Electronic Supplementary Information

for the paper

Direct Experimental and Computational Evidence for the Dihydride Pathway in TangPHOS-Rh Catalyzed Asymmetric Hydrogenation

by

Ilya D. Gridnev,*[a] Christina Kohrt,[b] Yuanyuan Liu,[a] and Detlef Heller*[b]

Contents

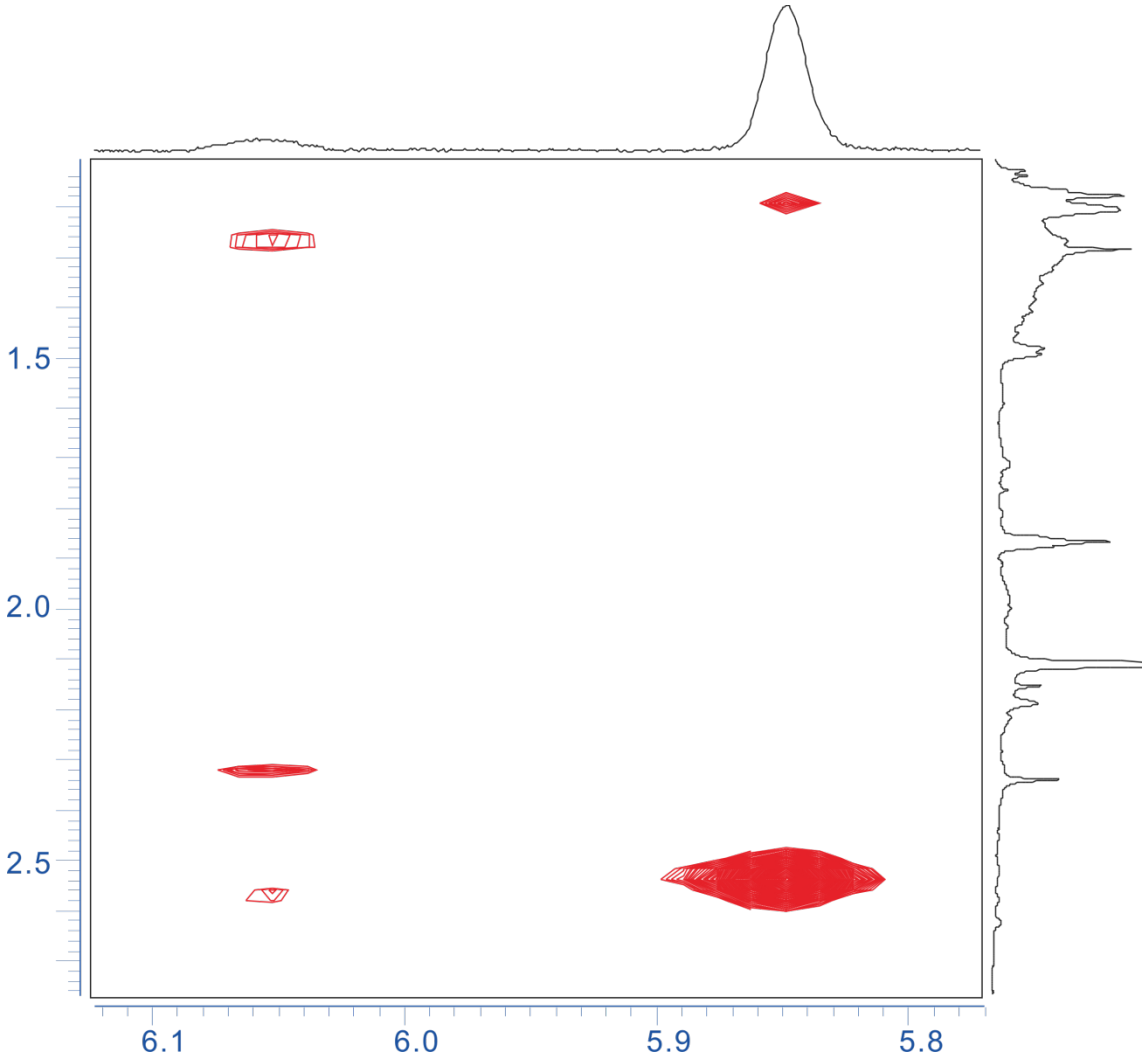

Figure S1. Section plot of phase sensitive 2D ^{1}H–^{1}H ROESY spectrum (600 MHz, CD_3OD, 203K) of the sample obtained by adding 2 equivalents of MAC to a solution of **2** in CD_3OD.

