42457400
N	2.33807100	0.62625000	0.02424100
N	3.16059200	-1.60206900	0.18638500
H	1.15855400	-1.03507500	0.43698000
C	6.04319400	0.36079000	-0.55006000
N	6.59249300	-0.84978800	-0.48256400
H	5.70880100	-2.68258400	-0.10045900
H	1.45434300	1.19324600	0.10277900

T1-TS2 (O-Up)

Zero-point correction= 0.141916 (Hartree/Particle)
Thermal correction to Energy= 0.159669
Thermal correction to Enthalpy= 0.160613
Thermal correction to Gibbs Free Energy= 0.092838
Sum of electronic and zero-point Energies= -1977.911250
Sum of electronic and thermal Energies= -1977.893497
Sum of electronic and thermal Enthalpies= -1977.892553
Sum of electronic and thermal Free Energies= -1977.960328

Mo	1.50604400	-0.42951700	0.15664200
S	3.97297800	-0.17544900	-0.46545200
S	1.85499600	2.05593900	0.58960200
S	1.43375200	-2.05078600	-1.37930400
C	4.46510000	1.42369600	0.07994700
H	5.52732200	1.65567600	-0.00816900
C	3.58601400	2.34952800	0.51784100
H	3.92044700	3.34785600	0.80301500
O	1.57391500	-1.19546300	1.69564800
O	-0.23646600	0.17913400	-0.05416800
C	-3.45068100	0.62705400	-0.83837400
C	-4.02026900	0.08624100	0.34025300
C	-3.33387700	-1.00624800	0.97938300
C	-1.56826000	-0.61709900	-0.77568300
N	-4.34684400	1.57576500	-1.25559900
H	-5.96080100	0.67002800	1.32286000
O	-3.69737700	-1.64478800	1.98428700
N	-2.16915000	-1.34153000	0.29156800
N	-2.32881300	0.28364100	-1.46812300
H	-0.91689000	-1.25848400	-1.38459900
C	-5.23353200	0.79071700	0.52946300
N	-5.44046400	1.69966600	-0.41995500
H	-4.22300100	2.21394800	-2.02423400
H	-1.57917900	-2.02175500	0.75627100

T1-IM2 (O-Up)

Zero-point correction= 0.142244 (Hartree/Particle)
Thermal correction to Energy= 0.160427
Thermal correction to Enthalpy= 0.161371
Thermal correction to Gibbs Free Energy= 0.092700
Sum of electronic and zero-point Energies= -1977.911800
Sum of electronic and thermal Energies= -1977.893617
Sum of electronic and thermal Enthalpies= -1977.892673
Sum of electronic and thermal Free Energies= -1977.961344

Mo	1.51890800	-0.44588900	0.13751400
S	3.96552500	-0.11680300	-0.43254000
S	1.75578400	2.03719900	0.58239900
S	1.46790600	-2.02087700	-1.42542300
C	4.39757300	1.48916900	0.14557800
H	5.45508200	1.74922400	0.09119400
C	3.47839300	2.38337800	0.56399100
H	3.77293600	3.38825400	0.86835300
O	1.58978500	-1.23988000	1.65731300
O	-0.28368900	0.11708600	-0.09478000
C	-3.40799200	0.60706800	-0.84255200
C	-3.99331500	0.08722800	0.34516700
C	-3.30984200	-0.98446100	1.01910600
C	-1.47722900	-0.60366000	-0.70713600
N	-4.32294600	1.52763400	-1.29929200
H	-5.95489300	0.66313400	1.28481500
O	-3.68830700	-1.59936800	2.03752000
N	-2.13757500	-1.33598900	0.36063600
N	-2.27573300	0.28011800	-1.44213700
H	-0.94702200	-1.32347700	-1.35851700
C	-5.21837400	0.77775700	0.49837700
N	-5.42972500	1.66064000	-0.47453000
H	-4.18380400	2.17092200	-2.06069200
H	-1.55960500	-2.00141500	0.85992400

T1-TS3 (O-Up)

Zero-point correction= 0.138398 (Hartree/Particle)
Thermal correction to Energy= 0.155637
Thermal correction to Enthalpy= 0.156581
Thermal correction to Gibbs Free Energy= 0.091345
Sum of electronic and zero-point Energies= -1977.908653
Sum of electronic and thermal Energies= -1977.891414
Sum of electronic and thermal Enthalpies= -1977.890469
Sum of electronic and thermal Free Energies= -1977.955706

Mo	-1.59172600	-0.42445900	-0.10301800
S	-3.79044700	-0.34557300	1.05583100
S	-2.48715300	1.64212800	-1.18878100
S	-0.58543300	-1.19228500	1.77893600
C	-4.74306200	0.83807100	0.15058600
H	-5.79918500	0.90817200	0.41375100
C	-4.20232800	1.66086500	-0.77139900
H	-4.81343900	2.40732400	-1.28015100
O	-1.68524100	-1.72885300	-1.20829800
O	0.16755700	0.44155300	-0.41327000
C	3.48189500	0.97166300	0.43329700
C	4.18398200	-0.08288900	-0.20969200
C	3.40834700	-1.13059100	-0.82887400
C	1.39041200	0.10366800	0.14322600
N	4.46877200	1.82109500	0.87453700
H	6.40734600	-0.30905700	-0.45993400
O	3.84529100	-2.10696000	-1.47015500
N	2.05094800	-0.92129400	-0.65583500
N	2.18032300	1.15401800	0.59339400
H	0.92272300	-0.50819600	1.15904600
C	5.55307000	0.24642800	-0.09234700
N	5.74544300	1.39225600	0.55955300
H	4.33286400	2.68120600	1.37924800
H	1.43758500	-1.63222300	-1.03753300

T1-PC (O-Up)

Zero-point correction= 0.140605 (Hartree/Particle)
Thermal correction to Energy= 0.158939
Thermal correction to Enthalpy= 0.159883
Thermal correction to Gibbs Free Energy= 0.091498
Sum of electronic and zero-point Energies= -1977.960906
Sum of electronic and thermal Energies= -1977.942572
Sum of electronic and thermal Enthalpies= -1977.941628
Sum of electronic and thermal Free Energies= -1978.010013

Mo	-1.58567700	0.29125400	0.19326300
S	-4.01102400	0.34721700	0.34246000
S	-1.94977200	-1.85484500	-0.87761300
S	-1.68084400	2.64887100	-0.48566300
C	-4.52531400	-1.29527900	-0.10452800
H	-5.58395200	-1.52515600	0.02522600
C	-3.67616400	-2.20385800	-0.62298000
H	-4.01726200	-3.19735900	-0.91587000
O	-1.01961500	0.08075100	1.79644800
O	0.34506900	0.32518200	-0.85062400
C	3.76346000	-0.01014800	-0.88269600
C	4.12392900	-0.25820500	0.45880800
C	3.06938100	-0.31060400	1.44065400
C	1.54681400	0.14689500	-0.50880500
N	4.94390700	-0.01445500	-1.57349000
H	6.19299500	-0.59167600	1.28522300
O	3.18875300	-0.51274700	2.65810300
N	1.81785000	-0.09706200	0.85112500
N	2.55270500	0.19285500	-1.41276400
H	-0.41206500	2.79969100	-0.94305400
C	5.53374400	-0.39439300	0.44924900
N	6.04244200	-0.25040500	-0.77154100
H	5.05895300	0.12523800	-2.56385400
H	0.99889300	-0.11175400	1.46539300

T1-IM1' (O-Down)

Zero-point correction= 0.142189 (Hartree/Particle)
Thermal correction to Energy= 0.160818
Thermal correction to Enthalpy= 0.161762
Thermal correction to Gibbs Free Energy= 0.089616
Sum of electronic and zero-point Energies= -1977.933300
Sum of electronic and thermal Energies= -1977.914672
Sum of electronic and thermal Enthalpies= -1977.913727
Sum of electronic and thermal Free Energies= -1977.985873

Mo	-1.95597600	0.01673100	0.67318700
S	-3.31890200	1.28326300	-1.11404900
S	-3.35559600	-1.90359400	-0.41060800
S	-0.60521000	1.87119600	0.52338000
C	-4.54157200	0.17355400	-1.73047900
H	-5.27096200	0.59944100	-2.42223900
C	-4.56305700	-1.14467900	-1.43498700
H	-5.31546000	-1.80211400	-1.87494600
O	-2.80289800	0.16663800	2.17415800
O	-0.76865700	-1.27506600	0.81647300
C	4.36200000	-1.03818100	-0.08816000
C	4.64652100	0.31540800	-0.31201000
C	3.56015900	1.27339400	-0.25669700
C	2.18418600	-0.71282900	0.22659800
N	5.55080900	-1.69268600	-0.19871600
H	6.66217500	1.22192700	-0.76342100
O	3.64318000	2.49060200	-0.42309300
N	2.33866100	0.62634600	0.02387100
N	3.16062000	-1.60224500	0.18489400
H	1.15857800	-1.03496200	0.43502600
C	6.04401600	0.36051800	-0.54871600
N	6.59301200	-0.85022800	-0.48180200
H	1.45500700	1.19340600	0.10209900
H	5.70875300	-2.68307700	-0.10127300

T1-TS2 (O-Down)

Zero-point correction= 0.142101 (Hartree/Particle)
Thermal correction to Energy= 0.159794
Thermal correction to Enthalpy= 0.160738
Thermal correction to Gibbs Free Energy= 0.093335
Sum of electronic and zero-point Energies= -1977.910968
Sum of electronic and thermal Energies= -1977.893275
Sum of electronic and thermal Enthalpies= -1977.892331
Sum of electronic and thermal Free Energies= -1977.959734

Mo	-1.55686400	-0.54733900	-0.33387000
S	-3.85862900	0.00397300	0.64421700
S	-1.66365300	1.95601100	-0.75146500
S	-1.44603900	-2.13315300	1.24153900
C	-4.23415000	1.64281100	0.12526500
H	-5.23805000	2.00263600	0.35492000
C	-3.32361600	2.45305000	-0.45484200
H	-3.57440700	3.48200400	-0.71556100
O	-1.97484700	-1.29299100	-1.82560100
O	0.25862800	-0.16492100	-0.40106600
C	3.57495600	-0.48657000	-0.56643700
C	3.92303800	0.55241100	0.33051000
C	3.04720600	0.80017700	1.44672300
C	1.57978600	-0.94547200	0.37965200
N	4.61380000	-0.54192800	-1.45770800
H	5.76782300	1.84352300	0.28878800
O	3.20856200	1.62013900	2.36889700
N	1.95307100	-0.06222700	1.42759100
N	2.51458600	-1.29326500	-0.55361500
H	0.93748600	-1.75557300	0.74861700
C	5.16876700	1.04370400	-0.12871100
N	5.59438600	0.40019600	-1.21272800
H	1.24125000	0.12780000	2.12245900
H	4.66174800	-1.11937200	-2.28091500

T1-IM2 (O-Down)

Zero-point correction= 0.142345 (Hartree/Particle)
Thermal correction to Energy= 0.160469
Thermal correction to Enthalpy= 0.161413
Thermal correction to Gibbs Free Energy= 0.093059
Sum of electronic and zero-point Energies= -1977.911867
Sum of electronic and thermal Energies= -1977.893743
Sum of electronic and thermal Enthalpies= -1977.892799
Sum of electronic and thermal Free Energies= -1977.961153

Mo	-1.56311100	-0.56579200	-0.29016200
S	-3.87777600	0.02557300	0.56365400
S	-1.59208500	1.91086300	-0.76915900
S	-1.46600000	-2.05670100	1.35398900
C	-4.21168400	1.64785100	-0.03241500
H	-5.22447800	2.01921500	0.12700400
C	-3.26138800	2.43132100	-0.58306100
H	-3.48511600	3.45311300	-0.89077400
O	-1.94008000	-1.37209200	-1.75596000
O	0.31021600	-0.21947400	-0.31971400
C	3.52815500	-0.54876600	-0.52866000
C	3.91187400	0.56264500	0.27183300
C	3.04491600	0.94275700	1.35641900
C	1.47329300	-0.83365500	0.42722500
N	4.58465700	-0.72848100	-1.39162200
H	5.80378400	1.77258800	0.13966700
O	3.24006200	1.84366400	2.19828900
N	1.92521900	0.12461000	1.42341300
N	2.44412600	-1.30416900	-0.46706900
H	0.95352100	-1.65895400	0.95052400
C	5.17987500	0.95979300	-0.21263000
N	5.59795000	0.20305700	-1.22462300
H	1.23093000	0.41305400	2.10140000
H	4.61029900	-1.36509000	-2.17065300

T1-PC (O-Down)

Zero-point correction= 0.140513 (Hartree/Particle)
Thermal correction to Energy= 0.158933
Thermal correction to Enthalpy= 0.159877
Thermal correction to Gibbs Free Energy= 0.091254
Sum of electronic and zero-point Energies= -1977.957033
Sum of electronic and thermal Energies= -1977.938613
Sum of electronic and thermal Enthalpies= -1977.937669
Sum of electronic and thermal Free Energies= -1978.006291

Mo	-1.81256200	-0.65170300	-0.32727400
S	-3.68941400	0.28634500	0.88664500
S	-1.42114200	1.66491200	-0.99887900
S	-1.43972100	-2.10628600	1.62603300
C	-3.80646000	1.96801400	0.32306300
H	-4.67493900	2.53276100	0.66539000
C	-2.85989200	2.54975700	-0.43837700
H	-2.93473300	3.59358300	-0.74310400
O	-2.49953900	-1.52746700	-1.61662400
O	0.34415300	-0.91408400	-0.56586000
C	3.75662000	-0.59719200	-0.35427600
C	3.97740600	0.63101800	0.30386800
C	2.82377100	1.41372200	0.67113000
C	1.50397900	-0.48365700	-0.33314300
N	5.00540900	-1.09912400	-0.59577000
H	5.95569700	1.56507800	0.84098400
O	2.81371400	2.52302900	1.22372100
N	1.63689800	0.76079400	0.31621600
N	2.60366800	-1.18735000	-0.68836400
H	-0.20566400	-2.58554200	1.32783800
C	5.38468500	0.75744500	0.40058600
N	6.01847900	-0.28153800	-0.13673200
H	0.77029000	1.28421800	0.44305800
H	5.22293300	-1.97405800	-1.04389100

T1-TS3 (O-Down)

Zero-point correction= 0.138187 (Hartree/Particle)
Thermal correction to Energy= 0.155497
Thermal correction to Enthalpy= 0.156441
Thermal correction to Gibbs Free Energy= 0.090898
Sum of electronic and zero-point Energies= -1977.908546
Sum of electronic and thermal Energies= -1977.891236
Sum of electronic and thermal Enthalpies= -1977.890292
Sum of electronic and thermal Free Energies= -1977.955835

Mo	-1.62925800	-0.60282900	-0.15387200
S	-3.71874400	-0.14109300	1.11599700
S	-2.35559000	1.43641800	-1.40145700
S	-0.58922800	-1.23342600	1.76500000
C	-4.59233800	1.04491000	0.13811300
H	-5.61404300	1.26618500	0.44935000
C	-4.02711800	1.70041900	-0.89644800
H	-4.58324300	2.45838000	-1.44911400
O	-1.97325700	-1.99478700	-1.08427500
O	0.19277100	0.00353000	-0.65827200
C	3.59718700	-0.57080500	-0.47759000
C	4.11715100	0.58090500	0.17095400
C	3.17641000	1.52027800	0.73264800
C	1.39905300	-0.16502300	-0.00579400
N	4.70849200	-1.23545200	-0.93872900
H	6.27159000	1.18823500	0.38728200
O	3.44220400	2.59720700	1.30317500
N	1.87162600	1.09992700	0.54418400
N	2.34259000	-0.96282300	-0.64001200
H	0.92992600	-0.80586700	0.99867400
C	5.52031200	0.49488600	0.02911500
N	5.89703300	-0.59497400	-0.63823500
H	1.15135800	1.69494000	0.93440900
H	4.71437000	-2.10118600	-1.45209000

T10-RC

Zero-point correction= 0.140731 (Hartree/Particle)
Thermal correction to Energy= 0.159389
Thermal correction to Enthalpy= 0.160333
Thermal correction to Gibbs Free Energy= 0.088722
Sum of electronic and zero-point Energies= -1977.930935
Sum of electronic and thermal Energies= -1977.912277
Sum of electronic and thermal Enthalpies= -1977.911333
Sum of electronic and thermal Free Energies= -1977.982944

Mo	-2.06856800	-0.30402300	-0.66566300
S	-3.59127000	-0.61679400	1.32254500
S	-2.00444800	2.00122700	0.33885100
S	-1.44290100	-2.39553000	-0.26668100
C	-3.92224300	0.97919900	1.97816400
H	-4.65793300	1.02337600	2.78106500
C	-3.24388700	2.07340400	1.58007800
H	-3.40919800	3.04604000	2.04276800
O	-3.22940500	-0.30534200	-1.92475600
O	-0.51099800	0.41887400	-1.48543800
H	0.40735400	0.57049200	-1.11987500
C	4.40809300	-0.67521400	0.71407400
C	4.49990800	0.48483000	-0.08130100
C	3.33213100	1.05409500	-0.71892200
C	2.09081900	-0.72015000	0.27555900
N	5.57443700	-1.07030400	1.22184300
H	6.44285700	1.56892400	-0.45767000
O	3.32245400	2.06100500	-1.43911400
N	2.10874200	0.35357500	-0.46786100
N	3.16930100	-1.27768000	0.88609000
H	1.14438700	-1.23769200	0.42937300
C	5.88813700	0.75871200	0.00079900
N	6.50796200	-0.15356300	0.76374600
H	3.07304400	-2.11439700	1.44379400