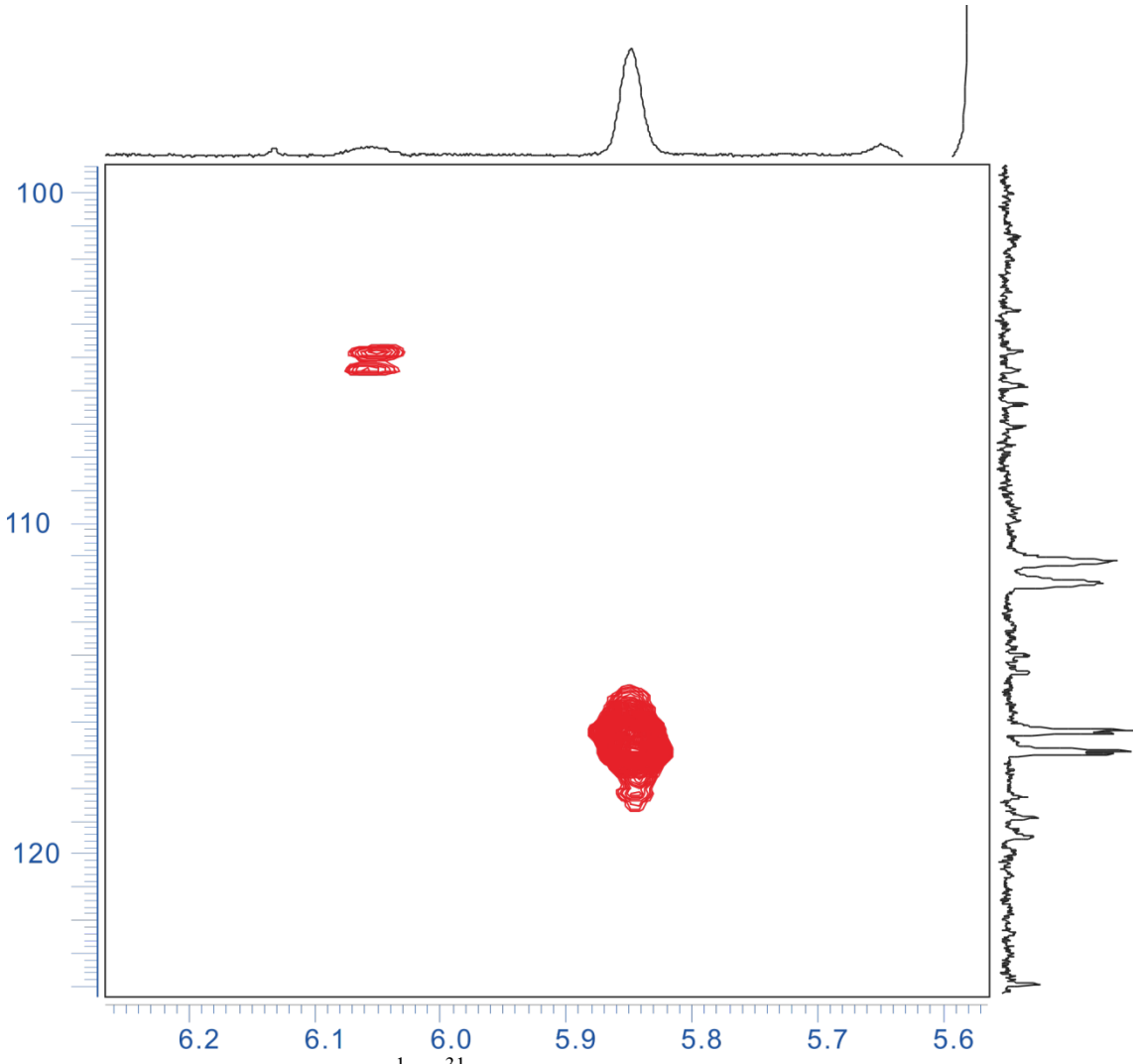

Figure S2. Section plot of 2D ^{1}H–^{31}P NMR spectrum (600 MHz, CD_3OD, 203 K) of the sample obtained by adding 2 equivalents of MAC to a solution of **2** in CD_3OD.

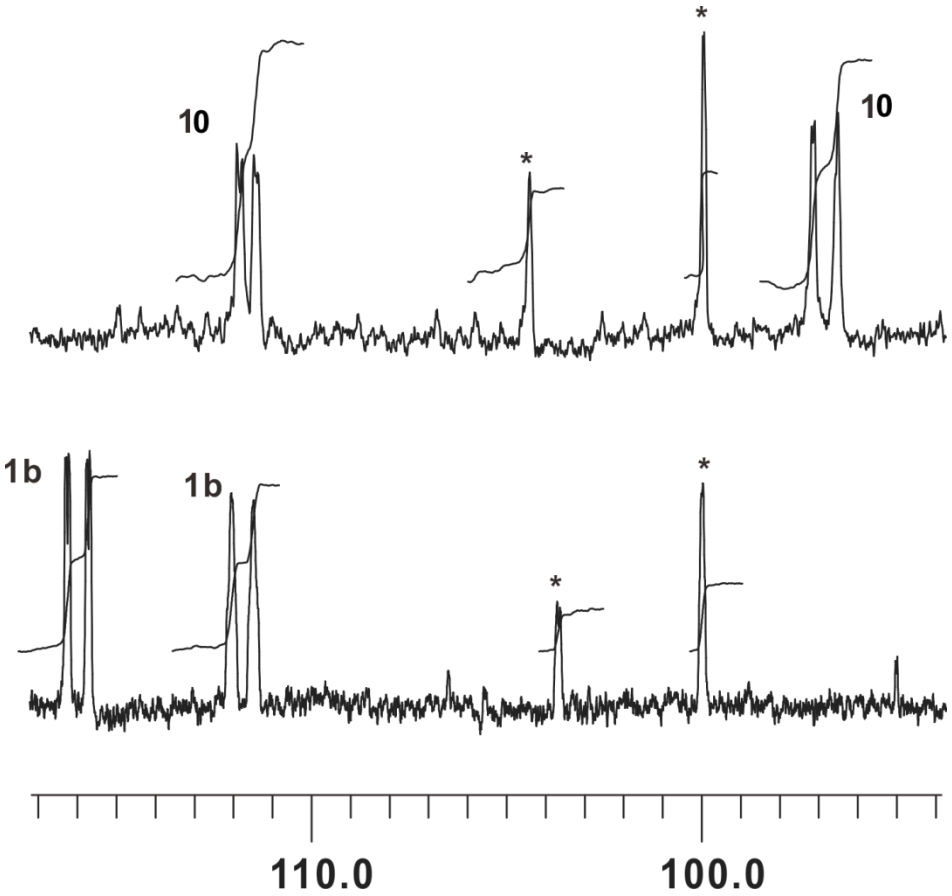

Figure S3. Section plots of ^{31}P NMR spectra (CD_3OD, 193 K) of the sample obtained by adding 2 equivalents of MAC to a solution of **2** in CD_3OD: bottom: 283 MHz; top: 243 MHz after 10 min hydrogenation at 193 K. The asterisks indicate the resonances of the complexes with one phosphorus atom of the TangPHOS ligand dissociated from Rh.
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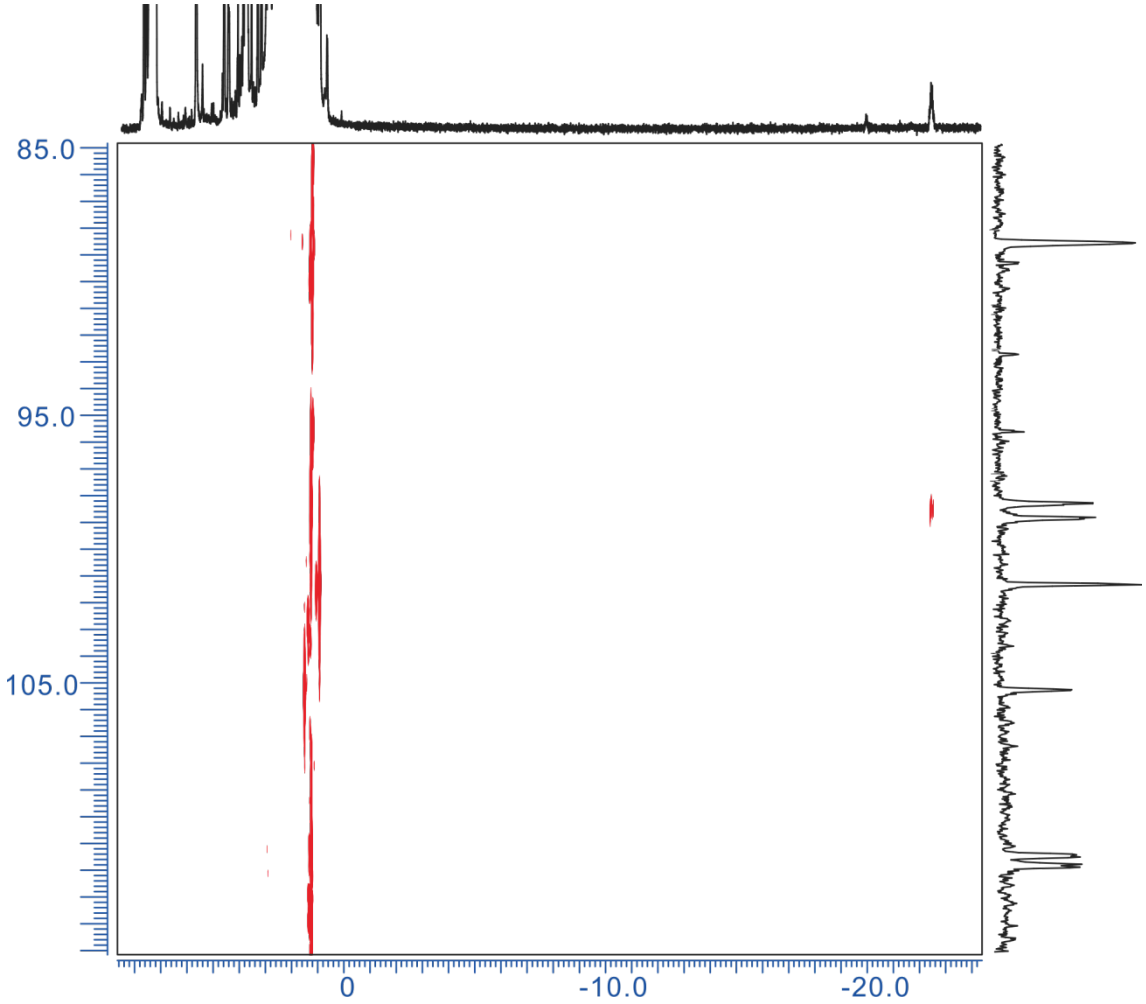


Figure S4. 2D ^{1}H–^{31}P HMBC NMR spectrum (600 MHz, CD_3OD, 203 K) of the sample obtained by adding 2 equivalents of MAC to a solution of **2** in CD_3OD followed by hydrogenation for 10 min at 193 K.

Summary for the calculation

All computations were carried out using the hybrid Becke functional (B3)[S1] for electron exchange and the correlation functional of Lee, Yang and Parr (LYP),[S2] as implemented in the GAUSSIAN 09 software package.[S3] For rhodium the SDD basis set with the associated effective core potential was employed.[S4] All other atoms were modeled at the 6-31G+(2d,2p) level of theory.[S5] The following additional diffuse function was applied for the phosphorus atom:

P 0
D 1 1.0
0.55 0.100D+01

Geometry optimizations were performed with the account of the solvent effects (CPCM, methanol) without applying any geometry constraints (C_1 symmetry).

Starting geometries for the transition state search were located either by QST2 or QST3 procedures, or by the guess based on the structure of the previously found TS. The transition states were subsequently fully optimized as saddle points of first order, employing the Berny algorithm.[S6] Frequency calculations were carried out to confirm the nature of the stationary points, yielding zero imaginary frequencies for all Rh complexes and one imaginary frequency for all transition states, which represented the vector for the appropriate bond formation.

(S1) (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.

(S2) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

(S3) Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A.

F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Gaussian, Inc., Wallingford CT, 2009.

(S4) Andrae, D.; Haeussermann, U.; Dolg, M.; Stoll. H.; Preuss, H. *Theor. Chim. Acta* **1990**, *77*, 123.

(S5) (a) Ditchfield, R.; Hehre, W. J.; Pople, J. A. *J. Chem. Phys.* **1971**, *54*, 724. (b) Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257. (c) Hariharan, P. C.; Pople, J. A. *Theo Chim. Acta* **1973**, *28*, 213. (d) Hariharan, P. C.; Pople, J. A. *Mol. Phys.* **1974**, *27*, 209. (e) Gordon, M. S. *Chem. Phys. Lett.* **1980**, *76*, 163.

(S6) Peng, C. Y.; Schlegel, B. *Isr. J. Chem.* **1994**, *34*, 449

Comparing results for B3LYP and TPSS functionals (both for SDD(Rh)/6-31+G(2d,2p)(all others)/CPCM(MeOH):

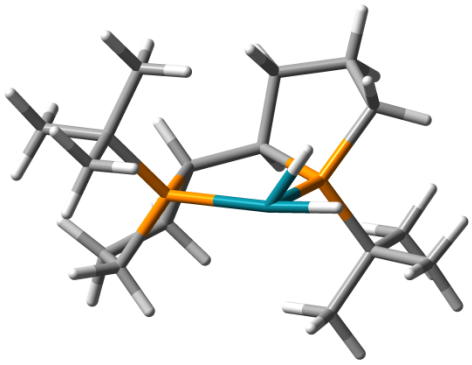
Compound	Relative stability B3LYP (ΔG^{298})	Relative stability TPSS (ΔG^{298})
1a	**0 kcal/mol**	**0 kcal/mol**
1b	**2.6 kcal/mol**	**4.6 kcal/mol**
1c	**1.5 kcal/mol**	**3.6 kcal/mol**

As can be seen from the above data, both functionals predict the similar trend in stabilities for the catalyst-substrate complexes, but TPSS suggests larger differences in the relative stabilities of **1a** and **1,b,c**. Since we were able to detect **1c** in equilibrium with **1a** by NMR, the results of B3LYP seem to conform to the experimental data slightly better. Besides using the same level of theory as in the previous publication makes possible the comparison of the similar data, *e.g.* the relative stabilities of monohydrides. Hence, we have used the B3LYP functional in this research.