T10-TS1

Zero-point correction= 0.137169 (Hartree/Particle)
Thermal correction to Energy= 0.155260
Thermal correction to Enthalpy= 0.156205
Thermal correction to Gibbs Free Energy= 0.086669
Sum of electronic and zero-point Energies= -1977.928175
Sum of electronic and thermal Energies= -1977.910083
Sum of electronic and thermal Enthalpies= -1977.909139
Sum of electronic and thermal Free Energies= -1977.978675

Mo	-1.88588600	-0.26324700	-0.65680300
S	-3.60255700	-0.83055100	1.16082200
S	-2.28640700	2.02189500	0.38799000
S	-1.18328700	-2.37551300	-0.27480300
C	-4.22681600	0.69508400	1.77054500
H	-5.05096400	0.62925500	2.48218900
C	-3.67599200	1.88565300	1.45337300
H	-4.04328600	2.81369500	1.89274000
O	-2.86578400	-0.28321200	-2.06988000
O	-0.32290300	0.56384500	-1.10900100
H	0.88265100	0.64934800	-0.74610700
C	4.35231600	-0.70092500	0.59309500
C	4.38363900	0.58535200	0.01404800
C	3.19312300	1.20867900	-0.50933200
C	2.03557500	-0.81102600	0.18583500
N	5.53925000	-1.12324800	1.01723100
H	6.27044700	1.80639500	-0.17219000
O	3.10061800	2.31221200	-1.04733500
N	2.01794400	0.39113900	-0.35528400
N	3.14590900	-1.38990700	0.66717600
H	1.09681100	-1.36803600	0.23359700
C	5.75792700	0.90384900	0.13753800
N	6.42420400	-0.10004900	0.72517200
H	3.10231600	-2.31589800	1.07041200

T10-TS2 (O-Down)

Zero-point correction= 0.142003 (Hartree/Particle)
Thermal correction to Energy= 0.159632
Thermal correction to Enthalpy= 0.160577
Thermal correction to Gibbs Free Energy= 0.093032
Sum of electronic and zero-point Energies= -1977.912611
Sum of electronic and thermal Energies= -1977.894981
Sum of electronic and thermal Enthalpies= -1977.894037
Sum of electronic and thermal Free Energies= -1977.961581

Mo	-1.53786200	-0.49058500	-0.26965700
S	-3.94603400	-0.26360100	0.56821300
S	-1.98471600	1.95229900	-0.76897400
S	-1.29354700	-2.01834100	1.36538800
C	-4.52317300	1.29756500	0.00031400
H	-5.57758400	1.51398800	0.17589300
C	-3.70927100	2.21818000	-0.55710200
H	-4.08726500	3.19621000	-0.85605600
O	-1.73724300	-1.33740200	-1.75403500
O	0.19015000	0.14446000	-0.24727800
C	3.66262900	-0.55290000	-0.57829300
C	4.13235900	0.54327500	0.18022100
C	3.36687500	1.06252300	1.26881100
C	1.61421500	-0.62960900	0.65268100
N	4.51270200	-0.92728300	-1.52721400
H	6.11143100	1.56429100	-0.19247200
O	3.62926800	1.99057100	2.04643600
N	2.15680900	0.33453300	1.46675600
N	2.45108700	-1.16793500	-0.27116500
H	0.86910800	-1.29762200	1.11073600
C	5.38414700	0.79850900	-0.43562300
N	5.59890300	-0.06446300	-1.43271600
H	1.53373700	0.73145700	2.15823700
H	2.06894500	-1.85970100	-0.90144500

T10-IM1

Zero-point correction= 0.141986 (Hartree/Particle)
Thermal correction to Energy= 0.160419
Thermal correction to Enthalpy= 0.161363
Thermal correction to Gibbs Free Energy= 0.090818
Sum of electronic and zero-point Energies= -1977.926773
Sum of electronic and thermal Energies= -1977.908340
Sum of electronic and thermal Enthalpies= -1977.907396
Sum of electronic and thermal Free Energies= -1977.977941

Mo	1.79726300	-0.15875000	0.52365300
S	3.77986400	-1.20310100	-0.75633100
S	2.99972600	1.92792400	-0.36207600
S	0.82694700	-2.18863400	0.07955900
C	4.87352100	0.11225000	-1.16653200
H	5.82114500	-0.17346700	-1.62622200
C	4.55386600	1.41357900	-0.99941600
H	5.23761100	2.20508100	-1.30942700
O	2.28766300	-0.19620400	2.17765100
O	0.38557000	0.91878000	0.39719400
H	-1.37843300	1.36018500	0.24837400
C	-4.38698200	-0.79300300	-0.28843900
C	-4.61874500	0.59530900	-0.14594300
C	-3.54286800	1.52089200	0.06576300
C	-2.06865600	-0.46266300	-0.02981500
N	-5.49778000	-1.49463200	-0.47563200
H	-6.67349500	1.51960900	-0.22907400
O	-3.58076500	2.74145300	0.20935800
N	-2.26862400	0.84625400	0.10395700
N	-3.08774200	-1.29195200	-0.22425900
H	-1.04902000	-0.87467900	0.02174600
C	-6.02737600	0.65164800	-0.27123600
N	-6.52988600	-0.57484600	-0.46355300
H	-2.89554200	-2.28233800	-0.32076700

T10-IM2 (O-Down)

Zero-point correction= 0.142812 (Hartree/Particle)
Thermal correction to Energy= 0.160639
Thermal correction to Enthalpy= 0.161583
Thermal correction to Gibbs Free Energy= 0.093691
Sum of electronic and zero-point Energies= -1977.917610
Sum of electronic and thermal Energies= -1977.899784
Sum of electronic and thermal Enthalpies= -1977.898840
Sum of electronic and thermal Free Energies= -1977.966732

Mo	-1.54227300	-0.53955400	-0.27807900
S	-3.90168900	-0.01900300	0.43911800
S	-1.55444100	1.93700000	-0.63841400
S	-1.49598700	-2.06156600	1.33226100
C	-4.21522000	1.62442600	-0.10572200
H	-5.24172700	1.97582900	-0.00295500
C	-3.23681900	2.43942200	-0.54821800
H	-3.44488300	3.47235400	-0.82603500
O	-1.82001200	-1.31460100	-1.78033400
O	0.35600700	-0.18422100	-0.21628200
C	3.57924500	-0.57549500	-0.56212600
C	3.94967800	0.53773600	0.22358600
C	3.13791500	0.96053200	1.32568200
C	1.43898000	-0.78134500	0.57175900
N	4.45905000	-0.83352000	-1.52835700
H	5.81812500	1.75811800	-0.11985600
O	3.34393900	1.89258100	2.12458500
N	2.00229600	0.14456800	1.51119100
N	2.44487100	-1.33334500	-0.27160100
H	0.91224400	-1.58451100	1.12437500
C	5.16804000	0.93173900	-0.38564500
N	5.46121900	0.12780200	-1.41280000
H	1.34128300	0.52169000	2.17796700
H	2.08183300	-1.89579900	-1.03030600

T10-TS3 (O-Down)

Zero-point correction= 0.138077 (Hartree/Particle)
Thermal correction to Energy= 0.155274
Thermal correction to Enthalpy= 0.156218
Thermal correction to Gibbs Free Energy= 0.090870
Sum of electronic and zero-point Energies= -1977.913281
Sum of electronic and thermal Energies= -1977.896084
Sum of electronic and thermal Enthalpies= -1977.895140
Sum of electronic and thermal Free Energies= -1977.960488

Mo	-1.60427100	-0.53257500	-0.14312900
S	-3.71236300	-0.36031300	1.13383900
S	-2.53752000	1.45026700	-1.31254000
S	-0.47532200	-1.10453300	1.74882900
C	-4.71642600	0.75694800	0.20037500
H	-5.75602200	0.84650000	0.51620300
C	-4.22823400	1.51135500	-0.80442300
H	-4.86362300	2.22165600	-1.33336300
O	-1.77343800	-1.92431900	-1.11974800
O	0.16828200	0.29108500	-0.62821800
C	3.64425100	-0.61540200	-0.53790700
C	4.20844500	0.50364600	0.11717500
C	3.37562100	1.54980300	0.63611400
C	1.38243000	0.11038300	-0.04036400
N	4.56652700	-1.48231200	-0.95448300
H	6.42393700	0.79246000	0.43030000
O	3.71820000	2.59976300	1.20805000
N	2.00620400	1.30685100	0.41533600
N	2.27453200	-0.72858300	-0.72813000
H	0.95262600	-0.52853000	1.02455800
C	5.59238200	0.21081000	0.04882900
N	5.79607700	-0.95277100	-0.57963600
H	1.37344300	1.97787400	0.83151200
H	1.89374200	-1.60833000	-1.05092300

T10-TS2 (O-Up)

Zero-point correction= 0.142064 (Hartree/Particle)
Thermal correction to Energy= 0.159667
Thermal correction to Enthalpy= 0.160611
Thermal correction to Gibbs Free Energy= 0.093358
Sum of electronic and zero-point Energies= -1977.912547
Sum of electronic and thermal Energies= -1977.894944
Sum of electronic and thermal Enthalpies= -1977.894000
Sum of electronic and thermal Free Energies= -1977.961253

Mo	-1.55431100	-0.45846200	-0.20162600
S	-3.93538600	-0.14153600	0.67650400
S	-1.96199100	1.97047600	-0.80266200
S	-1.30759800	-1.92823000	1.48487000
C	-4.49317800	1.40689100	0.05632600
H	-5.53789100	1.65379200	0.24867000
C	-3.67406400	2.28427400	-0.55988300
H	-4.03863200	3.25702400	-0.89105200
O	-1.79473100	-1.36427200	-1.64466800
O	0.18424500	0.14802000	-0.23395700
C	3.52989400	0.74593800	0.83201800
C	4.16902200	0.13991200	-0.27278800
C	3.56577500	-0.96185900	-0.95401100
C	1.61795800	-0.67292000	0.60662900
N	4.24315800	1.72997200	1.36685400
H	6.18361400	0.78777900	-1.06039600
O	3.98627600	-1.61907900	-1.91621900
N	2.32372200	-1.34079700	-0.36477200
N	2.30627200	0.27091600	1.29873000
H	0.86740000	-1.25902300	1.15792400
C	5.37009100	0.89002000	-0.35173300
N	5.40587500	1.81746400	0.60939400
H	1.81089700	-2.04878400	-0.87555500
H	1.80278600	0.79950200	1.99729300

T10-PC (O-Down)

Zero-point correction= 0.140243 (Hartree/Particle)
Thermal correction to Energy= 0.158549
Thermal correction to Enthalpy= 0.159493
Thermal correction to Gibbs Free Energy= 0.091089
Sum of electronic and zero-point Energies= -1977.959890
Sum of electronic and thermal Energies= -1977.941584
Sum of electronic and thermal Enthalpies= -1977.940640
Sum of electronic and thermal Free Energies= -1978.009044

Mo	1.54850900	0.16868900	-0.30970400
S	3.93368200	0.10199000	-0.70031100
S	2.04319300	-1.34462200	1.51002500
S	1.67135500	2.59823800	-0.59973000
C	4.52100900	-1.21810900	0.33743100
H	5.56513200	-1.50623900	0.21051800
C	3.74525400	-1.80714900	1.26703100
H	4.12795900	-2.59851100	1.91137500
O	0.82264700	-0.65284100	-1.62778300
O	-0.32604700	0.64043400	0.80299700
C	-3.27210500	-0.58705400	-0.78649700
C	-4.26478300	-0.16365700	0.13126600
C	-3.91800500	0.54821400	1.31652400
C	-1.52051300	0.35545100	0.53723100
N	-3.78128100	-1.23363200	-1.82688500
H	-6.47285200	-0.54684100	-0.14413500
O	-4.64114200	0.99093200	2.22241900
N	-2.51201200	0.75145100	1.41726900
N	-1.91740700	-0.32106400	-0.56554100
H	0.42904100	2.94475300	-0.17632200
C	-5.44918900	-0.63882300	-0.48826600
N	-5.15825200	-1.26246100	-1.63133600
H	-2.18645500	1.24928500	2.23534200
H	-1.18290100	-0.61859000	-1.21290000

T10-IM2 (O-Up)

Zero-point correction= 0.142812 (Hartree/Particle)
Thermal correction to Energy= 0.160652
Thermal correction to Enthalpy= 0.161597
Thermal correction to Gibbs Free Energy= 0.093742
Sum of electronic and zero-point Energies= -1977.917428
Sum of electronic and thermal Energies= -1977.899588
Sum of electronic and thermal Enthalpies= -1977.898644
Sum of electronic and thermal Free Energies= -1977.966498

Mo	-1.51883500	-0.45868700	-0.15739600
S	-3.93949400	-0.05441000	0.38916300
S	-1.63650600	2.02419900	-0.53775800
S	-1.50885800	-2.02665800	1.40649100
C	-4.30313300	1.57877600	-0.15789800
H	-5.35076100	1.87521200	-0.11240000
C	-3.34228700	2.44436700	-0.53721600
H	-3.58634200	3.46768000	-0.82169300
O	-1.61218600	-1.24276300	-1.67694900
O	0.32990000	0.05029300	0.09198200
C	3.44971300	0.63902000	0.87320200
C	3.99910500	0.11401000	-0.31706500
C	3.35682100	-0.96266000	-1.00891700
C	1.44688000	-0.72139900	0.65854000
N	4.18751700	1.62234700	1.38520000
H	5.90887600	0.86235700	-1.26204300
O	3.72544800	-1.54479900	-2.04567800
N	2.18891200	-1.41269000	-0.35576900
N	2.29824300	0.10149500	1.44935800
H	0.92241500	-1.45824400	1.29728100
C	5.16668900	0.90420900	-0.47236700
N	5.27194800	1.78760500	0.52509700
H	1.63951400	-2.05304700	-0.91521200
H	1.80072700	0.70974000	2.08666200

T10-TS3 (O-Up)

Zero-point correction= 0.138081 (Hartree/Particle)
Thermal correction to Energy= 0.155274
Thermal correction to Enthalpy= 0.156218
Thermal correction to Gibbs Free Energy= 0.090908
Sum of electronic and zero-point Energies= -1977.913080
Sum of electronic and thermal Energies= -1977.895887
Sum of electronic and thermal Enthalpies= -1977.894942
Sum of electronic and thermal Free Energies= -1977.960253

Mo	-1.61993200	-0.47687600	-0.08702600
S	-3.70874500	-0.19281500	1.19987800
S	-2.51586800	1.47597000	-1.33675900
S	-0.47715300	-1.00933600	1.80691500
C	-4.69382600	0.91054500	0.22967200
H	-5.72632300	1.04309100	0.55345900
C	-4.19757000	1.60609300	-0.81287200
H	-4.81992100	2.31009200	-1.36531300
O	-1.82487000	-1.90334800	-1.00527200
O	0.16150700	0.29626200	-0.62123000
C	3.53569200	1.08931300	0.32657600
C	4.23879300	-0.03399500	-0.16651900
C	3.53942900	-1.14256900	-0.74909700
C	1.38419600	0.04352200	-0.07775400
N	4.34623100	2.01905200	0.83097400
H	6.48478600	-0.23791000	-0.10483900
O	4.01192500	-2.18048500	-1.24439800
N	2.14260600	-0.95671500	-0.75127700
N	2.15398300	1.17490500	0.23791400
H	0.95462200	-0.49249400	1.04208300
C	5.58228300	0.32671800	0.10017300
N	5.63931400	1.52937900	0.68358100
H	1.60060100	-1.75103600	-1.06884400
H	1.67421800	1.91240600	0.73576400

T10-PC (O-Up)

Zero-point correction= 0.140236 (Hartree/Particle)
Thermal correction to Energy= 0.158605
Thermal correction to Enthalpy= 0.159549
Thermal correction to Gibbs Free Energy= 0.091054
Sum of electronic and zero-point Energies= -1977.959400
Sum of electronic and thermal Energies= -1977.941031
Sum of electronic and thermal Enthalpies= -1977.940087
Sum of electronic and thermal Free Energies= -1978.008582

Mo	-1.59592400	0.29320100	0.18929500
S	-4.00467800	0.34484100	0.39089100
S	-1.96677300	-1.85354100	-0.86045500
S	-1.70839800	2.61953800	-0.57351900
C	-4.52572600	-1.30132600	-0.03717000
H	-5.57995800	-1.53213800	0.11993600
C	-3.68767600	-2.20866500	-0.57313700
H	-4.02904000	-3.20506100	-0.85338800
O	-0.98850700	0.11493700	1.78169400
O	0.37003900	0.29811800	-0.86873200
C	3.89859700	-0.05454600	-0.90681200
C	4.18887400	-0.24208100	0.46005400
C	3.14735500	-0.25733500	1.44278900
C	1.54288200	0.12471500	-0.45570000
N	4.97950700	-0.06698700	-1.67723700
H	6.27947400	-0.53481900	1.26162700
O	3.23733200	-0.40837700	2.66530100
N	1.85058500	-0.06464100	0.86768800
N	2.58472600	0.12278900	-1.33724800
H	-0.43198900	2.78351500	-1.00539600
C	5.60200800	-0.37309100	0.43136200
N	6.05770400	-0.27019500	-0.81972200
H	1.04635300	-0.06263800	1.50167400
H	2.36511000	0.25308400	-2.31428000

S3. Cartesian coordinates of concerted mechanisms of neutral allopurinol.