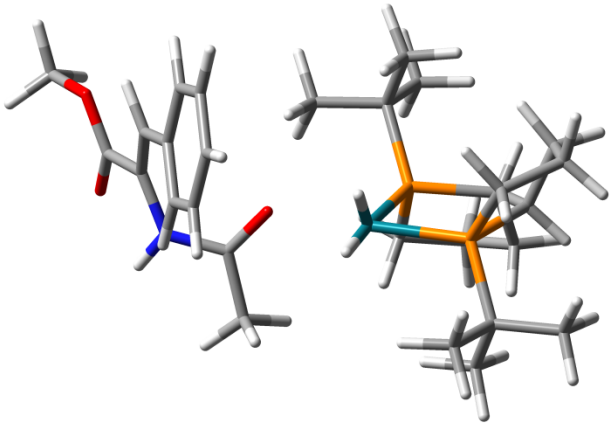
We have also attempted to use wB97XD functional with the same basis set, but it resulted in very long convergence and impossibility of the frequency analysis in certain cases.

Structures of the Transition States:

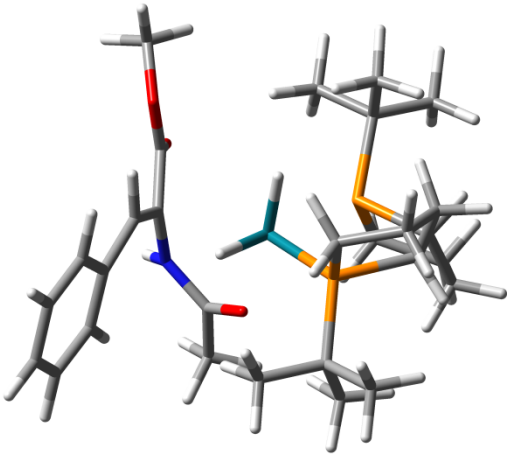
TS1, ν = 710.9*i*



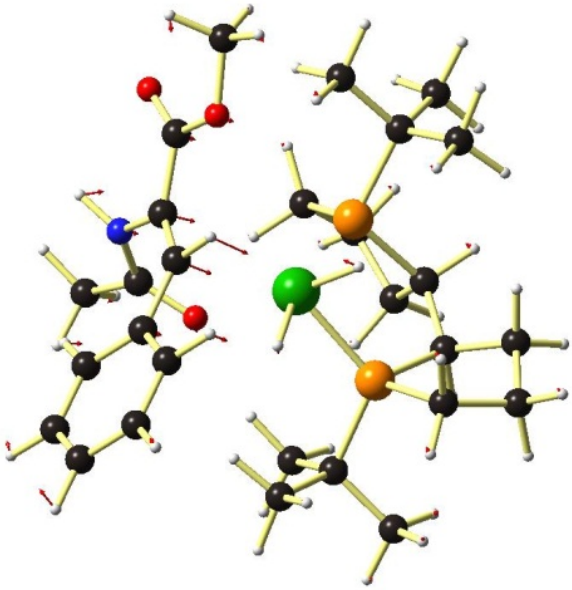
TS2, ν = 804.5*i*



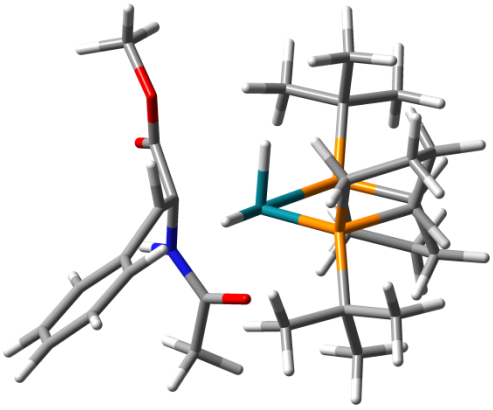
TS3, ν = 61.2*i*



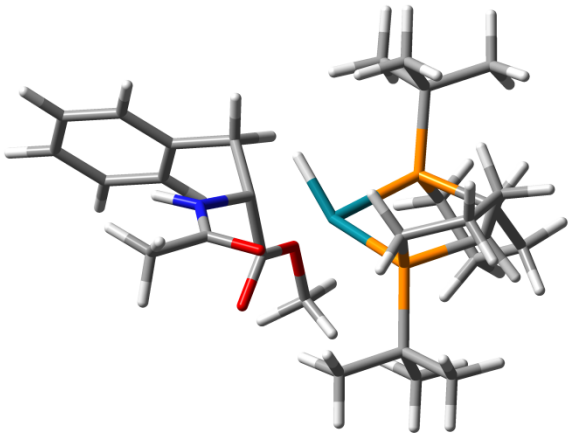
Displacement vectors in the **TS3**



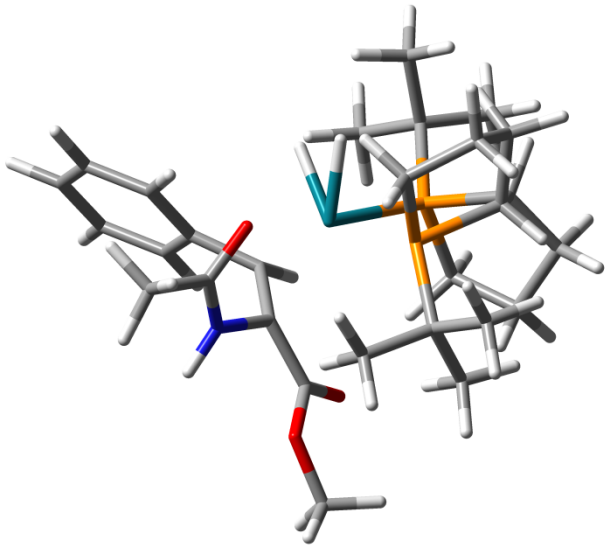
TS4, $\nu = 264.6i$



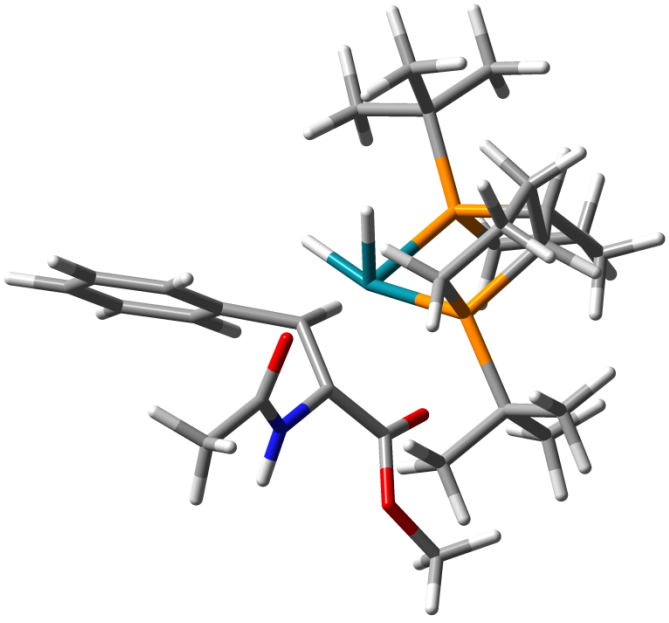
TS5, $\nu = 833.0i$



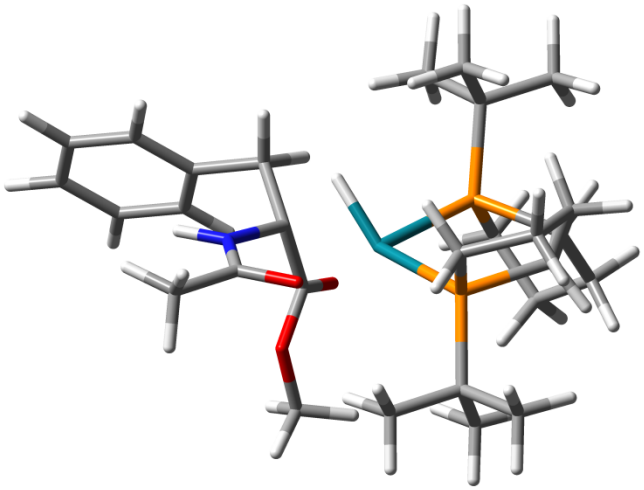
TS6, ν = 787.2*i*



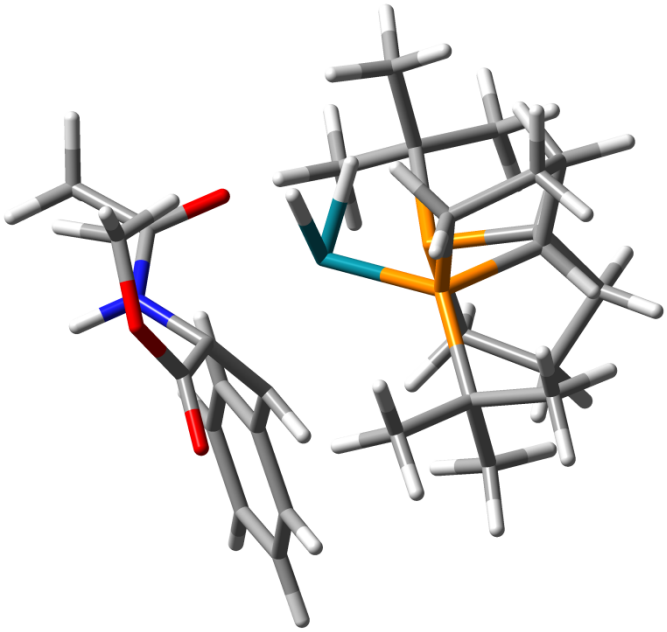
TS7, ν = 521.4*i*



TS8, ν = 875.0*i*

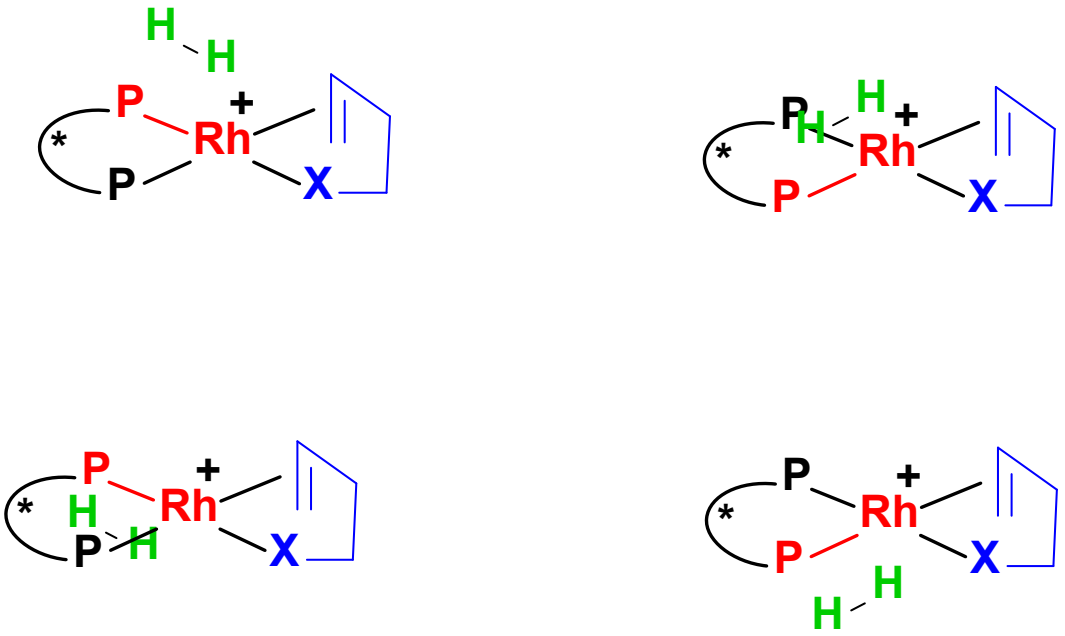


TS9, ν = 845.5*i*



Possible pathways for the H_2 approach to 1c.