T1-RC (O-Down)

Zero-point correction= 0.154799 (Hartree/Particle)
Thermal correction to Energy= 0.173966
Thermal correction to Enthalpy= 0.174911
Thermal correction to Gibbs Free Energy= 0.101757
Sum of electronic and zero-point Energies= -1978.554709
Sum of electronic and thermal Energies= -1978.535542
Sum of electronic and thermal Enthalpies= -1978.534597
Sum of electronic and thermal Free Energies= -1978.607751

Mo	2.11004800	0.05673300	-0.70515800
S	3.50839400	-1.35854700	0.75632700
C	4.36465800	-0.29758100	1.86461200
H	5.11118800	-0.78076600	2.49149500
C	4.06095900	1.00567600	1.99281000
H	4.54810000	1.64569600	2.72480800
S	2.80201000	1.74164700	1.01850300
S	0.78404000	-1.66455900	-1.05012300
O	0.74637900	1.48472600	-0.88572600
H	0.89940500	2.33701600	-0.45622600
C	-2.24783300	0.55579600	-0.41733900
H	-1.24309900	0.85981300	-0.71571000
N	-3.24220200	1.40611600	-0.51102400
O	3.13719800	0.23008600	-2.05561700
C	-3.55606000	-1.33270200	0.51704600
C	-4.66122900	-0.40687700	0.41948400
C	-4.42224300	0.87959600	-0.08401800
N	-2.36267700	-0.72088400	0.05701200
H	-1.51453300	-1.29245200	0.05998700
O	-3.56446700	-2.49089200	0.92364000
C	-6.05003100	-0.43227200	0.71038100
H	-6.63941600	-1.24259400	1.11643100
N	-5.62048800	1.51649700	-0.06552800
N	-6.62651500	0.72844500	0.41732000
H	-5.81383000	2.46142500	-0.36013400

T1-TS (O-Down)

Zero-point correction= 0.150390 (Hartree/Particle)
Thermal correction to Energy= 0.168165
Thermal correction to Enthalpy= 0.169109
Thermal correction to Gibbs Free Energy= 0.102772
Sum of electronic and zero-point Energies= -1978.489983
Sum of electronic and thermal Energies= -1978.472209
Sum of electronic and thermal Enthalpies= -1978.471264
Sum of electronic and thermal Free Energies= -1978.537601

Mo	1.74026400	-0.58943800	-0.08023200
S	3.74701600	-0.15764800	1.16334000
C	4.68945500	0.92111700	0.12014500
H	5.72009400	1.09631200	0.42247100
C	4.15360400	1.54613600	-0.94243600
H	4.72959500	2.23688400	-1.55417000
S	2.46747700	1.29744500	-1.42869400
S	0.46234000	-0.82834800	1.80716800
O	-0.28296200	-0.05350500	-0.86879200
H	-0.44658400	-0.57663300	-1.67338400
C	-1.53273100	-0.11513500	-0.10511900
H	-0.87803000	-0.66274900	1.02448700
N	-2.41505900	-0.98119200	-0.62333600
O	1.98573600	-2.08224000	-0.86485900
C	-3.25187900	1.58165000	0.55360500
C	-4.19439700	0.57112700	0.13023400
C	-3.69854600	-0.62318000	-0.42440000
N	-1.92627700	1.16830900	0.31880200
H	-1.20496500	1.78004700	0.68571700
O	-3.48974600	2.68499000	1.04326100
C	-5.60386600	0.43883200	0.08738700
H	-6.35512400	1.14256400	0.41869200
N	-4.79490300	-1.35970100	-0.74905800
N	-5.97072700	-0.72422500	-0.44107300
H	-4.81068600	-2.28279800	-1.15378900

T1-PC (O-Down)

Zero-point correction= 0.152113 (Hartree/Particle)
Thermal correction to Energy= 0.170886
Thermal correction to Enthalpy= 0.171830
Thermal correction to Gibbs Free Energy= 0.099621
Sum of electronic and zero-point Energies= -1978.546209
Sum of electronic and thermal Energies= -1978.527436
Sum of electronic and thermal Enthalpies= -1978.526492
Sum of electronic and thermal Free Energies= -1978.598701

Mo	1.93944500	-0.07726800	0.05431500
S	3.53625500	-0.11210300	-1.64927400
C	5.08047200	0.38847800	-0.88937700
H	5.92058700	0.54423500	-1.56179400
C	5.16863600	0.55412200	0.43646700
H	6.08673500	0.85559900	0.93493600
S	3.74496400	0.28039500	1.49044500
S	0.85379900	-2.17620400	0.39721700
O	-1.38709000	2.23508500	0.03098200
H	-0.43921400	1.82201600	-0.00635600
C	-2.35524200	1.35346300	0.00767300
H	-0.32980800	-1.50882300	0.38149100
N	-2.16123400	0.05326900	-0.02401700
O	0.97850700	1.37259700	-0.06203200
C	-4.84960800	1.24546500	-0.00336600
C	-4.63817400	-0.17693200	-0.04697400
C	-3.31811100	-0.65782200	-0.05568800
N	-3.60991900	1.93023200	0.02002400
H	-3.65442300	2.94209100	0.04429700
O	-5.90504400	1.87717100	0.01231700
C	-5.45124600	-1.34023300	-0.09297200
H	-6.53036600	-1.40754200	-0.10232400
N	-3.41630000	-2.00860500	-0.10317700
N	-4.71574500	-2.44307900	-0.12738400
H	-2.65946300	-2.67652700	-0.12854600

T1-TS (O-Up)

Zero-point correction= 0.150634 (Hartree/Particle)
Thermal correction to Energy= 0.168240
Thermal correction to Enthalpy= 0.169184
Thermal correction to Gibbs Free Energy= 0.103471
Sum of electronic and zero-point Energies= -1978.492301
Sum of electronic and thermal Energies= -1978.474695
Sum of electronic and thermal Enthalpies= -1978.473750
Sum of electronic and thermal Free Energies= -1978.539464

Mo	1.68285000	-0.43688800	-0.12993200
S	3.77795400	-0.47014000	1.05301000
C	4.76780400	0.76757300	0.26032200
H	5.81280400	0.80137100	0.56239200
C	4.26205100	1.65946900	-0.60766600
H	4.87229300	2.43838300	-1.05853200
S	2.56269000	1.61446200	-1.10928000
S	0.48627400	-0.99455500	1.74053400
O	-0.22380200	0.55647300	-0.57338900
H	-0.19709600	1.52934000	-0.53346400
C	-1.49955400	0.17134100	0.05848400
H	-0.84925000	-0.38260000	1.16802700
N	-2.24343400	1.22885000	0.41171800
O	1.70308700	-1.73914200	-1.22741500
C	-3.43185200	-1.22354900	-0.69548800
C	-4.22677200	-0.13811000	-0.16680000
C	-3.56839600	0.99918500	0.33669000
N	-2.05610800	-0.93272500	-0.61167600
H	-1.42963800	-1.68787500	-0.87427800
O	-3.82336600	-2.28040900	-1.18799500
C	-5.60740100	0.14346700	-0.02437200
H	-6.45079600	-0.47700900	-0.29479800
N	-4.55429300	1.84946700	0.73041300
N	-5.81017400	1.34029700	0.51691300
H	-4.44328900	2.75858000	1.15135200

T1-RC (O-Up)

Zero-point correction= 0.154895 (Hartree/Particle)
Thermal correction to Energy= 0.173848
Thermal correction to Enthalpy= 0.174792
Thermal correction to Gibbs Free Energy= 0.102179
Sum of electronic and zero-point Energies= -1978.559508
Sum of electronic and thermal Energies= -1978.540555
Sum of electronic and thermal Enthalpies= -1978.539611
Sum of electronic and thermal Free Energies= -1978.612224

Mo	-2.02938700	-0.25658200	0.55066000
S	-4.02699400	-0.93189800	-0.73875300
C	-4.78272500	0.54154700	-1.32702700
H	-5.75534100	0.41425800	-1.79780500
C	-4.16518600	1.73487100	-1.27874400
H	-4.60848400	2.63330500	-1.70207900
S	-2.55759600	1.90149800	-0.59381400
S	-1.12128900	-2.20815400	0.15445600
O	-0.32653400	0.79251800	0.71962000
H	-0.39406000	1.75789000	0.73848900
C	2.51426200	-1.09616200	-0.37910300
H	1.62664400	-1.70875200	-0.51279200
N	3.68395400	-1.57486900	-0.73486100
O	-2.69177600	-0.24403000	2.12216300
C	3.28957100	1.10215500	0.41028300
C	4.59276200	0.60212700	0.03128700
C	4.69089800	-0.68796500	-0.50749800
N	2.28905600	0.13240200	0.15886400
H	1.30445800	0.39326300	0.39467400
O	3.01040700	2.20024100	0.88603500
C	5.92471700	1.09136500	0.04851200
H	6.28564300	2.05171100	0.38968300
N	6.00858000	-0.88661500	-0.76749500
N	6.77702600	0.19254400	-0.43293900
H	6.43659000	-1.71003400	-1.16189100

T1-PC (O-Up)

Zero-point correction= 0.152351 (Hartree/Particle)
Thermal correction to Energy= 0.171676
Thermal correction to Enthalpy= 0.172620
Thermal correction to Gibbs Free Energy= 0.098195
Sum of electronic and zero-point Energies= -1978.533418
Sum of electronic and thermal Energies= -1978.514092
Sum of electronic and thermal Enthalpies= -1978.513148
Sum of electronic and thermal Free Energies= -1978.587573

Mo	-2.29784900	0.59973300	0.00023400
S	-2.53584100	-1.10638600	-1.58880400
C	-2.51132900	-2.64470600	-0.67088900
H	-2.50994700	-3.55916600	-1.26019300
C	-2.51162900	-2.64503200	0.66972800
H	-2.51049700	-3.55978600	1.25858300
S	-2.53649700	-1.10718600	1.58840700
S	-4.13902800	2.14986200	-0.00033300
O	1.03340200	-1.55799100	0.00055200
H	1.23601700	-2.50553200	0.00040500
C	2.18263900	-0.88286500	0.00031300
H	-3.33600500	3.23956200	0.00084800
N	3.32759900	-1.53084600	0.00021500
O	-0.66520200	1.16232600	0.00054300
C	3.09488700	1.39448600	0.00005900
C	4.37166800	0.71365500	-0.00007100
C	4.39265000	-0.68610800	0.00000200
N	2.02058600	0.46609900	0.00016100
H	1.04066300	0.82764200	0.00032100
O	2.88886300	2.60273100	0.00009000
C	5.73799100	1.09760900	-0.00028300
H	6.15511100	2.09522500	-0.00041100
N	5.70099400	-1.04306700	-0.00010000
N	6.54173400	0.04068400	-0.00031400
H	6.08200000	-1.97622300	-0.00005700

T2-RC (O-Down)

Zero-point correction= 0.154564 (Hartree/Particle)
Thermal correction to Energy= 0.173720
Thermal correction to Enthalpy= 0.174664
Thermal correction to Gibbs Free Energy= 0.100751
Sum of electronic and zero-point Energies= -1978.550209
Sum of electronic and thermal Energies= -1978.531053
Sum of electronic and thermal Enthalpies= -1978.530109
Sum of electronic and thermal Free Energies= -1978.604022

Mo	1.90026700	-0.30329000	-0.25211100
S	4.19778800	-1.00221400	0.32766400
C	5.21377100	0.43074500	0.29785100
H	6.27889000	0.25044600	0.42800400
C	4.70687400	1.67213600	0.20342400
H	5.33406700	2.55957800	0.24701100
S	2.98018600	1.93754400	0.04861300
S	1.12427300	-2.00588600	0.88224900
O	0.34642700	0.93205200	-0.01377300
H	0.48339300	1.88749700	0.03622500
C	-2.61041000	-1.10844200	-0.16210200
H	-1.72849000	-1.73717200	-0.25452500
N	-3.79101700	-1.65596900	-0.21583800
O	1.86278200	-0.69521100	-1.91312700
C	-3.30487800	1.22354600	0.15516900
C	-4.63890400	0.65064500	0.10305200
C	-4.82092900	-0.75523400	-0.07979400
N	-2.33382700	0.22657900	0.01128700
H	-1.33469000	0.52451700	0.02280500
O	-3.01590500	2.41080100	0.30213600
C	-5.91880000	1.17400600	0.19192900
H	-6.27851700	2.18292200	0.33071800
N	-6.12087300	-1.08376000	-0.10274700
N	-6.74754900	0.10961000	0.06454800
H	-7.75575400	0.11853400	0.08218400

T2-TS (O-Down)

Zero-point correction= 0.150338 (Hartree/Particle)
Thermal correction to Energy= 0.168029
Thermal correction to Enthalpy= 0.168973
Thermal correction to Gibbs Free Energy= 0.103022
Sum of electronic and zero-point Energies= -1978.479049
Sum of electronic and thermal Energies= -1978.461358
Sum of electronic and thermal Enthalpies= -1978.460414
Sum of electronic and thermal Free Energies= -1978.526365

Mo	1.74416000	-0.61040700	-0.08082000
S	3.73836000	-0.08597100	1.15663100
C	4.63914700	1.01644300	0.10222900
H	5.66132300	1.23631900	0.40449500
C	4.08139800	1.60656800	-0.96912600
H	4.63118900	2.31307600	-1.58715800
S	2.40791500	1.28609100	-1.45478500
S	0.48063600	-0.87352100	1.80717600
O	-0.27949600	-0.13491600	-0.87375300
H	-0.45833200	-0.68098600	-1.66014300
C	-1.53211500	-0.19524300	-0.08890000
H	-0.88299600	-0.74334100	1.00640500
N	-2.42669100	-1.02142600	-0.62462000
O	2.04902700	-2.10348100	-0.84248400
C	-3.17596900	1.55816800	0.58246300
C	-4.15134800	0.58100300	0.13128700
C	-3.72641600	-0.65932400	-0.44948700
N	-1.87827500	1.10845900	0.35766100
H	-1.13485000	1.68000100	0.74493700
O	-3.40654700	2.65703900	1.08932800
C	-5.53337900	0.54809600	0.09906000
H	-6.27795000	1.25972500	0.42483700
N	-4.78060000	-1.40882100	-0.81728100
N	-5.85164600	-0.64000200	-0.46860300
H	-6.77498200	-1.00416400	-0.64327500

T2-PC (O-down)

Zero-point correction= 0.151706 (Hartree/Particle)
Thermal correction to Energy= 0.170743
Thermal correction to Enthalpy= 0.171687
Thermal correction to Gibbs Free Energy= 0.098125
Sum of electronic and zero-point Energies= -1978.534052
Sum of electronic and thermal Energies= -1978.515015
Sum of electronic and thermal Enthalpies= -1978.514071
Sum of electronic and thermal Free Energies= -1978.587633

Mo	2.43098800	-0.57974800	0.00015200
S	3.35718100	0.86301600	-1.58509400
C	3.98406500	2.26978200	-0.67005900
H	4.35563700	3.10321000	-1.26134200
C	3.98480100	2.26963600	0.66931100
H	4.35702000	3.10293500	1.26036900
S	3.35892900	0.86265800	1.58473500
S	3.47531800	-2.74275400	-0.00083800
O	-1.28862100	1.15244000	0.00100200
H	-0.54216000	0.44489100	0.00094100
C	-2.50858600	0.66827800	0.00063800
H	2.29524200	-3.40588200	0.00018700
N	-2.80085300	-0.60072000	0.00066500
O	0.70208800	-0.41271900	0.00097700
C	-4.84540600	1.52407000	-0.00023200
C	-5.18021900	0.11677300	-0.00024000
C	-4.14339400	-0.87274400	0.00024200
N	-3.45812500	1.69282100	0.00021800
H	-3.10842300	2.64365100	0.00030900
O	-5.61222400	2.48835400	-0.00056400
C	-6.36991200	-0.59465000	-0.00047700
H	-7.40170300	-0.27493400	-0.00075700
N	-4.65814300	-2.11056200	0.00025800
N	-6.00375900	-1.89616600	-0.00014900
H	-6.61184700	-2.70025900	-0.00031600

T2-RC (O-Up)

Zero-point correction= 0.154775 (Hartree/Particle)
Thermal correction to Energy= 0.173747
Thermal correction to Enthalpy= 0.174691
Thermal correction to Gibbs Free Energy= 0.101544
Sum of electronic and zero-point Energies= -1978.549933
Sum of electronic and thermal Energies= -1978.530962
Sum of electronic and thermal Enthalpies= -1978.530018
Sum of electronic and thermal Free Energies= -1978.603164

Mo	2.02208900	0.28515800	0.50213600
S	4.11302100	0.89580000	-0.66839900
C	4.90035800	-0.60379300	-1.13715800
H	5.90356900	-0.49898100	-1.54523400
C	4.27654800	-1.79341600	-1.07759300
H	4.74480000	-2.71024000	-1.42857400
S	2.62646700	-1.92862200	-0.49473200
S	1.15646700	2.21576800	-0.05303100
O	0.31056000	-0.75286700	0.59881500
H	0.36089600	-1.71889600	0.62588900
C	-2.62354200	1.18438600	-0.32573900
H	-1.75910500	1.83442700	-0.43427800
N	-3.80772300	1.64732600	-0.60837000
O	2.56627100	0.35024500	2.11780800
C	-3.26667200	-1.09542800	0.31210900
C	-4.60426900	-0.61653800	0.00885300
C	-4.81371100	0.72608800	-0.43421600
N	-2.32160600	-0.08295600	0.11051000
H	-1.32282700	-0.32135000	0.29981100
O	-2.95471900	-2.22288700	0.69396700
C	-5.86569400	-1.18884400	0.04251100
H	-6.20261700	-2.17885200	0.31261200
N	-6.11243100	0.97236600	-0.66002100
N	-6.71106100	-0.20933800	-0.35980800
H	-7.71300100	-0.27232600	-0.45480800

T2-TS (O-Up)

Zero-point correction= 0.150531 (Hartree/Particle)
Thermal correction to Energy= 0.168079
Thermal correction to Enthalpy= 0.169023
Thermal correction to Gibbs Free Energy= 0.103611
Sum of electronic and zero-point Energies= -1978.481593
Sum of electronic and thermal Energies= -1978.464045
Sum of electronic and thermal Enthalpies= -1978.463101
Sum of electronic and thermal Free Energies= -1978.528513

Mo	1.67030400	-0.41532400	-0.13449300
S	3.79049800	-0.53164200	1.00293000
C	4.78687800	0.71852500	0.23898100
H	5.83812100	0.72266800	0.52085400
C	4.27962100	1.65209900	-0.58334600
H	4.89519400	2.43791600	-1.01491700
S	2.56985500	1.65978200	-1.04809200
S	0.50116100	-1.03761800	1.72697900
O	-0.21960300	0.61378100	-0.51279700
H	-0.20726500	1.58474100	-0.43540700
C	-1.50101500	0.19833100	0.12196900
H	-0.85177100	-0.37055800	1.18974400
N	-2.25318600	1.23533600	0.47756000
O	1.65014700	-1.67139000	-1.28594100
C	-3.37690100	-1.21096900	-0.71578800
C	-4.19878600	-0.13865100	-0.18107800
C	-3.59495200	1.03258300	0.38516300
N	-2.02314100	-0.91327500	-0.58974000
H	-1.37457800	-1.65045700	-0.85037100
O	-3.76973800	-2.25599600	-1.23579600
C	-5.56257400	0.07081200	-0.09100300
H	-6.40501500	-0.53585600	-0.38966800
N	-4.52815600	1.90828400	0.79820800
N	-5.70239500	1.28710300	0.48922300
H	-6.56360800	1.75714100	0.71952500

T2-PC (O-Up)

Zero-point correction= 0.152933 (Hartree/Particle)
Thermal correction to Energy= 0.171753
Thermal correction to Enthalpy= 0.172697
Thermal correction to Gibbs Free Energy= 0.102036
Sum of electronic and zero-point Energies= -1978.521693
Sum of electronic and thermal Energies= -1978.502873
Sum of electronic and thermal Enthalpies= -1978.501929
Sum of electronic and thermal Free Energies= -1978.572590

Mo	1.77398800	0.27060500	0.29940000
S	3.98370100	-0.41592400	0.64589100
C	4.26299600	-1.72351800	-0.54370000
H	5.19994200	-2.26847200	-0.44892000
C	3.37579600	-1.98971300	-1.51334800
H	3.53309100	-2.77313700	-2.25129700
S	1.84457400	-1.07435300	-1.64509800
S	2.26050600	2.66494700	0.22760400
O	-0.60165300	1.22013300	-0.40611700
H	-0.63576400	1.83310400	-1.15907200
C	-1.82846900	0.67850300	-0.23855600
H	1.02031000	3.09340300	0.56166900
N	-2.81588700	1.09654900	-0.96997900
O	0.80795400	-0.48609800	1.51759600
C	-3.02469800	-0.95835600	1.12051500
C	-4.16057400	-0.52293100	0.32575000
C	-4.00816300	0.47646700	-0.68281300
N	-1.85645500	-0.27128200	0.74528800
H	-0.95048000	-0.50999000	1.19792200
O	-3.02560000	-1.80126500	2.01034400
C	-5.50028300	-0.87391800	0.28715800
H	-6.07435500	-1.58698600	0.86039200
N	-5.16526700	0.73342200	-1.30347800
N	-6.04273800	-0.10611200	-0.68649800
H	-7.00353300	-0.09747500	-0.99180800

T10-RC

Zero-point correction= 0.154079 (Hartree/Particle)
Thermal correction to Energy= 0.173226
Thermal correction to Enthalpy= 0.174170
Thermal correction to Gibbs Free Energy= 0.101548
Sum of electronic and zero-point Energies= -1978.528438
Sum of electronic and thermal Energies= -1978.509291
Sum of electronic and thermal Enthalpies= -1978.508347
Sum of electronic and thermal Free Energies= -1978.580969

Mo	2.05359400	-0.04304900	0.67838800
S	3.60396600	1.33985500	-0.63800100
C	4.53216600	0.26392800	-1.67162500
H	5.34518600	0.73192100	-2.22219200
C	4.20800100	-1.02957500	-1.83731700
H	4.74193000	-1.68024700	-2.52549200
S	2.84656800	-1.73411700	-0.98546700
S	0.73187900	1.69727300	0.92295300
O	0.62332300	-1.44531600	0.71068500
H	0.81476500	-2.28373000	0.26886000
C	-2.13281900	-0.31670500	0.24837100
H	-1.09706800	-0.58027100	0.48107500
N	-3.07890100	-1.23220500	0.39540500
O	2.94583700	-0.26015300	2.11363600
C	-3.77123000	1.37914200	-0.58197600
C	-4.75151600	0.35628000	-0.40507200
C	-4.40171600	-0.92871000	0.07952000
N	-2.44378500	0.89789100	-0.20607800
H	-1.67730900	1.56749300	-0.27771400
O	-3.86884900	2.53277400	-0.97922800
C	-6.14721400	0.20715800	-0.58381800
H	-6.86314300	0.93475400	-0.94273900
N	-5.43383500	-1.75020100	0.18260100
N	-6.53093900	-1.02742000	-0.23695500
H	-2.83819600	-2.15401000	0.74011700

T10-TS

Zero-point correction= 0.149442 (Hartree/Particle)
Thermal correction to Energy= 0.167297
Thermal correction to Enthalpy= 0.168241
Thermal correction to Gibbs Free Energy= 0.101261
Sum of electronic and zero-point Energies= -1978.460357
Sum of electronic and thermal Energies= -1978.442502
Sum of electronic and thermal Enthalpies= -1978.441558
Sum of electronic and thermal Free Energies= -1978.508538

Mo	1.63928100	-0.39283700	-0.06103700
S	3.76522900	-0.73080200	0.96445800
C	4.88750100	0.24629100	-0.00343800
H	5.94565100	0.09327800	0.19763700
C	4.46705000	1.16703200	-0.88602100
H	5.15827800	1.78569200	-1.45292200
S	2.74143400	1.43870500	-1.20146100
S	0.45839700	-0.63228100	1.92595400
O	-0.23087800	0.78158400	-0.46667400
H	-0.30404600	1.06998000	-1.39531000
C	-1.52251800	0.43283300	0.04601100
H	-0.81053600	-0.13760700	1.35257100
N	-2.11806800	-0.62019600	-0.56108900
O	1.37301700	-1.72882300	-1.08746900
C	-3.75846200	1.50338300	0.50802000
C	-4.32133900	0.29566800	-0.00323500
C	-3.50057000	-0.74741900	-0.50771700
N	-2.31307200	1.49478200	0.40081400
H	-1.84787100	2.28234900	0.83852500
O	-4.28677600	2.50299200	0.98509100
C	-5.60867900	-0.26092600	-0.16935100
H	-6.56875500	0.17022400	0.08211400
N	-4.19553200	-1.79621700	-0.92643500
N	-5.51966300	-1.48249800	-0.71380900
H	-1.53992900	-1.41302500	-0.83186400

T10-PC

Zero-point correction= 0.150121 (Hartree/Particle)
Thermal correction to Energy= 0.169073
Thermal correction to Enthalpy= 0.170017
Thermal correction to Gibbs Free Energy= 0.097112
Sum of electronic and zero-point Energies= -1978.524061
Sum of electronic and thermal Energies= -1978.505109
Sum of electronic and thermal Enthalpies= -1978.504165
Sum of electronic and thermal Free Energies= -1978.577071

Mo	2.15989900	-0.53421800	0.04919900
S	3.18404000	0.64439800	-1.66264100
C	4.06761100	1.99102800	-0.87917200
H	4.52713700	2.71665500	-1.54493700
C	4.14226300	2.07050700	0.45486100
H	4.66792200	2.86660900	0.97527000
S	3.35937100	0.83161700	1.48509300
S	2.96588900	-2.77418700	0.13694500
O	-1.21687800	1.68636100	0.15597700
H	-0.41220800	0.97876400	0.14195000
C	-2.36490000	1.08259700	0.09355500
H	1.72837800	-3.31777000	0.22262100
N	-2.48273500	-0.24533300	0.01828500
O	0.44314600	-0.11027100	0.11786400
C	-4.86377500	1.38056900	0.04453400
C	-4.92934200	-0.03706100	-0.03418800
C	-3.75543200	-0.82920700	-0.04577600
N	-3.48353300	1.83994200	0.10647800
H	-3.35505500	2.84297900	0.16340000
O	-5.73947100	2.24207300	0.06835200
C	-5.93496200	-1.03608700	-0.11316800
H	-7.00980200	-0.90922100	-0.13422400
N	-4.00029400	-2.12387100	-0.12056700
N	-5.38193100	-2.24797200	-0.16293200
H	-1.63463100	-0.80884500	0.00893300

S4. Cartesian coordinates of concerted mechanisms of deprotonated allopurinol.

I-RC

Zero-point correction= 0.141480 (Hartree/Particle)
Thermal correction to Energy= 0.159800
Thermal correction to Enthalpy= 0.160744
Thermal correction to Gibbs Free Energy= 0.090343
Sum of electronic and zero-point Energies= -1977.951572
Sum of electronic and thermal Energies= -1977.933252
Sum of electronic and thermal Enthalpies= -1977.932308
Sum of electronic and thermal Free Energies= -1978.002709

Mo	-2.10571800	-0.68012000	0.32380600
S	-3.56788300	0.83180400	-1.04723100
C	-3.13982200	2.49187400	-0.65592000
H	-3.77154000	3.25966700	-1.10217300
C	-2.05245600	2.81231100	0.07129100
H	-1.76244500	3.84840900	0.24061900
S	-1.00625500	1.57871500	0.75369300
S	-2.61818600	-2.20883800	-1.19096600
O	-0.36986600	-1.20588500	0.86901400
H	0.56708300	-1.00016400	0.54967900
C	3.07459100	-1.89189300	0.10055200
H	2.57359700	-2.85540400	0.21205500
N	2.24595700	-0.82904500	0.16236700
O	-3.09354300	-0.96415700	1.69516500
C	5.11881800	-0.75851500	-0.22223000
C	4.31348700	0.45235900	-0.17278400
C	2.92709000	0.33282100	0.01724800
N	4.39229000	-1.94238900	-0.07290900
O	6.35857000	-0.76200000	-0.38266700
C	4.53157800	1.85216100	-0.26377900
H	5.46633100	2.37770500	-0.41197500
N	2.42101300	1.59582700	0.02725700
N	3.39741200	2.54108800	-0.14344100
H	1.44661000	1.85921600	0.15272000

I-PC

Zero-point correction= 0.139999 (Hartree/Particle)
Thermal correction to Energy= 0.158668
Thermal correction to Enthalpy= 0.159612
Thermal correction to Gibbs Free Energy= 0.089230
Sum of electronic and zero-point Energies= -1977.919084
Sum of electronic and thermal Energies= -1977.900415
Sum of electronic and thermal Enthalpies= -1977.899471
Sum of electronic and thermal Free Energies= -1977.969853

Mo	-1.81065300	-0.36837600	0.37465300
S	-3.98030100	-0.58749000	-0.64298900
C	-4.65491600	1.05941300	-0.63727600
H	-5.69289900	1.15437200	-0.95886700
C	-3.93397300	2.14776900	-0.30711000
H	-4.36161300	3.14944000	-0.33404800
S	-2.23825800	2.02517500	0.22162500
S	-1.03774100	-2.11539700	-1.15384500
O	0.41157400	0.47621400	0.32305300
H	0.31181400	1.43516800	0.19704800
C	1.77270900	0.22414300	0.18990000
H	0.27499000	-2.13213600	-0.81967500
N	2.46386200	1.35052900	-0.06635900
O	-2.03086200	-0.88873100	1.97900800
C	3.51513500	-1.33027100	0.25463200
C	4.37811500	-0.18590600	-0.02541300
C	3.77782300	1.07314400	-0.16467300
N	2.15605000	-1.02092700	0.34926200
O	3.94207100	-2.48916800	0.40313500
C	5.76245500	0.05578700	-0.21364900
H	6.57536800	-0.65875700	-0.18602600
N	4.79043500	1.95367000	-0.41429500
N	6.02425400	1.34133100	-0.45038300
H	4.71201000	2.94386200	-0.57813200

I-TS

Zero-point correction= 0.135552 (Hartree/Particle)
Thermal correction to Energy= 0.153316
Thermal correction to Enthalpy= 0.154261
Thermal correction to Gibbs Free Energy= 0.088320
Sum of electronic and zero-point Energies= -1977.864812
Sum of electronic and thermal Energies= -1977.847048
Sum of electronic and thermal Enthalpies= -1977.846104
Sum of electronic and thermal Free Energies= -1977.912044

Mo	1.74138700	-0.55099800	-0.17238900
S	3.75434800	-0.11370000	1.16692800
C	4.57758100	1.22637500	0.35447900
H	5.56267100	1.48634300	0.74302100
C	4.01709200	1.93677300	-0.64331800
H	4.53352500	2.78215100	-1.09732800
S	2.41048500	1.56268600	-1.28449600
S	0.58191400	-1.22817000	1.68241700
O	-0.15246000	0.06325300	-0.77022900
H	-0.26757200	1.02648000	-0.81267300
C	-1.67086100	-0.30003800	0.09100300
H	-0.79454800	-0.82537900	1.00868300
N	-2.10165600	0.91675100	0.51622500
O	2.13424800	-1.88192400	-1.16013200
C	-3.71430200	-1.22590700	-0.61682600
C	-4.30252000	0.01512100	-0.11758800
C	-3.43716800	0.99278000	0.40622600
N	-2.33128100	-1.28576200	-0.48773000
O	-4.38637900	-2.14686100	-1.12451600
C	-5.59351600	0.58897900	-0.02137800
H	-6.54027400	0.15769200	-0.32207600
N	-4.23518400	2.04237200	0.77320900
N	-5.56887100	1.81091400	0.51517100
H	-3.94218500	2.91139600	1.18842800

III-RC

Zero-point correction= 0.140506 (Hartree/Particle)
Thermal correction to Energy= 0.158355
Thermal correction to Enthalpy= 0.159299
Thermal correction to Gibbs Free Energy= 0.088928
Sum of electronic and zero-point Energies= -1977.926705
Sum of electronic and thermal Energies= -1977.908855
Sum of electronic and thermal Enthalpies= -1977.907911
Sum of electronic and thermal Free Energies= -1977.978282

Mo	-2.12703800	-0.42792100	0.55514900
S	-4.03891600	0.22575000	-0.95725500
C	-3.79114800	1.90439200	-1.41422100
H	-4.59497600	2.36660200	-1.98751100
C	-2.64217000	2.55935500	-1.15472800
H	-2.47652900	3.57804500	-1.50535100
S	-1.31243700	1.80679900	-0.29150700
S	-2.58406700	-2.49883800	-0.09308800
O	-0.28487200	-0.52521300	0.97143200
H	0.60400300	-0.35755000	0.53485000
C	2.57843700	-0.84767700	-1.28133500
H	1.71959600	-1.25014500	-1.82041200
N	2.27755700	-0.30433100	-0.09628300
O	-2.87912900	-0.17332100	2.07586800
C	4.90348600	-0.50424400	-1.32122700
C	4.69264500	0.11887300	-0.01275500
C	3.37685700	0.18869700	0.54764200
N	3.75513700	-0.98184500	-1.91528600
O	6.03657600	-0.59239000	-1.84639900
C	5.51446400	0.71735100	0.92871900
H	6.58028300	0.89630600	0.94402500
N	3.37954100	0.78728500	1.75498200
N	4.69405000	1.09088300	1.94654100
H	4.94991000	1.56304400	2.79827000

III-TS

Zero-point correction= 0.135220 (Hartree/Particle)
Thermal correction to Energy= 0.152982
Thermal correction to Enthalpy= 0.153926
Thermal correction to Gibbs Free Energy= 0.088070
Sum of electronic and zero-point Energies= -1977.848527
Sum of electronic and thermal Energies= -1977.830765
Sum of electronic and thermal Enthalpies= -1977.829821
Sum of electronic and thermal Free Energies= -1977.895676