In general there are four possible pathways for the molecule of dihydrogen to approach a Rh(I) catalyst-substrate complex with C_2-symmetric diphosphine ligand (Scheme S1)



However, in the real compound, *e.g.* **1c**, only one pathway is possible (Fig. S5)

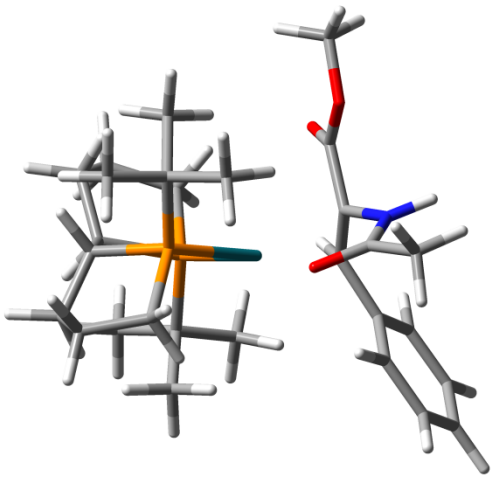


Fig. S5. Optimized structure of **1c**

Approach from the upper side (Fig. S5) is effectively blocked by the carboxymethyl group of the coordinated substrate and both substituents on the phosphorus atoms, because the substrate is bent accordingly with respect of the chelate plane of the complex.

Approach from the bottom side is open for both possibilities sterically. However, only one molecular hydride complex **11** (with the H_2 molecule over the Rh–P bond *trans*- to the coordinated double bond) could be located. Attempts to locate the second possible molecular hydride complex inevitably resulted in **11**. This is in accord with the previously found regularities (ref. 8 in the paper).

Compound, Mechanism	ZPVE Corrected Energy, a.u.	Free Energy (298 K), a. u.	System of the same content	Normalized Free Energy (298 K), a. u. for the system of the same content
1a	-2167.216536	-2167.287119	**1a + $(MeOH)_2$ + H_2**	-2399.890083
Dihydride				
2	-1653.215615	-1653.275042	**2 + MAC+ H_2**	-2399.897341
4	-1654.388798	-1654.453135	**4 + MAC**	-2399.895149
TS1	-1654.383283	-1654.44724	**TS1 + MAC**	-2399.889255
5	-1654.386521	-1654.447199	**5 + MAC**	-2399.889213
3	-746.601649	-746.649305	**3 + 2**	-2399.924347
Semi-Dihydride				
6	-2167.207454	-2167.282415	**6 + $(MeOH)_2$ + H_2**	-2399.889542
7	-2168.384014	-2168.46031	**7 + $(MeOH)_2$**	-2399.887152
TS2	-2168.378198	-2168.453991	**TS2 + $MeOH)_2$**	-2399.880833
8	-2168.385195	-2168.460703	**8 + $(MeOH)_2$**	-2399.887545
TS3	-2168.372065	-2168.443587	**TS3 + $MeOH)_2$**	-2399.870429
9	-2168.377643	-2168.448902	**9 + $(MeOH)_2$**	-2399.875744
TS4	-2168.378166	-2168.448315	**TS4 + $MeOH)_2$**	-2399.875157
10	-2168.39795	-2168.46874	**10 + $(MeOH)_2$**	-2399.895582
TS5	-2168.376954	-2168.448011	**TS5 + $MeOH)_2$**	-2399.874853
MAC	-745.399528	-745.444733		
$(MeOH)_2$	-231.394557	-231.426842		
Semi-Unsaturated				
1c	-2167.213445	-2167.284594	**1c + $(MeOH)_2$ + H_2**	-2399.891721
11	-2168.369253	-2168.439662	**11 + $(MeOH)_2$**	-2399.866504
TS6	-2168.367437	-2168.367437	**TS6 + $MeOH)_2$**	-2399.864946
12	-2168.374597	-2168.444783	**12 + $(MeOH)_2$**	-2399.871625
TS7	-2168.37312	-2168.442815	**TS7 + $MeOH)_2$**	-2399.869657
13	-2169.094639	-2168.456555	**13 + $(MeOH)_2$**	-2399.883397
TS8	-2168.377805	-2168.336441	**TS8 + $MeOH)_2$**	-2399.924347
Unsaturated				
1b	-2167.212431	-2167.282956	**1b + $(MeOH)_2$ + H_2**	-2399.890083
14	-2168.355124	-2168.423207	**14 + $(MeOH)_2$**	-2399.850049
TS9	-2168.341336	-2168.410993	**TS9 + $MeOH)_2$**	-2399.837835
15	-2168.363502	-2168.437271	**15 + $(MeOH)_2$**	-2399.864113