Mo	1.73296800	-0.52306600	-0.18154900
S	3.77984500	-0.19848900	1.14283600
C	4.63676700	1.13888800	0.36123700
H	5.63599300	1.35277900	0.74204600
C	4.08569000	1.90083900	-0.60356900
H	4.62457900	2.74344500	-1.03659300
S	2.45668100	1.60687400	-1.22914500
S	0.58290800	-1.23120600	1.66734700
O	-0.14429300	0.16863400	-0.72765100
H	-0.25445300	1.13278100	-0.68274100
C	-1.68121800	-0.23814800	0.12321400
H	-0.78946100	-0.76999100	1.02796100
N	-2.13595800	0.94622300	0.55491400
O	2.07220500	-1.82857500	-1.22224400
C	-3.65658900	-1.22843500	-0.63648400
C	-4.29301800	-0.00685400	-0.12350800
C	-3.48769900	1.03479100	0.44675500
N	-2.29222300	-1.25235700	-0.48756800
O	-4.31873800	-2.14843100	-1.16637300
C	-5.58982600	0.46669900	-0.06647700
H	-6.52782900	0.03098100	-0.38198900
N	-4.24165600	2.08768500	0.83840400
N	-5.51184100	1.70096200	0.50373600
H	-6.27072500	2.32662800	0.71652100

III-PC

Zero-point correction= 0.139760 (Hartree/Particle)
Thermal correction to Energy= 0.158406
Thermal correction to Enthalpy= 0.159350
Thermal correction to Gibbs Free Energy= 0.089262
Sum of electronic and zero-point Energies= -1977.904811
Sum of electronic and thermal Energies= -1977.886165
Sum of electronic and thermal Enthalpies= -1977.885221
Sum of electronic and thermal Free Energies= -1977.955309

Mo	-1.79192300	-0.33247600	0.37172000
S	-4.00391800	-0.65221800	-0.52700200
C	-4.71473000	0.97847500	-0.57409900
H	-5.76971800	1.03585000	-0.84579300
C	-4.00158400	2.09682500	-0.34073000
H	-4.45261800	3.08702400	-0.39934200
S	-2.27709200	2.03829600	0.09798800
S	-1.05608600	-2.14460800	-1.10050300
O	0.41542200	0.52775300	0.21381300
H	0.33286500	1.48919600	0.09523200
C	1.78096800	0.26953500	0.12375300
H	0.26771600	-2.12502100	-0.81307900
N	2.48488200	1.37937100	-0.09021700
O	-1.93190900	-0.76670100	2.01078300
C	3.46425100	-1.33002200	0.22003000
C	4.36146100	-0.19258100	-0.01800600
C	3.82009300	1.12399400	-0.16284100
N	2.12588500	-1.00076100	0.27782000
O	3.89025300	-2.49343700	0.35872600
C	5.72907200	-0.03600300	-0.15186000
H	6.54047100	-0.74956800	-0.11689100
N	4.78590700	2.04227200	-0.37255000
N	5.93175900	1.29295400	-0.35804300
H	6.80925100	1.76386500	-0.50322800

S5. Cartesian coordinates of allopurinol oxidation using the cytochrome P450.

^{2}T1-RC

Zero-point correction= 0.388603 (Hartree/Particle)
Thermal correction to Energy= 0.418706
Thermal correction to Enthalpy= 0.419650
Thermal correction to Gibbs Free Energy= 0.323189
Sum of electronic and zero-point Energies= -2073.077947
Sum of electronic and thermal Energies= -2073.047844
Sum of electronic and thermal Enthalpies= -2073.046900
Sum of electronic and thermal Free Energies= -2073.143362

C	-0.33073600	1.23419500	2.38993600
C	-0.78606400	2.50367100	2.89665900
C	-0.17385600	3.46402500	2.15119800
C	3.62749400	-0.01692000	-2.37946100
C	-0.31640600	-1.23461500	2.40983600
C	1.50608600	-3.42445200	0.31559100
C	2.25931900	2.77691400	-0.68682600
C	-0.74067400	-2.50011300	2.95370300
C	3.67947400	2.48670500	-2.40834100
C	1.44947600	3.41175400	0.24173100
C	3.24406400	1.21761000	-1.87977400
C	3.23891900	-1.25020500	-1.87010800
C	3.68795500	-2.52183400	-2.38156200
C	-0.73650600	0.00201900	2.88389700
C	3.10110100	-3.48173600	-1.61624900
C	0.69681900	-2.78378300	1.24862100
C	2.28796400	-2.79566600	-0.64285500
C	-0.10756900	-3.46540700	2.23258400
C	0.65251000	2.77688000	1.18999300
C	3.07179000	3.45254100	-1.66809500
Fe	1.35109400	-0.01180300	0.18411700
H	1.43381600	4.49742000	0.22802900
H	-1.48851500	2.62333100	3.71087800
H	-1.43439500	-2.61384300	3.77624800
H	3.19763100	-4.55732800	-1.68956200
H	4.36304700	2.60354800	-3.23941300
H	1.52124000	-4.51001600	0.33496500
H	3.37220900	1.32938900	2.01104100
H	-1.45654200	0.00483800	3.69463200
H	-0.16771900	-4.54057400	2.34174600
H	3.15090600	4.52769900	-1.76539300
H	4.36913500	-2.64417200	-3.21378000
H	-0.26317500	4.53993000	2.22894800
H	4.30206200	-0.02118600	-3.23018600
N	0.54863600	1.41989200	1.35356200
N	2.38962900	1.41225600	-0.81781200
N	2.39041100	-1.43606600	-0.80870800
N	0.55627800	-1.42758100	1.37247200
O	0.10464000	-0.01140400	-0.87401000
S	3.47641400	0.05571100	1.56954400
C	-3.00641600	-0.04317000	-2.24173900
H	-2.12772400	-0.06042200	-2.88112500
C	-5.18233600	-0.02942900	-1.84273100
C	-5.04127400	0.00461300	-0.44792100
C	-3.71586200	0.01636100	0.12317100
H	-1.74754900	-0.00617300	-0.63326300
O	-3.39342300	0.04502900	1.30585800
N	-4.19550600	-0.05431200	-2.78304100
N	-2.73931800	-0.01072800	-0.90665500
C	-6.36921300	0.01907900	0.04955200
H	-6.70379700	0.04483400	1.07769900
N	-6.51620700	-0.03285900	-2.08120100
N	-7.25668500	-0.00356600	-0.93614400
H	-6.97846700	-0.05423100	-2.97817400

^{2}T1-TS1

Zero-point correction= 0.387163 (Hartree/Particle)
Thermal correction to Energy= 0.416353
Thermal correction to Enthalpy= 0.417297
Thermal correction to Gibbs Free Energy= 0.327032
Sum of electronic and zero-point Energies= -2073.039427
Sum of electronic and thermal Energies= -2073.010237
Sum of electronic and thermal Enthalpies= -2073.009292
Sum of electronic and thermal Free Energies= -2073.099558

C	-0.33200000	-2.23203200	-1.96084700
C	-0.29633300	-3.66585000	-2.13751200
C	0.71854300	-4.13189600	-1.36239000
C	3.11985500	1.45817700	1.81788300
C	-1.25216700	0.00583000	-2.48001500
C	-0.17992700	3.15586600	-1.28694800
C	2.85518700	-1.94997300	0.91705600
C	-2.14359400	0.86564000	-3.22313400
C	4.11875000	-0.77867300	2.36379900
C	2.32712700	-3.03886600	0.22576300
C	3.20773000	0.08077500	1.64578800
C	2.26672400	2.31379100	1.12890700
C	2.26785500	3.74918800	1.27003200
C	-1.23170200	-1.38052900	-2.58721400
C	1.35433700	4.23004500	0.38171100
C	-0.75435900	2.06629200	-1.92320700
C	0.79011200	3.08641300	-0.29044800
C	-1.82439600	2.14635300	-2.88721100
C	1.29713900	-2.98504500	-0.70126200
C	3.90084700	-2.04277900	1.90815300
Fe	0.94266000	0.05007500	-0.38818700
H	2.74343200	-4.01649200	0.45004300
H	-0.96876000	-4.22416800	-2.77606600
H	-2.89129800	0.51739300	-3.92454900
H	1.07928900	5.25848900	0.18615100
H	4.82548700	-0.44274100	3.11178300
H	-0.53299100	4.14312800	-1.56911000
H	3.27350300	-0.82689400	-1.99644300
H	-1.96641500	-1.83493800	-3.24518200
H	-2.26059900	3.06873900	-3.24919300
H	4.38933400	-2.96176600	2.20574900
H	2.90156900	4.30140700	1.95215300
H	1.05178000	-5.15308300	-1.22904200
H	3.79329500	1.91045900	2.54009400
N	0.65454500	-1.83496400	-1.09391100
N	2.45294800	-0.65032300	0.76703100
N	1.34511000	1.92716100	0.18610000
N	-0.41647500	0.75567400	-1.69256000
O	-0.19658300	-0.31254200	0.84902400
S	2.42090900	0.16614900	-2.33444900
C	-1.28800000	0.79871800	1.79233500
H	-0.49953000	1.50185700	2.03682800
C	-3.30450200	0.47464300	0.86434300
C	-3.70926500	-0.50863000	1.78891500
C	-2.82778200	-0.82761600	2.89633500
H	-0.96634200	-0.26760200	3.53395000
O	-3.00154900	-1.64458100	3.78911000
N	-2.17493100	1.19730900	0.85415900
N	-1.67714500	-0.01329200	2.85810700
C	-4.97087100	-0.94016500	1.33424800
H	-5.62460100	-1.68731800	1.76291200
N	-4.32063000	0.56521800	-0.04020900
N	-5.33771200	-0.29300100	0.22583100
H	-4.34159900	1.13563400	-0.87341800

^{2}T1-Int

Zero-point correction= 0.389697 (Hartree/Particle)
Thermal correction to Energy= 0.418530
Thermal correction to Enthalpy= 0.419474
Thermal correction to Gibbs Free Energy= 0.329430
Sum of electronic and zero-point Energies= -2073.041265
Sum of electronic and thermal Energies= -2073.012432
Sum of electronic and thermal Enthalpies= -2073.011488
Sum of electronic and thermal Free Energies= -2073.101532

C	0.54814800	2.92692000	-1.11549000
C	0.32483000	3.69186600	-2.32279400
C	0.45674000	2.82823800	-3.36579600
C	1.57747400	-3.25289100	-0.34310000
C	0.72904300	2.76592700	1.35412800
C	1.43998500	-0.08438000	3.32542500
C	1.15715100	-0.89630200	-2.95683500
C	0.74529700	3.37928700	2.66155600
C	1.46691400	-3.12489400	-2.84298000
C	0.93126500	0.35395900	-3.51079900
C	1.43744500	-2.53788900	-1.52486900
C	1.57254200	-2.70368900	0.93193200
C	1.79205300	-3.45123600	2.14479200
C	0.50461300	3.45603000	0.16813100
C	1.77131300	-2.55678400	3.16990100
C	1.18071100	1.17805200	2.79487600
C	1.52844900	-1.25867400	2.59296400
C	1.03323900	2.39477500	3.55706900
C	0.75331100	1.53431100	-2.79237700
C	1.29803200	-2.10798500	-3.72879000
Fe	1.11655900	0.08219200	-0.09262700
H	0.86690700	0.41187800	-4.59318500
H	0.09758900	4.75004400	-2.34779500
H	0.56169100	4.42918600	2.85086600
H	1.90556600	-2.74152800	4.22805600
H	1.59699900	-4.18075000	-3.04238700
H	1.56936100	-0.15978200	4.40080200
H	3.42425300	0.81290500	-1.47820400
H	0.29188300	4.51760400	0.25352000
H	1.13170100	2.46732200	4.63261600
H	1.25863500	-2.15397400	-4.80960400
H	1.95020000	-4.52125000	2.18587000
H	0.35711700	3.02748700	-4.42518300
H	1.72082500	-4.32596500	-0.42286000
N	0.81502500	1.62003400	-1.43514100
N	1.25451800	-1.17973700	-1.60974500
N	1.39500100	-1.36807900	1.21974500
N	0.99322000	1.42396700	1.46515000
O	-0.71693100	0.03258400	-0.13163400
S	3.23888500	0.76885500	-0.13902300
C	-1.55350400	-0.15886700	0.97096400
H	-1.01311300	-0.06329900	1.91527000
C	-3.71580400	0.49538900	0.43915700
C	-4.13827100	-0.81012700	0.05020200
C	-3.22822700	-1.93993700	0.25791400
H	-1.36058600	-2.25545100	0.96355600
O	-3.46250900	-3.10626300	-0.03685500
N	-2.57041000	0.88674500	0.93978000
N	-2.07503100	-1.53719400	0.90827700
C	-5.43822800	-0.65717600	-0.42162000
H	-6.11344700	-1.40813900	-0.80756600
N	-4.80473500	1.30387000	0.17696100
N	-5.84296700	0.62984600	-0.34841300
H	-4.86222900	2.30475900	0.29913500

^{2}T1-TS2

Zero-point correction= 0.384372 (Hartree/Particle)
Thermal correction to Energy= 0.412926
Thermal correction to Enthalpy= 0.413870
Thermal correction to Gibbs Free Energy= 0.325908
Sum of electronic and zero-point Energies= -2073.054892
Sum of electronic and thermal Energies= -2073.026339
Sum of electronic and thermal Enthalpies= -2073.025394
Sum of electronic and thermal Free Energies= -2073.113356

C	-3.14961300	-0.54555100	-1.91851300
C	-3.97033100	0.12668200	-2.89936200
C	-3.75118500	1.46036200	-2.73873200
C	0.74694000	1.93201300	2.46229700
C	-2.28398500	-2.59353300	-0.83591500
C	0.07380100	-2.82047400	1.79985500
C	-1.39383000	2.98937300	-0.16306300
C	-2.20991100	-4.03046900	-0.69582900
C	-0.10300500	4.02772600	1.36235700
C	-2.31158900	2.81347200	-1.18924600
C	-0.01836200	2.59269400	1.49372800
C	0.85720400	0.56183500	2.60494600
C	1.59552500	-0.12478000	3.62753300
C	-3.07920600	-1.92797300	-1.75882200
C	1.41042500	-1.46259000	3.43223800
C	-0.85005500	-2.98845300	0.76538000
C	0.55072700	-1.61674100	2.29048000
C	-1.31680800	-4.27665000	0.29992400
C	-2.79894000	1.59462500	-1.65947200
C	-0.95552700	4.27379900	0.32880700
Fe	-1.14332400	-0.00105900	0.31144900
H	-2.69412400	3.71168100	-1.66528600
H	-4.61730500	-0.37094900	-3.61040800
H	-2.77169200	-4.73926600	-1.29068100
H	1.80285800	-2.28278300	4.02001000
H	0.42735500	4.73788100	1.98352000
H	0.42636000	-3.72274700	2.29127100
H	-3.77519700	-0.47342400	1.21208400
H	-3.69090900	-2.53585100	-2.41902100
H	-0.99209700	-5.23064300	0.69543800
H	-1.27227800	5.22881600	-0.07032000
H	2.17085700	0.36444900	4.40308300
H	-4.18162200	2.28687000	-3.28958700
H	1.28890800	2.55133300	3.17059400
N	-2.45101400	0.36548900	-1.17589800
N	-0.79449700	1.97894000	0.55198700
N	0.25385700	-0.36780300	1.75202900
N	-1.45292200	-1.98463200	0.06806800
O	0.22289600	-0.13949700	-1.06308000
S	-2.75593800	0.04823200	1.93070800
C	1.51562900	-0.12841500	-0.71507800
H	1.48050500	-0.32910900	0.45413100
C	3.57458700	-0.97904600	-1.27802000
C	4.24666800	0.27153800	-1.28439800
C	3.47696600	1.49522200	-1.06163600
H	1.50643700	1.96558200	-0.72861000
O	3.90893800	2.63951100	-1.08212000
N	2.29582600	-1.24277000	-1.08496000
N	2.13998800	1.18416600	-0.85779000
C	5.58329400	-0.03016900	-1.55726100
H	6.42533200	0.64065200	-1.65298400
N	4.55541500	-1.91059900	-1.53431400
N	5.76181100	-1.35478100	-1.71524600
H	4.43759600	-2.90981600	-1.63094500

^{2}T1-PC

Zero-point correction= 0.391501 (Hartree/Particle)
Thermal correction to Energy= 0.420803
Thermal correction to Enthalpy= 0.421748
Thermal correction to Gibbs Free Energy= 0.330436
Sum of electronic and zero-point Energies= -2073.178427
Sum of electronic and thermal Energies= -2073.149124
Sum of electronic and thermal Enthalpies= -2073.148180
Sum of electronic and thermal Free Energies= -2073.239492

C	-3.10310900	1.15454000	1.63952600
C	-4.05500800	0.77931700	2.66119400
C	-4.05415200	-0.57932900	2.71825000
C	0.39918900	-2.46138100	-2.15539500
C	-1.83885200	2.85814500	0.37335300
C	0.57313400	2.38538500	-2.17612900
C	-1.91012900	-2.81113300	0.51231700
C	-1.52633900	4.23438500	0.06458600
C	-0.75687100	-4.22218000	-0.80765000
C	-2.80785200	-2.36731900	1.47500600
C	-0.47090600	-2.84663400	-1.14299200
C	0.71741000	-1.15185700	-2.49532700
C	1.62259500	-0.76996700	-3.54674500
C	-2.78261300	2.46618900	1.31431700
C	1.68093200	0.59678700	-3.54805600
C	-0.30960100	2.82290300	-1.19680300
C	0.80847200	1.05436800	-2.49979200
C	-0.57598800	4.21271300	-0.90786300
C	-3.10523300	-1.03483200	1.72829300
C	-1.64708900	-4.19988000	0.22076800
Fe	-1.21574400	0.00405100	-0.41550100
H	-3.32693400	-3.11902400	2.06174500
H	-4.63190000	1.47967100	3.25185900
H	-1.98772800	5.09146800	0.53854700
H	2.23984300	1.24446800	-4.21218400
H	-0.32351800	-5.07971700	-1.30674200
H	1.09535900	3.14182200	-2.75403900
H	-3.66834300	-0.79956900	-1.41126300
H	-3.30911500	3.25280600	1.84630600
H	-0.09440700	5.04758300	-1.40100000
H	-2.09828900	-5.03489900	0.74157600
H	2.12661900	-1.46364600	-4.20832200
H	-4.63057600	-1.22924000	3.36435500
H	0.86634300	-3.25211900	-2.73475000
N	-2.54287100	0.03534700	1.08037700
N	-1.17605200	-2.00089800	-0.31940000
N	0.24910800	-0.02671000	-1.84277800
N	-1.07721900	2.01322000	-0.39399000
O	0.25516200	0.00105900	1.36316700
S	-2.78695600	0.04731800	-1.99083000
C	1.48955900	-0.00367800	1.41878400
H	1.74599000	-0.04837800	-0.59339500
C	3.63194700	-0.03796200	0.38679700
C	4.32264600	-0.01163800	1.59279800
C	3.58850700	0.02114600	2.84028200
H	1.59863000	0.04590000	3.44738100
O	4.02302200	0.04667500	3.97652200
N	2.26892500	-0.03737500	0.28528000
N	2.17629600	0.02186900	2.61422100
C	5.69084400	-0.02477500	1.20649500
H	6.56324600	-0.01224600	1.84507600
N	4.54673100	-0.06421800	-0.60020300
N	5.83094300	-0.05606300	-0.10838700
H	4.38995500	-0.08525900	-1.59827000

^{4}T1-RC

Zero-point correction= 0.388695 (Hartree/Particle)
Thermal correction to Energy= 0.418706
Thermal correction to Enthalpy= 0.419651
Thermal correction to Gibbs Free Energy= 0.322735
Sum of electronic and zero-point Energies= -2073.077745
Sum of electronic and thermal Energies= -2073.047734
Sum of electronic and thermal Enthalpies= -2073.046790
Sum of electronic and thermal Free Energies= -2073.143705

C	0.34030700	-1.25013400	2.36850300
C	0.79855500	-2.52257500	2.86569400
C	0.17962000	-3.47901500	2.12073400
C	-3.65457300	0.03151400	-2.36203700
C	0.33482600	1.21977400	2.39770700
C	-1.49926800	3.42218900	0.32806400
C	-2.27931200	-2.77255500	-0.69126400
C	0.77214400	2.48193000	2.94000500
C	-3.72062900	-2.47162800	-2.39342200
C	-1.46191900	-3.41439200	0.22586900
C	-3.27076800	-1.20583900	-1.86932900
C	-3.25820600	1.26201000	-1.85167000
C	-3.71072000	2.53708400	-2.35099300
C	0.75284300	-0.02073200	2.86435800
C	-3.11457600	3.49155500	-1.58601100
C	-0.68152700	2.77666800	1.25057900
C	-2.29202900	2.79893400	-0.62522900
C	0.13707400	3.45223800	2.22752600
C	-0.65394400	-2.78637000	1.16961700
C	-3.10887300	-3.44188200	-1.66242700
Fe	-1.36133600	0.00794700	0.18178300
H	-1.45153300	-4.50007100	0.20799600
H	1.50755200	-2.64661200	3.67356500
H	1.47562600	2.58989900	3.75498700
H	-3.21060200	4.56768400	-1.65175100
H	-4.41629700	-2.58335200	-3.21509800
H	-1.51225100	4.50772200	0.35151800
H	-3.35329200	-1.32394200	2.01875700
H	1.47944200	-0.02912200	3.66913200
H	0.20475200	4.52683600	2.33789200
H	-3.19597800	-4.51643400	-1.75953100
H	-4.40062400	2.66536900	-3.17507600
H	0.26869200	-4.55534100	2.19272200
H	-4.33893700	0.04042200	-3.20487300
N	-0.54721900	-1.43070000	1.33810200
N	-2.40179600	-1.40668900	-0.82026000
N	-2.39751100	1.44022800	-0.79891000
N	-0.54663600	1.42014100	1.36996000
O	-0.10155700	0.02310500	-0.86348400
S	-3.44789300	-0.04599200	1.58775900
C	3.00555300	0.05323700	-2.23569600
H	2.12371800	0.07412000	-2.87063200
C	5.18329300	0.02971200	-1.84750000
C	5.04897800	-0.00367500	-0.45198200
C	3.72642600	-0.00933100	0.12565500
H	1.75455200	0.02103400	-0.62145600
O	3.40992700	-0.03654100	1.31006800
N	4.19194200	0.05903900	-2.78288500
N	2.74494700	0.02229100	-0.89922900
C	6.37929600	-0.02436300	0.03890900
H	6.71887400	-0.05170000	1.06537300
N	6.51593800	0.02693900	-2.09256300
N	7.26192300	-0.00582300	-0.95119200
H	6.97384400	0.04614000	-2.99182400

^{4}T1-TS1

Zero-point correction= 0.387693 (Hartree/Particle)
Thermal correction to Energy= 0.416649
Thermal correction to Enthalpy= 0.417593
Thermal correction to Gibbs Free Energy= 0.327125
Sum of electronic and zero-point Energies= -2073.041460
Sum of electronic and thermal Energies= -2073.012504
Sum of electronic and thermal Enthalpies= -2073.011560
Sum of electronic and thermal Free Energies= -2073.102028

C	-0.40612100	-2.24139500	-1.95801800
C	-0.39252800	-3.67268000	-2.15056800
C	0.63498600	-4.15913500	-1.40469600
C	3.13991500	1.34562400	1.84279500
C	-1.26458300	0.01358000	-2.48901100
C	-0.12451000	3.12778700	-1.25591000
C	2.85212200	-2.04141000	0.84023800
C	-2.14053800	0.90279300	-3.21542300
C	4.11575100	-0.91122400	2.32122100
C	2.31005300	-3.10981500	0.13848500
C	3.20412500	-0.02636000	1.63678500
C	2.32000400	2.22823900	1.14781300
C	2.33243800	3.66234200	1.30511800
C	-1.27924000	-1.37392000	-2.59840800
C	1.43109300	4.16269300	0.41519800
C	-0.71549200	2.05393700	-1.90563000
C	0.85856400	3.03591000	-0.27948200
C	-1.79229500	2.17073000	-2.85873200
C	1.24107300	-3.02708500	-0.74410800
C	3.90358200	-2.15867900	1.82116900
Fe	0.96468700	-0.02818500	-0.41029800
H	2.73214600	-4.09300800	0.32179000
H	-1.08282800	-4.21395800	-2.78473600
H	-2.89999600	0.58149600	-3.91721000
H	1.16493200	5.19618100	0.23405500
H	4.82343100	-0.59876700	3.07850900
H	-0.47490500	4.12174600	-1.51608800
H	3.55914200	0.71956400	-1.44362900
H	-2.01903200	-1.81289200	-3.26075000
H	-2.21268900	3.10834100	-3.19972400
H	4.39668700	-3.08528200	2.08560400
H	2.96249300	4.20001100	2.00219600
H	0.96349800	-5.18445100	-1.29351100
H	3.81121700	1.76886200	2.58387200
N	0.59417700	-1.87195100	-1.09408300
N	2.44391600	-0.73514700	0.73703100
N	1.41289400	1.86651700	0.18410900
N	-0.40702800	0.73243500	-1.70429000
O	-0.19657700	-0.24103200	0.82155800
S	2.47586200	0.42367000	-2.19657200
C	-1.33190700	0.88520600	1.75159400
H	-0.54294900	1.59765800	1.96363400
C	-3.35024900	0.51164600	0.84982500
C	-3.72715000	-0.46721200	1.79565200
C	-2.82846500	-0.74707900	2.89857700
H	-0.97313900	-0.13162100	3.51224200
O	-2.97632200	-1.54605300	3.81126000
N	-2.23668900	1.24954400	0.81234600
N	-1.69091700	0.08771500	2.83130900
C	-4.98582100	-0.92597200	1.36556000
H	-5.62168000	-1.67733400	1.81314700
N	-4.38210400	0.57166400	-0.04101900
N	-5.37799900	-0.30106700	0.25113700
H	-4.42137200	1.12512600	-0.88509400

^{4}T1-Int1

Zero-point correction= 0.389106 (Hartree/Particle)
Thermal correction to Energy= 0.418462
Thermal correction to Enthalpy= 0.419406
Thermal correction to Gibbs Free Energy= 0.327191
Sum of electronic and zero-point Energies= -2073.066544
Sum of electronic and thermal Energies= -2073.037188
Sum of electronic and thermal Enthalpies= -2073.036244
Sum of electronic and thermal Free Energies= -2073.128459

C	1.49616300	-2.76611700	1.08316000
C	1.59061200	-3.54504200	2.29457100
C	1.48576400	-2.67259300	3.33280900
C	0.41738200	3.42820100	0.36194000
C	1.60662500	-2.54098000	-1.36296300
C	1.38627300	0.41739200	-3.31103600
C	0.91837200	1.05865000	2.95575200
C	1.81392500	-3.08635600	-2.67934600
C	0.40915400	3.25042900	2.85568400
C	1.14331000	-0.19823200	3.49701100
C	0.55616700	2.69818400	1.53345700
C	0.60665300	2.91880600	-0.91596600
C	0.58483000	3.70575800	-2.12242400
C	1.61426800	-3.28994700	-0.19469700
C	0.88672000	2.86378000	-3.15037500
C	1.53701500	-0.85389000	-2.77512200
C	1.07924500	1.55594400	-2.58043300
C	1.77922000	-2.04147400	-3.55245700
C	1.31405500	-1.35947400	2.75886900
C	0.64217800	2.23805800	3.73562500
Fe	1.09652000	0.08138600	0.08807800
H	1.15318200	-0.28345400	4.57874200
H	1.72792600	-4.61836200	2.32427300
H	1.96874100	-4.13679100	-2.88977700
H	0.97204500	3.09129000	-4.20519200
H	0.15607600	4.28200800	3.06383200
H	1.49772900	0.52533000	-4.38501500
H	3.35888500	1.64814500	0.65976900
H	1.75771900	-4.36151400	-0.28784900
H	1.89519200	-2.05659600	-4.62855000
H	0.61743200	2.26490200	4.81741400
H	0.37495000	4.76704200	-2.15841200
H	1.51345200	-2.87859900	4.39511800
H	0.17687300	4.48235300	0.45257100
N	1.32041100	-1.44169500	1.39135700
N	0.87452900	1.36243400	1.61576900
N	0.88829300	1.60654400	-1.21781900
N	1.43621900	-1.18012500	-1.44286800
O	-0.71300700	-0.27633200	0.08952800
S	3.37750900	0.41944900	0.09803900
C	-1.62475000	-0.17725300	-0.96427400
H	-1.10423100	-0.11099100	-1.92459200
C	-3.58935300	-1.30655500	-0.45147900
C	-4.28003900	-0.14114000	-0.00443000
C	-3.63479900	1.16598600	-0.16039800
H	-1.88963700	1.90804100	-0.85377400
O	-4.11244700	2.23924400	0.19051500
N	-2.39282000	-1.41976500	-0.96955400
N	-2.42846600	1.04921100	-0.82407200
C	-5.51109500	-0.59184200	0.46003600
H	-6.32889900	-0.02241400	0.87922100
N	-4.47562900	-2.34254000	-0.22594900
N	-5.62895600	-1.93215100	0.32934500
H	-4.31592700	-3.32603200	-0.39130900

^{4}T1-TS2

Zero-point correction= 0.382729 (Hartree/Particle)
Thermal correction to Energy= 0.412159
Thermal correction to Enthalpy= 0.413103
Thermal correction to Gibbs Free Energy= 0.321362
Sum of electronic and zero-point Energies= -2073.048915
Sum of electronic and thermal Energies= -2073.019485
Sum of electronic and thermal Enthalpies= -2073.018541
Sum of electronic and thermal Free Energies= -2073.110282

C	-3.13554100	-1.11592900	-1.75768400
C	-4.12939600	-0.68892400	-2.71364900
C	-4.15304800	0.67145800	-2.67216200
C	0.53340000	2.35039800	2.09075600
C	-1.90662500	-2.87016700	-0.53000300
C	0.56313600	-2.49034000	1.99936400
C	-1.98198200	2.79760100	-0.38403200
C	-1.59902300	-4.25206800	-0.26356200
C	-0.74106700	4.15726000	0.91253500
C	-2.90402400	2.39128000	-1.33907000
C	-0.42185700	2.77451800	1.16425200
C	0.88471300	1.03900800	2.34710800
C	1.75834400	0.59671800	3.39481900
C	-2.82792300	-2.44154900	-1.47541300
C	1.76169700	-0.76954400	3.37514700
C	-0.37064500	-2.88707400	1.04036700
C	0.89293700	-1.18587700	2.31280300
C	-0.64932000	-4.26283100	0.71322200
C	-3.17221800	1.07420800	-1.69243400
C	-1.70796800	4.17103300	-0.04816000
Fe	-1.18888000	-0.04981000	0.32323700
H	-3.46429900	3.16826700	-1.84979800
H	-4.72516900	-1.35594800	-3.32342600
H	-2.05742000	-5.09286700	-0.76811000
H	2.29104700	-1.44425400	4.03591800
H	-0.27259600	4.99697400	1.40946900
H	1.05392000	-3.27718100	2.56402700
H	-2.90315100	-1.32812800	2.29031900
H	-3.35651700	-3.20639800	-2.03584600
H	-0.16527900	-5.11457600	1.17370400
H	-2.19815700	5.02465900	-0.49826300
H	2.28375400	1.25533400	4.07456600
H	-4.77219300	1.35327100	-3.24091500
H	1.01854100	3.11951200	2.68365000
N	-2.55789000	-0.02795200	-1.16012600
N	-1.18753300	1.96262700	0.36809200
N	0.41353000	-0.06501900	1.63061300
N	-1.15306900	-2.05559400	0.28327100
O	0.24825500	0.00040400	-1.23671300
S	-2.78587800	0.00744700	2.11966600
C	1.52526700	0.03018100	-0.92449900
H	1.48025100	-0.08059600	0.27563600
C	3.62718600	-0.85496500	-1.22737000
C	4.29548700	0.39442700	-1.27895800
C	3.50986000	1.62662200	-1.24319100
H	1.51989400	2.11814400	-1.14559800
O	3.94204200	2.76986300	-1.31619500
N	2.33078200	-1.11581700	-1.14111500
N	2.15686200	1.32983900	-1.15540900
C	5.65496400	0.08134900	-1.39044700
H	6.50027600	0.75147500	-1.46184000
N	4.62719000	-1.79484100	-1.29905900
N	5.85202700	-1.24694500	-1.41362600
H	4.51822900	-2.79876600	-1.32596600

^{4}T1-PC

Zero-point correction= 0.390063 (Hartree/Particle)
Thermal correction to Energy= 0.420479
Thermal correction to Enthalpy= 0.421423
Thermal correction to Gibbs Free Energy= 0.324396
Sum of electronic and zero-point Energies= -2073.179926
Sum of electronic and thermal Energies= -2073.149511
Sum of electronic and thermal Enthalpies= -2073.148566
Sum of electronic and thermal Free Energies= -2073.245593