Cartesian coordinates of the optimized structures

1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.484063	-1.972726	0.567074
2	6	0	-2.816060	-0.577983	1.154395
3	15	0	-0.936131	-1.966604	-0.497181
4	15	0	-1.704836	0.849734	0.593647
5	6	0	-1.789327	-2.497969	-2.069163
6	1	0	-1.526500	-3.534674	-2.288629
7	1	0	-1.447152	-1.889262	-2.907287
8	6	0	-1.518167	1.577925	2.295175
9	6	0	0.107972	-3.457300	0.042416
10	6	0	0.714495	-3.170704	1.427699
11	1	0	1.356204	-2.290077	1.416628
12	1	0	-0.055204	-3.028757	2.191855
13	1	0	1.323307	-4.028348	1.733754
14	6	0	1.232574	-3.656457	-0.991478
15	1	0	1.863860	-4.494212	-0.675754
16	1	0	0.838638	-3.897101	-1.983067
17	1	0	1.861313	-2.769606	-1.081265
18	6	0	-0.742965	-4.740541	0.129537
19	1	0	-1.189619	-5.021787	-0.826360
20	1	0	-0.090517	-5.565293	0.436318
21	1	0	-1.538683	-4.664219	0.874584
22	6	0	-2.817981	2.063852	-0.368876
23	6	0	-3.327337	1.389359	-1.654590
24	1	0	-2.507751	1.017582	-2.276128
25	1	0	-4.011271	0.566164	-1.440514
26	1	0	-3.884219	2.124959	-2.244925
27	6	0	-1.990850	3.300526	-0.758841
28	1	0	-2.634225	3.997125	-1.306833
29	1	0	-1.606728	3.826277	0.116125
30	1	0	-1.154072	3.037026	-1.408783
31	6	0	-4.024670	2.522122	0.473235
32	1	0	-3.723095	3.078325	1.363419
33	1	0	-4.635868	3.195136	-0.138277
34	1	0	-4.667736	1.694632	0.781133
35	1	0	-1.578606	2.666728	2.274147
36	1	0	-0.525336	1.314422	2.664899
37	45	0	0.092645	0.139426	-0.623472
38	8	0	1.473036	-0.484898	-2.175825
39	6	0	2.363259	0.358363	-2.449900
40	7	0	2.532650	1.428331	-1.673427
41	1	0	3.178171	2.149640	-1.966282
42	6	0	3.266090	0.153605	-3.631010
43	1	0	2.650909	-0.016766	-4.517077
44	1	0	3.928198	1.002267	-3.802084
45	1	0	3.868746	-0.743921	-3.468269
46	6	0	1.663420	1.724779	-0.561247
47	6	0	1.664186	0.931720	0.638987
48	1	0	1.177771	1.453793	1.452146
49	6	0	2.700523	0.016045	1.167625
50	6	0	2.795917	-0.066914	2.573630
51	6	0	3.619365	-0.734881	0.409663
52	6	0	3.765634	-0.850260	3.195284
53	1	0	2.103040	0.501748	3.184899
54	6	0	4.594531	-1.514106	1.030888
55	1	0	3.579069	-0.732801	-0.667404
56	6	0	4.674905	-1.578364	2.424250
57	1	0	3.813029	-0.887649	4.278132
58	1	0	5.290663	-2.078854	0.420299
59	1	0	5.433287	-2.189332	2.901127
60	6	0	1.417900	3.187205	-0.496575
61	8	0	1.693044	3.946005	-1.413120
62	8	0	0.939618	3.612665	0.681930
63	6	0	0.808255	5.039378	0.841025
64	1	0	0.375252	5.179331	1.829269
65	1	0	1.789698	5.512659	0.784101
66	1	0	0.155740	5.456413	0.073399
67	6	0	-2.717103	-0.546922	2.700087
68	1	0	-3.576639	-1.054969	3.147361
69	1	0	-1.821151	-1.098315	3.007547
70	6	0	-3.579769	-2.626163	-0.320321
71	1	0	-3.561121	-3.707015	-0.152890
72	1	0	-4.575362	-2.280839	-0.026479
73	6	0	-2.596939	0.907276	3.169972
74	1	0	-3.554854	1.421889	3.057790
75	1	0	-2.324268	0.961993	4.227665
76	6	0	-3.302696	-2.346385	-1.809495
77	1	0	-3.874107	-3.026859	-2.446885
78	1	0	-3.616860	-1.335001	-2.069726
79	1	0	-3.835200	-0.306481	0.867005
80	1	0	-2.286008	-2.632455	1.413991

MAC

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.444403	1.879960	1.388067
2	6	0	-0.235979	2.246278	0.438684
3	7	0	-0.897260	1.367768	-0.389789
4	1	0	-1.624058	1.771759	-0.965822
5	6	0	-0.366469	3.704218	0.054764
6	1	0	-1.177922	3.895255	-0.648571
7	1	0	-0.517510	4.294795	0.959109
8	1	0	0.572767	4.027448	-0.403489
9	6	0	-1.053861	-0.013503	-0.150304
10	6	0	-0.067254	-0.916892	0.055943
11	1	0	-0.420203	-1.906402	0.321771
12	6	0	1.385797	-0.808705	-0.044440
13	6	0	2.155227	-1.842540	0.525186
14	6	0	2.060066	0.217469	-0.734157
15	6	0	3.545005	-1.839337	0.437573
16	1	0	1.651576	-2.651836	1.043045
17	6	0	3.447631	0.208072	-0.839762
18	1	0	1.498364	1.009597	-1.209350
19	6	0	4.197349	-0.812149	-0.247030
20	1	0	4.115801	-2.639836	0.894006
21	1	0	3.947316	1.000937	-1.384680
22	1	0	5.278585	-0.808613	-0.324151
23	6	0	-2.485994	-0.426721	-0.181408
24	8	0	-3.383689	0.352149	-0.456416
25	8	0	-2.690132	-1.720368	0.087826
26	6	0	-4.058491	-2.176127	0.046540
27	1	0	-4.014766	-3.234007	0.293548
28	1	0	-4.658552	-1.635766	0.779089
29	1	0	-4.473411	-2.032000	-0.951344