C	-3.18281200	0.58371200	2.00217600
C	-4.06522600	-0.08973100	2.92346900
C	-4.02424500	-1.41169700	2.60934000
C	0.43278800	-1.82499100	-2.59821000
C	-2.09036900	2.60649300	1.13879200
C	0.32085700	2.87960700	-1.44427200
C	-1.93852000	-2.89062600	-0.18761700
C	-1.83415300	4.02162000	1.17726000
C	-0.69824500	-3.89036800	-1.77636100
C	-2.81930100	-2.74760400	0.87469600
C	-0.46696800	-2.47055900	-1.76369800
C	0.70957200	-0.46619500	-2.56420700
C	1.62215200	0.20299200	-3.45057800
C	-2.95710700	1.95011700	2.00016200
C	1.59194300	1.53131000	-3.12298800
C	-0.60380600	3.02627700	-0.42159300
C	0.66060800	1.67252000	-2.03728200
C	-0.91239700	4.28223300	0.20929000
C	-3.11779000	-1.54570100	1.49506900
C	-1.60962700	-4.15083100	-0.79806400
Fe	-1.47288400	0.10243200	-0.47195300
H	-3.29875800	-3.64430400	1.25378100
H	-4.63031900	0.40292900	3.70416700
H	-2.30138100	4.71178400	1.86784600
H	2.12600500	2.35117100	-3.58706600
H	-0.20862300	-4.58629700	-2.44547100
H	0.81198800	3.77570800	-1.80975200
H	-3.41337000	-0.75133100	-2.37508700
H	-3.48472000	2.54975400	2.73473300
H	-0.46571500	5.23081900	-0.05966900
H	-2.02351400	-5.10504300	-0.49838700
H	2.18656800	-0.28368400	-4.23630200
H	-4.54861500	-2.23489800	3.07728400
H	0.96003500	-2.42792100	-3.33055000
N	-2.60826700	-0.31983200	1.14067500
N	-1.24036200	-1.86776600	-0.79210800
N	0.14735200	0.43881500	-1.68307400
N	-1.33603800	2.00847300	0.15353000
O	0.82206500	-0.58901800	2.27887100
S	-3.19153700	0.54132800	-2.04666400
C	1.98121600	-0.47744900	1.91181900
H	1.54568800	0.03688900	-0.03740900
C	3.63070300	-0.00986000	0.23690300
C	4.70513800	-0.22694800	1.09301500
C	4.46422600	-0.59901600	2.47132000
H	2.83115000	-0.94664400	3.69874600
O	5.28189900	-0.82415000	3.34687600
N	2.31765700	-0.12371000	0.60713000
N	3.07150900	-0.68959500	2.74825200
C	5.84767200	0.00355400	0.28050100
H	6.88914700	-0.06059100	0.56428900
N	4.13895000	0.31850300	-0.96651800
N	5.51467600	0.33100500	-0.95722200
H	3.63610100	0.53810800	-1.81801200

^{2}T2-RC

Zero-point correction= 0.388545 (Hartree/Particle)
Thermal correction to Energy= 0.418636
Thermal correction to Enthalpy= 0.419580
Thermal correction to Gibbs Free Energy= 0.322104
Sum of electronic and zero-point Energies= -2073.070208
Sum of electronic and thermal Energies= -2073.040117
Sum of electronic and thermal Enthalpies= -2073.039173
Sum of electronic and thermal Free Energies= -2073.136649

C	-0.32559700	1.24589400	2.38341300
C	-0.78173900	2.51776900	2.88343000
C	-0.17052700	3.47459100	2.13263000
C	3.63026700	-0.02783200	-2.38182700
C	-0.30806300	-1.22293000	2.41759400
C	1.51683400	-3.42244500	0.33525800
C	2.26134300	2.77397100	-0.70319100
C	-0.72989800	-2.48592000	2.96925800
C	3.67907400	2.47563100	-2.42530600
C	1.45176200	3.41315400	0.22246900
C	3.24619100	1.20903700	-1.88851200
C	3.24395500	-1.25866500	-1.86483900
C	3.69346900	-2.53272600	-2.37013500
C	-0.72978800	0.01594400	2.88420400
C	3.10901600	-3.48892100	-1.59855700
C	0.70746000	-2.77740500	1.26543600
C	2.29672700	-2.79823500	-0.62755500
C	-0.09546600	-3.45452700	2.25369700
C	0.65604800	2.78280800	1.17489700
C	3.07141900	3.44494000	-1.68972900
Fe	1.35720900	-0.01085900	0.18437400
H	1.43462700	4.49869900	0.20228200
H	-1.48378800	2.64135100	3.69743900
H	-1.42248900	-2.59601800	3.79330500
H	3.20607100	-4.56482000	-1.66644200
H	4.36060700	2.58841800	-3.25860400
H	1.53296900	-4.50787700	0.36045900
H	3.37931700	1.34552300	2.00241100
H	-1.44912100	0.02262800	3.69562000
H	-0.15367100	-4.52914400	2.36925700
H	3.14847700	4.51960700	-1.79384600
H	4.37286300	-2.65890200	-3.20323200
H	-0.26060800	4.55085900	2.20441000
H	4.30293700	-0.03613300	-3.23401200
N	0.55348500	1.42681800	1.34608200
N	2.39335400	1.40870200	-0.82628000
N	2.39763200	-1.43940300	-0.80099600
N	0.56498900	-1.42090800	1.38143500
O	0.11088200	-0.01809000	-0.87203800
S	3.48649400	0.06942100	1.56872300
C	-3.03656000	-0.07373300	-2.25863400
H	-2.15404400	-0.10247700	-2.89336600
C	-5.23846200	-0.05329300	-1.87935100
C	-5.04726200	0.00680800	-0.46398600
C	-3.71480600	0.02846000	0.10716000
H	-1.75991400	-0.00782400	-0.64826200
O	-3.41055400	0.07838400	1.29549400
N	-4.21420400	-0.09458600	-2.79976100
N	-2.75227200	-0.01677600	-0.91339800
C	-6.32564100	0.03206500	0.06995100
H	-6.68517500	0.07618600	1.08751200
N	-6.53629100	-0.06455900	-2.20328100
N	-7.15486400	-0.01187100	-0.99781700
H	-8.16435800	-0.00937700	-0.98440500

^{2}T2-TS1

Zero-point correction= 0.386854 (Hartree/Particle)
Thermal correction to Energy= 0.416160
Thermal correction to Enthalpy= 0.417104
Thermal correction to Gibbs Free Energy= 0.325467
Sum of electronic and zero-point Energies= -2073.031318
Sum of electronic and thermal Energies= -2073.002012
Sum of electronic and thermal Enthalpies= -2073.001068
Sum of electronic and thermal Free Energies= -2073.092705

C	0.50640800	-1.66604600	2.47837300
C	0.66619700	-3.02787800	2.92917300
C	-0.18593600	-3.78595600	2.18580800
C	-3.10119300	0.66719500	-2.13717900
C	1.06615800	0.74462500	2.58853200
C	-0.31074100	3.40463100	0.71847600
C	-2.43007700	-2.43735900	-0.57589100
C	1.76837600	1.85448100	3.19060300
C	-3.72640500	-1.75959400	-2.28655000
C	-1.79716200	-3.27629400	0.33079400
C	-3.00846100	-0.64916300	-1.70501000
C	-2.45898000	1.76148900	-1.56791000
C	-2.65004300	3.12701200	-1.98952100
C	1.20539400	-0.57729600	2.99156700
C	-1.88354400	3.90347900	-1.17406200
C	0.36897600	2.54783000	1.57586200
C	-1.21361500	3.01145400	-0.26220700
C	1.32918800	2.97736500	2.56479800
C	-0.85881200	-2.88376600	1.28192600
C	-3.37165500	-2.86801500	-1.58257800
Fe	-0.92277300	0.05189600	0.42520300
H	-2.04066200	-4.33363300	0.28265700
H	1.34437900	-3.34389500	3.71148800
H	2.49545700	1.76406700	3.98709700
H	-1.77018000	4.97995300	-1.17852300
H	-4.41100200	-1.68141200	-3.12149800
H	-0.10738400	4.46721300	0.81089300
H	-3.15789100	-0.89891600	2.13314700
H	1.91685300	-0.77787200	3.78717200
H	1.62062500	4.00562900	2.73518400
H	-3.70156500	-3.88968600	-1.72114100
H	-3.29917200	3.43591300	-2.79894300
H	-0.35215100	-4.85477500	2.22832800
H	-3.76137400	0.86661900	-2.97629100
N	-0.43082900	-1.59874600	1.48428700
N	-2.23186000	-1.08015700	-0.65786900
N	-1.57440000	1.70907100	-0.51545600
N	0.22406000	1.18783900	1.60348900
O	0.29883500	-0.33495900	-0.72688500
S	-2.91962200	0.39074100	1.80563800
C	1.37923000	0.77282300	-1.69307300
H	0.59109700	1.47891000	-1.93052300
C	3.42626300	0.44173800	-0.77990500
C	3.75947800	-0.56798600	-1.74029700
C	2.84521000	-0.88885000	-2.82586200
H	0.98289100	-0.30689400	-3.41819800
O	2.99905400	-1.72589100	-3.70509500
N	2.28084500	1.16943900	-0.77905700
N	1.72298400	-0.05723200	-2.77291000
C	5.00434200	-1.02766200	-1.36659800
H	5.65408400	-1.78147900	-1.78652400
N	4.41017300	0.59615300	0.12911700
N	5.33614100	-0.30584400	-0.26358100
H	6.18755800	-0.37729100	0.27431300

^{2}T2-Int

Zero-point correction= 0.387901 (Hartree/Particle)
Thermal correction to Energy= 0.417192
Thermal correction to Enthalpy= 0.418136
Thermal correction to Gibbs Free Energy= 0.327087
Sum of electronic and zero-point Energies= -2073.055734
Sum of electronic and thermal Energies= -2073.026444
Sum of electronic and thermal Enthalpies= -2073.025499
Sum of electronic and thermal Free Energies= -2073.116548

C	0.49903500	1.68766600	2.51037200
C	0.91521900	1.53192700	3.88492400
C	0.41476100	0.33931900	4.30805700
C	-2.80837400	-2.18471300	-1.19053200
C	0.41787700	2.98270000	0.39336500
C	-1.17792300	2.13279100	-2.64186300
C	-1.63921000	-2.02873100	2.14137600
C	0.74075100	4.15540700	-0.38377200
C	-2.79585800	-3.52857600	0.92970500
C	-0.96279900	-1.45113200	3.21049300
C	-2.46206000	-2.36156400	0.14476800
C	-2.53813000	-1.06536000	-1.97218900
C	-2.97130800	-0.89928500	-3.33844600
C	0.80188100	2.79060100	1.71702800
C	-2.52555300	0.32056000	-3.74809000
C	-0.47868500	2.69254000	-1.57530700
C	-1.81417200	0.89550500	-2.63374500
C	0.18133000	3.97549500	-1.61045800
C	-0.30137900	-0.22504000	3.18798500
C	-2.28793500	-3.31937400	2.17370200
Fe	-0.99955700	0.31087100	0.26814200
H	-0.93589500	-2.01061700	4.14108200
H	1.51074800	2.24897300	4.43517200
H	1.32345400	4.99314400	-0.02326800
H	-2.65546800	0.79768900	-4.71098500
H	-3.34742400	-4.38373200	0.56072600
H	-1.22622600	2.70963700	-3.56090600
H	-3.23096900	2.12784800	-0.07801700
H	1.39568900	3.57669400	2.17414300
H	0.20655800	4.63452100	-2.46871600
H	-2.33330200	-3.96722500	3.03963400
H	-3.54507100	-1.62863800	-3.89582300
H	0.51227200	-0.12891200	5.27909200
H	-3.36449400	-2.98888800	-1.66394000
N	-0.23877900	0.60981400	2.10814400
N	-1.76335000	-1.45933600	0.90283100
N	-1.83572500	0.04013900	-1.55726500
N	-0.32364100	2.10323800	-0.34764900
O	0.54512300	-0.64165200	-0.19144500
S	-3.10289000	1.19290700	0.89058400
C	1.33649800	-0.40167500	-1.30529300
H	0.77514800	0.08194200	-2.11320500
C	3.56014800	-0.07734700	-0.61391700
C	3.88359400	-1.46656300	-0.80951400
C	2.92390400	-2.37974600	-1.44002100
H	1.04653300	-2.30750000	-2.15734200
O	3.11360200	-3.57529600	-1.64142700
N	2.40804400	0.51404600	-0.91689300
N	1.79724100	-1.70026700	-1.84663300
C	5.16647000	-1.61023300	-0.35650600
H	5.82548100	-2.46500500	-0.30962300
N	4.61971100	0.59293700	-0.06570300
N	5.55026200	-0.36419400	0.07077000
H	6.44307500	-0.10919200	0.46797900

^{2}T2-TS2

Zero-point correction= 0.384175 (Hartree/Particle)
Thermal correction to Energy= 0.412814
Thermal correction to Enthalpy= 0.413759
Thermal correction to Gibbs Free Energy= 0.324683
Sum of electronic and zero-point Energies= -2073.047200
Sum of electronic and thermal Energies= -2073.018561
Sum of electronic and thermal Enthalpies= -2073.017616
Sum of electronic and thermal Free Energies= -2073.106692

C	2.68041400	1.79680200	-1.66390200
C	3.65752300	1.72096200	-2.72612000
C	3.99411900	0.40775300	-2.85066800
C	0.13810300	-2.77174700	1.85918900
C	1.13221900	3.09488300	-0.22442200
C	-0.94174000	1.91980200	2.39713300
C	2.50541000	-2.40245600	-0.75436400
C	0.55158200	4.34617900	0.20861000
C	1.66689400	-4.13726500	0.40689200
C	3.26054200	-1.68891900	-1.67730200
C	1.08401900	-2.88564900	0.83607500
C	-0.43949800	-1.60091100	2.31977200
C	-1.32061300	-1.49486600	3.45086200
C	2.07625500	2.97905200	-1.23245800
C	-1.61479300	-0.17284900	3.61647300
C	-0.22696700	2.61758900	1.41741700
C	-0.92426600	0.55021900	2.58479500
C	-0.29137400	4.04988200	1.23345400
C	3.21847600	-0.31006400	-1.86577700
C	2.55316200	-3.83554900	-0.58156800
Fe	1.13695600	0.11771900	0.32565000
H	3.93479000	-2.25618200	-2.31246700
H	4.02329100	2.56857500	-3.29150200
H	0.77514900	5.31263300	-0.22473400
H	-2.23674200	0.28388100	4.37577600
H	1.42044900	-5.10729100	0.81961000
H	-1.55377700	2.50708300	3.07510900
H	3.79382700	-0.13027600	1.25582300
H	2.37679100	3.89486300	-1.73318300
H	-0.90876100	4.72042000	1.81721600
H	3.18465200	-4.50645700	-1.14993600
H	-1.65268400	-2.33293900	4.05046700
H	4.69281800	-0.04842900	-3.54034000
H	-0.14541400	-3.68950400	2.36639500
N	2.43247800	0.55597700	-1.15471100
N	1.60651800	-1.84754900	0.12006400
N	-0.23688300	-0.34101300	1.76073200
N	0.63419500	2.05783400	0.52476300
O	-0.19500100	-0.12868200	-1.05574300
S	2.72856000	0.31296900	1.96046900
C	-1.49186700	-0.23594700	-0.72998600
H	-1.47168100	-0.33639700	0.45040900
C	-3.60581200	0.67272700	-1.01534900
C	-4.19155800	-0.58954600	-1.37885500
C	-3.36499300	-1.79110700	-1.52178100
H	-1.37206100	-2.23959500	-1.33399100
O	-3.75607900	-2.89710700	-1.87261200
N	-2.30970700	0.90531600	-0.78361000
N	-2.04958500	-1.49239500	-1.23222200
C	-5.52742500	-0.33066400	-1.55366000
H	-6.35795000	-0.96124700	-1.83462000
N	-4.55244400	1.65138700	-0.96448400
N	-5.67389500	1.00637200	-1.29713400
H	-6.53348900	1.53760000	-1.33813300

^{2}T2-PC

Zero-point correction= 0.391550 (Hartree/Particle)
Thermal correction to Energy= 0.420959
Thermal correction to Enthalpy= 0.421904
Thermal correction to Gibbs Free Energy= 0.329199
Sum of electronic and zero-point Energies= -2073.180822
Sum of electronic and thermal Energies= -2073.151413
Sum of electronic and thermal Enthalpies= -2073.150468
Sum of electronic and thermal Free Energies= -2073.243173

C	-3.16056600	0.53919100	-1.85825300
C	-3.92576000	1.63373700	-2.41050200
C	-3.62907500	2.73434100	-1.66773500
C	0.65074100	0.39481400	3.15860500
C	-2.37431800	-1.80180700	-1.91411600
C	-0.07126000	-3.40799200	0.24235700
C	-1.26743300	2.73507600	1.30946300
C	-2.35653200	-3.12001000	-2.50531100
C	-0.00139700	2.81133500	3.16870600
C	-2.14353200	3.14349000	0.31190500
C	-0.02206800	1.48036700	2.60977100
C	0.68486100	-0.88790600	2.62549300
C	1.39680600	-2.00016400	3.20165500
C	-3.15000300	-0.74825800	-2.38017400
C	1.21389400	-3.06389300	2.36827000
C	-0.96019000	-3.00057200	-0.74458800
C	0.38325500	-2.60881900	1.28375600
C	-1.47534700	-3.86265200	-1.78260400
C	-2.68883200	2.31040700	-0.65657600
C	-0.76898500	3.59076300	2.35872800
Fe	-1.23508700	-0.16445400	0.36516800
H	-2.44451700	4.18677000	0.30483100
H	-4.59035200	1.55244200	-3.26145900
H	-2.94822700	-3.41867900	-3.36150000
H	1.59429900	-4.07224700	2.47155800
H	0.53577800	3.09367900	4.06546800
H	0.25931100	-4.44208400	0.22370700
H	-3.52595900	0.40851100	1.80821900
H	-3.78893500	-0.94256400	-3.23643900
H	-1.19387900	-4.89926900	-1.91858100
H	-0.99554500	4.64531100	2.45339000
H	1.96177900	-1.95777900	4.12422500
H	-4.00042000	3.74529900	-1.77911300
H	1.19857100	0.56408100	4.08069500
N	-2.42066600	0.97128200	-0.78782500
N	-0.78988500	1.45631100	1.46972800
N	0.08662400	-1.27064000	1.44076400
N	-1.51003000	-1.74723600	-0.85007100
O	0.33642000	0.51471900	-1.12129400
S	-2.90462500	-0.78839300	1.70022500
C	1.56941900	0.52993800	-1.16728800
H	1.88879300	-0.50336900	0.55636900
C	3.74410500	0.01554500	-0.30687000
C	4.38078700	0.65586900	-1.39853200
C	3.61254700	1.28077700	-2.46072600
H	1.61207200	1.56168600	-2.91998800
O	4.03215800	1.85981800	-3.44660400
N	2.36881700	-0.03877400	-0.21218200
N	2.22444200	1.14596600	-2.22677600
C	5.73545100	0.50293300	-1.14056100
H	6.60812700	0.82463300	-1.68933200
N	4.59840800	-0.49834500	0.56627400
N	5.80888600	-0.17890700	0.02035400
H	6.64117400	-0.46926900	0.51210600

^{4}T2-RC

Zero-point correction= 0.388637 (Hartree/Particle)
Thermal correction to Energy= 0.418636
Thermal correction to Enthalpy= 0.419580
Thermal correction to Gibbs Free Energy= 0.321728
Sum of electronic and zero-point Energies= -2073.070016
Sum of electronic and thermal Energies= -2073.040016
Sum of electronic and thermal Enthalpies= -2073.039072
Sum of electronic and thermal Free Energies= -2073.136924

C	0.33678400	-1.25744100	2.36306100
C	0.79774600	-2.53114900	2.85453000
C	0.18113600	-3.48557300	2.10509000
C	-3.65687100	0.03685700	-2.36481800
C	0.32456100	1.21235800	2.40455000
C	-1.51491000	3.41999000	0.34485900
C	-2.27758900	-2.77164100	-0.70510100
C	0.75759800	2.47313800	2.95358600
C	-3.71650600	-2.46620700	-2.40846300
C	-1.45966800	-3.41585100	0.20977000
C	-3.27096400	-1.20180100	-1.87719400
C	-3.26445200	1.26587700	-1.84785200
C	-3.71899600	2.54224800	-2.34235800
C	0.74604300	-0.02929800	2.86472700
C	-3.12679400	3.49452500	-1.57179200
C	-0.69634300	2.77205100	1.26519100
C	-2.30450900	2.79933900	-0.61247100
C	0.11976400	3.44518400	2.24589600
C	-0.65381100	-2.79035000	1.15703400
C	-3.10365500	-3.43839600	-1.68110000
Fe	-1.36740200	0.00695800	0.18207500
H	-1.44627800	-4.50139100	0.18634400
H	1.50666500	-2.65735800	3.66215900
H	1.45974000	2.57926200	3.77002400
H	-3.22478200	4.57073400	-1.63313500
H	-4.40981100	-2.57563300	-3.23243300
H	-1.53039600	4.50537300	0.37322200
H	-3.35999600	-1.34150600	2.01044200
H	1.47209400	-0.03984900	3.67004900
H	0.18391900	4.51942900	2.36178200
H	-3.18726800	-4.51267900	-1.78405900
H	-4.40700400	2.67264000	-3.16768800
H	0.27258300	-4.56204200	2.17195100
H	-4.33915600	0.04807700	-3.20929700
N	-0.55033300	-1.43536300	1.33200200
N	-2.40354700	-1.40547600	-0.82743900
N	-2.40654900	1.44112800	-0.79253400
N	-0.55760000	1.41554200	1.37785900
O	-0.10751500	0.03069900	-0.86109100
S	-3.45880100	-0.06146300	1.58665000
C	3.03609200	0.08704800	-2.25279000
H	2.15067100	0.12080900	-2.88322000
C	5.23958500	0.05607900	-1.88398000
C	5.05478800	-0.00637800	-0.46785700
C	3.72500500	-0.02333100	0.10953000
H	1.76675500	0.02236700	-0.63703400
O	3.42636100	-0.07453300	1.29931100
N	4.21120400	0.10395900	-2.79943500
N	2.75789800	0.02855300	-0.90627600
C	6.33556500	-0.03862300	0.05997100
H	6.69971300	-0.08668200	1.07570800
N	6.53589300	0.06230300	-2.21400200
N	7.15989500	0.00402600	-1.01161100
H	8.16942500	-0.00302500	-1.00299100

^{4}T2-TS1

Zero-point correction= 0.387695 (Hartree/Particle)
Thermal correction to Energy= 0.416671
Thermal correction to Enthalpy= 0.417616
Thermal correction to Gibbs Free Energy= 0.326346
Sum of electronic and zero-point Energies= -2073.033042
Sum of electronic and thermal Energies= -2073.004065
Sum of electronic and thermal Enthalpies= -2073.003121
Sum of electronic and thermal Free Energies= -2073.094390

C	0.40195000	-1.97379800	2.28154100
C	0.49506100	-3.37906800	2.59953200
C	-0.38637500	-4.02455800	1.78910900
C	-3.04232500	0.93808700	-2.14388500
C	1.00080600	0.38852600	2.68618100
C	-0.25004500	3.26512300	1.05592500
C	-2.51545300	-2.32147600	-0.85770600
C	1.71802300	1.41357100	3.40855600
C	-3.72805700	-1.43817600	-2.53600100
C	-1.95558400	-3.27322600	-0.01590700
C	-2.98458500	-0.41563300	-1.84089900
C	-2.38524700	1.94883700	-1.45019400
C	-2.51244600	3.35764700	-1.72956500
C	1.11636400	-0.97499600	2.92984400
C	-1.74167200	4.01118700	-0.81572600
C	0.36320000	2.30862700	1.85192100
C	-1.13688700	3.00349500	0.01907700
C	1.31772200	2.60564200	2.89371800
C	-1.01001600	-3.01508100	0.96714800
C	-3.44298000	-2.61835800	-1.92176900
Fe	-0.98021500	-0.03585400	0.40526600
H	-2.25970400	-4.30559900	-0.15841100
H	1.14974500	-3.79629200	3.35397800
H	2.43184200	1.22353300	4.19957500
H	-1.58486800	5.07647500	-0.70441600
H	-4.38339400	-1.25624200	-3.37829500
H	-0.00668300	4.30501300	1.25046100
H	-3.70329900	0.61164800	1.12972400
H	1.80909700	-1.28390800	3.70663000
H	1.63579700	3.60262500	3.16976300
H	-3.81172800	-3.60852200	-2.15706100
H	-3.12179900	3.77614300	-2.52053200
H	-0.60457500	-5.08341300	1.73447700
H	-3.67693000	1.23514400	-2.97346600
N	-0.51726400	-1.77650700	1.28297400
N	-2.25005800	-0.97513400	-0.82139900
N	-1.54387200	1.75254300	-0.38386600
N	0.17962800	0.95387900	1.75133900
O	0.32535400	-0.21797800	-0.68397900
S	-2.69614600	0.38903300	2.00375700
C	1.45653700	0.98088200	-1.52130200
H	0.68323800	1.73033100	-1.64370000
C	3.50104700	0.46864300	-0.69285100
C	3.78500900	-0.42370900	-1.77935100
C	2.84701400	-0.56778500	-2.88124400
H	1.00264400	0.16326400	-3.36829500
O	2.95795400	-1.28196100	-3.86767000
N	2.38451800	1.22339800	-0.57453000
N	1.75322300	0.28754800	-2.69898300
C	5.01814800	-0.96671400	-1.49123300
H	5.63503400	-1.68240700	-2.01461100
N	4.50727600	0.47480000	0.20876500
N	5.39223200	-0.40014300	-0.31225700
H	6.24798500	-0.56941000	0.19653400

^{4}T2-Int

Zero-point correction= 0.387581 (Hartree/Particle)
Thermal correction to Energy= 0.416957
Thermal correction to Enthalpy= 0.417901
Thermal correction to Gibbs Free Energy= 0.325609
Sum of electronic and zero-point Energies= -2073.055362
Sum of electronic and thermal Energies= -2073.025986
Sum of electronic and thermal Enthalpies= -2073.025042
Sum of electronic and thermal Free Energies= -2073.117334

C	0.55408900	0.59283000	2.92305100
C	0.96399300	-0.07104700	4.13960800
C	0.40828400	-1.31265600	4.10913500
C	-2.89042700	-1.52474000	-1.90118000
C	0.50847400	2.58557600	1.43742500
C	-1.12931800	2.97461200	-1.66602900
C	-1.74410300	-2.63524800	1.25344100
C	0.86890500	3.95338100	1.14924900
C	-2.95169100	-3.54405900	-0.41154100
C	-1.05058700	-2.51786200	2.45253900
C	-2.55891800	-2.18907500	-0.72491300
C	-2.57860600	-0.20587500	-2.22017900
C	-3.00916400	0.46886900	-3.42061600
C	0.89616800	1.89851900	2.58597500
C	-2.52797600	1.74075700	-3.35059600
C	-0.41162900	3.08106300	-0.47669200
C	-1.79785600	1.83843900	-2.11121000
C	0.29327200	4.26369400	-0.04387500
C	-0.33263500	-1.39842600	2.87168300
C	-2.44987400	-3.81944800	0.82192400
Fe	-1.00873000	0.19117000	0.35328400
H	-1.05560100	-3.37926900	3.11425200
H	1.59142100	0.37030300	4.90321600
H	1.48564400	4.57631100	1.78397800
H	-2.64593500	2.54691400	-4.06324900
H	-3.53632200	-4.18325900	-1.06059900
H	-1.16413700	3.85224400	-2.30515300
H	-3.10074300	2.13412000	0.81475800
H	1.52377400	2.43802800	3.28928100
H	0.33674600	5.19468400	-0.59423400
H	-2.53360600	-4.73270800	1.39682800
H	-3.60652700	0.01658000	-4.20185900
H	0.48349500	-2.10574400	4.84191700
H	-3.47571300	-2.07906000	-2.62936800
N	-0.23146800	-0.23402700	2.16854100
N	-1.82783800	-1.65211100	0.30207900
N	-1.84016300	0.64238500	-1.43306700
N	-0.27103800	2.07269300	0.43905400
O	0.54582300	-0.53197600	-0.40766000
S	-3.03902900	0.88335000	1.32441000
C	1.34894200	0.08863900	-1.35193000
H	0.80036400	0.84542700	-1.92533200
C	3.57817400	0.10382700	-0.60236700
C	3.87997800	-1.12037900	-1.29698500
C	2.90615100	-1.72468900	-2.21260400
H	1.02886800	-1.36855000	-2.84108600
O	3.07728900	-2.76509200	-2.84067400
N	2.43412400	0.78094600	-0.65830800
N	1.78915700	-0.92845200	-2.33404100
C	5.16109700	-1.43860500	-0.93705200
H	5.80663000	-2.26003600	-1.21212600
N	4.64814000	0.51052800	0.14681800
N	5.56454000	-0.44306800	-0.08408500
H	6.46156000	-0.36431700	0.37299200

^{4}T2-TS2

Zero-point correction= 0.383080 (Hartree/Particle)
Thermal correction to Energy= 0.412315
Thermal correction to Enthalpy= 0.413259
Thermal correction to Gibbs Free Energy= 0.322240
Sum of electronic and zero-point Energies= -2073.041153
Sum of electronic and thermal Energies= -2073.011918
Sum of electronic and thermal Enthalpies= -2073.010973
Sum of electronic and thermal Free Energies= -2073.101992

C	3.12608800	1.12451500	-1.75830900
C	4.12811200	0.70268500	-2.70792900
C	4.16841200	-0.65701700	-2.65699000
C	-0.50385800	-2.35649500	2.11349700
C	1.86921800	2.87451200	-0.55383600
C	-0.59829900	2.48332500	1.97219400
C	2.01904500	-2.79137200	-0.35624900
C	1.54265900	4.25534900	-0.30035400
C	0.78853300	-4.15655600	0.94485800
C	2.93683400	-2.38175700	-1.31462900
C	0.45614100	-2.77636300	1.19067500
C	-0.86900600	-1.04597800	2.35859800
C	-1.75301000	-0.60429300	3.39850700
C	2.80052200	2.44909100	-1.49013500
C	-1.77422700	0.76132800	3.36294900
C	0.33036300	2.88474500	1.01174600
C	-0.90594600	1.17660200	2.29943300
C	0.59054900	4.26191500	0.67296200
C	3.19008400	-1.06476500	-1.67698000
C	1.75693000	-4.16535600	-0.01502700
Fe	1.18589000	0.05244000	0.32431500
H	3.50454300	-3.15637200	-1.82087300
H	4.71719400	1.37285900	-3.32077900
H	1.99151400	5.09747000	-0.81114700
H	-2.31626800	1.43753700	4.01173100
H	0.32605700	-4.99882700	1.44331500
H	-1.10614900	3.26750600	2.52483900
H	2.88887800	-1.05714800	2.40803000
H	3.32275400	3.21498500	-2.05499100
H	0.09199500	5.11026300	1.12373800
H	2.25397600	-5.01647600	-0.46254400
H	-2.27326000	-1.26266500	4.08258800
H	4.79746400	-1.33518900	-3.21927700
H	-0.98410200	-3.12651400	2.70939500
N	2.56061900	0.03404500	-1.15430300
N	1.21920900	-1.95971000	0.39475400
N	-0.40693500	0.05553200	1.63554500
N	1.12219900	2.05797400	0.26139400
O	-0.24074800	-0.04151000	-1.23393600
S	2.78265000	0.25797800	2.11476100
C	-1.52230500	-0.06049200	-0.93657600
H	-1.50314700	0.05067600	0.25976900
C	-3.63329100	0.87157400	-1.19973500
C	-4.27559600	-0.41114200	-1.28757700
C	-3.49387200	-1.64986500	-1.29720700
H	-1.50645300	-2.14551600	-1.21346400
O	-3.94192100	-2.78527600	-1.40665500
N	-2.31130000	1.09484900	-1.12769000
N	-2.14807900	-1.36134700	-1.20228000
C	-5.61805400	-0.13788000	-1.37722700
H	-6.48257600	-0.77903200	-1.46744300
N	-4.54791100	1.87635700	-1.22694100
N	-5.71502000	1.22496400	-1.34062900
H	-6.56225100	1.77312800	-1.39540900

^{4}T2-PC

Zero-point correction= 0.389872 (Hartree/Particle)
Thermal correction to Energy= 0.420460
Thermal correction to Enthalpy= 0.421404
Thermal correction to Gibbs Free Energy= 0.321681
Sum of electronic and zero-point Energies= -2073.180229
Sum of electronic and thermal Energies= -2073.149641
Sum of electronic and thermal Enthalpies= -2073.148697
Sum of electronic and thermal Free Energies= -2073.248420

C	3.15763600	-0.69318200	-1.96716400
C	3.89163800	-1.82612400	-2.47549600
C	3.65394300	-2.86045000	-1.62489300
C	-0.59437800	-0.27630500	3.11628000
C	2.42232800	1.64802400	-2.10223100
C	0.19244100	3.37996400	0.04141900
C	1.45693400	-2.64833300	1.45763300
C	2.38354500	2.92883200	-2.75748900
C	0.14717700	-2.65442300	3.28751500
C	2.30881000	-3.11499800	0.46691800
C	0.14322700	-1.36015200	2.65950700
C	-0.64853800	0.96284300	2.49645200
C	-1.39908000	2.08953000	2.98289900
C	3.14520100	0.55769100	-2.56402100
C	-1.18049100	3.11618800	2.11364700
C	1.07996500	2.92437500	-0.92343400
C	-0.29582400	2.62061100	1.09346000
C	1.55026000	3.72065200	-2.02645000
C	2.77625300	-2.35825600	-0.59609300
C	0.96046300	-3.45366900	2.54100400
Fe	1.46056900	0.20635900	0.39830600
H	2.62668300	-4.15113800	0.52597600
H	4.50137900	-1.81243200	-3.36987200
H	2.92440800	3.17262400	-3.66297600
H	-1.57371600	4.12406100	2.14926100
H	-0.41244800	-2.90624700	4.17940200
H	-0.13802200	4.41147000	-0.02875900
H	3.19325000	0.08672500	2.67623400
H	3.73368400	0.69112200	-3.46615000
H	1.26560800	4.74937300	-2.20706800
H	1.20671400	-4.49667500	2.69417800
H	-2.01127300	2.08096200	3.87537500
H	4.02740700	-3.87539500	-1.67294800
H	-1.17435900	-0.41031400	4.02380900
N	2.48030500	-1.03648800	-0.82285500
N	0.95360700	-1.36846700	1.54393900
N	0.00254100	1.29192500	1.32285300
N	1.62471700	1.66114600	-0.98072700
O	-0.70245200	-0.86453000	-1.55385400
S	3.30367300	1.00572600	1.69051100
C	-1.90955200	-0.76268500	-1.39012000
H	-1.82151800	0.44517800	0.25940100
C	-3.83663000	0.06426300	-0.20490100
C	-4.72503100	-0.59931200	-1.08785100
C	-4.23393400	-1.39833600	-2.19802100
H	-2.40017100	-1.93656600	-2.98274700
O	-4.89254700	-2.01275100	-3.02034600
N	-2.47112900	-0.02140200	-0.36872800
N	-2.82510900	-1.39719400	-2.23712000
C	-5.98657900	-0.28005400	-0.60847400
H	-6.97209300	-0.55489300	-0.95423100
N	-4.46199600	0.74287400	0.74814200
N	-5.77915800	0.50697000	0.46664300
H	-6.47423200	0.92773600	1.06496600