2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.705901	1.678982	-0.309389
2	6	0	0.705912	1.678939	0.309606
3	15	0	-1.455822	-0.051568	-0.363137
4	15	0	1.455822	-0.051625	0.363126
5	6	0	-2.103701	0.110933	-2.105368
6	1	0	-3.104147	-0.313729	-2.204681
7	1	0	-1.436530	-0.459480	-2.755096
8	6	0	2.103686	0.110636	2.105384
9	6	0	-2.990342	-0.136785	0.744371
10	6	0	-2.566223	0.022232	2.215317
11	1	0	-1.804689	-0.710647	2.494853
12	1	0	-2.175751	1.022208	2.421778
13	1	0	-3.438597	-0.127323	2.861003
14	6	0	-3.615778	-1.534229	0.544932
15	1	0	-4.508547	-1.620944	1.173943
16	1	0	-3.924523	-1.707167	-0.489901
17	1	0	-2.925642	-2.331621	0.836031
18	6	0	-4.027087	0.945283	0.387650
19	1	0	-4.400062	0.844785	-0.634183
20	1	0	-4.887362	0.843639	1.058746
21	1	0	-3.633948	1.957309	0.515443
22	6	0	2.990348	-0.136690	-0.744390
23	6	0	2.566224	0.022459	-2.215319
24	1	0	1.804723	-0.710424	-2.494934
25	1	0	2.175709	1.022439	-2.421677
26	1	0	3.438606	-0.126992	-2.861019
27	6	0	3.615828	-1.534132	-0.545081
28	1	0	4.508610	-1.620756	-1.174086
29	1	0	3.924564	-1.707159	0.489740
30	1	0	2.925725	-2.331521	-0.836267
31	6	0	4.027053	0.945379	-0.387560
32	1	0	4.400026	0.844799	0.634266
33	1	0	4.887336	0.843827	-1.058659
34	1	0	3.633880	1.957403	-0.515262
35	1	0	3.104125	-0.314053	2.204653
36	1	0	1.436498	-0.459855	2.755027
37	45	0	-0.000007	-1.651889	-0.000110
38	6	0	0.768322	2.173297	1.775139
39	1	0	0.735986	3.266342	1.808541
40	1	0	-0.108701	1.810973	2.320317
41	6	0	-0.768305	2.173529	-1.774858
42	1	0	-0.735945	3.266577	-1.808123
43	1	0	0.108707	1.811251	-2.320086
44	6	0	-2.035501	1.615866	-2.437866
45	1	0	-2.021956	1.776279	-3.519665
46	1	0	-2.918970	2.128879	-2.046470
47	1	0	-1.363804	2.308062	0.297421
48	6	0	2.035502	1.615525	2.438084
49	1	0	2.021948	1.775792	3.519905
50	1	0	2.918985	2.128578	2.046769
51	1	0	1.363819	2.308090	-0.297126

4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	**6**	**0**	**0.671003**	**1.468775**	**0.883355**
2	**6**	**0**	**-0.738349**	**1.694233**	**0.297606**
3	**15**	**0**	**1.480679**	**-0.148828**	**0.327762**
4	**15**	**0**	**-1.499592**	**0.109183**	**-0.373294**
5	**6**	**0**	**2.170845**	**-0.563308**	**2.008207**
6	**1**	**0**	**3.194413**	**-0.936097**	**1.942662**
7	**1**	**0**	**1.553104**	**-1.363792**	**2.420459**
8	**6**	**0**	**-2.085037**	**0.870869**	**-1.966400**
9	**6**	**0**	**2.973922**	**0.235920**	**-0.777435**
10	**6**	**0**	**2.479422**	**0.827554**	**-2.109726**
11	**1**	**0**	**1.755138**	**0.170086**	**-2.598438**
12	**1**	**0**	**2.019203**	**1.809073**	**-1.974009**
13	**1**	**0**	**3.332477**	**0.957379**	**-2.784252**
14	**6**	**0**	**3.725656**	**-1.081994**	**-1.057669**
15	**1**	**0**	**4.622361**	**-0.858935**	**-1.645585**
16	**1**	**0**	**4.049621**	**-1.582275**	**-0.140916**
17	**1**	**0**	**3.116501**	**-1.780548**	**-1.635001**
18	**6**	**0**	**3.938316**	**1.228152**	**-0.097077**
19	**1**	**0**	**4.357440**	**0.831644**	**0.830548**
20	**1**	**0**	**4.775864**	**1.420019**	**-0.776551**
21	**1**	**0**	**3.469493**	**2.191423**	**0.117328**
22	**6**	**0**	**-3.050653**	**-0.351615**	**0.603688**
23	**6**	**0**	**-2.647651**	**-0.701113**	**2.048645**
24	**1**	**0**	**-1.877781**	**-1.477492**	**2.075808**
25	**1**	**0**	**-2.278314**	**0.172263**	**2.592710**
26	**1**	**0**	**-3.526473**	**-1.072741**	**2.586676**
27	**6**	**0**	**-3.644747**	**-1.604857**	**-0.075115**
28	**1**	**0**	**-4.540749**	**-1.918379**	**0.471268**
29	**1**	**0**	**-3.940083**	**-1.415462**	**-1.110976**
30	**1**	**0**	**-2.938431**	**-2.440368**	**-0.065534**
31	**6**	**0**	**-4.097571**	**0.776303**	**0.618004**
32	**1**	**0**	**-4.453955**	**1.026270**	**-0.383983**
33	**1**	**0**	**-4.965477**	**0.444519**	**1.198959**
34	**1**	**0**	**-3.719898**	**1.687380**	**1.089517**
35	**1**	**0**	**-3.071213**	**0.499028**	**-2.249746**
36	**1**	**0**	**-1.383560**	**0.575765**	**-2.750191**
37	**45**	**0**	**0.022827**	**-1.598282**	**-0.483793**
38	**1**	**0**	**1.251516**	**-2.855047**	**-0.841410**
39	**1**	**0**	**1.065814**	**-2.974044**	**-0.054221**
40	**1**	**0**	**-1.392808**	**2.066280**	**1.091216**
41	**6**	**0**	**0.720457**	**1.398600**	**2.428447**
42	**1**	**0**	**0.620247**	**2.401147**	**2.854575**
43	**1**	**0**	**-0.124376**	**0.807205**	**2.795506**
44	**6**	**0**	**2.030371**	**0.720377**	**2.851055**
45	**1**	**0**	**2.032201**	**0.485910**	**3.919054**
46	**1**	**0**	**2.875245**	**1.389812**	**2.664779**
47	**6**	**0**	**-0.793086**	**2.690497**	**-0.888734**
48	**1**	**0**	**-0.783690**	**3.719683**	**-0.518349**
49	**1**	**0**	**0.098140**	**2.567763**	**-1.510787**
50	**6**	**0**	**-2.038115**	**2.396075**	**-1.736542**
51	**1**	**0**	**-2.007485**	**2.932862**	**-2.688873**
52	**1**	**0**	**-2.938254**	**2.724574**	**-1.209022**
53	**1**	**0**	**1.321562**	**2.285634**	**0.558584**

TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	**6**	**0**	**0.618087**	**1.321289**	**1.084837**
2	**6**	**0**	**-0.781908**	**1.604926**	**0.503492**
3	**15**	**0**	**1.534345**	**-0.160783**	**0.345243**
4	**15**	**0**	**-1.541023**	**0.137953**	**-0.406932**
5	**6**	**0**	**2.344015**	**-0.660131**	**1.945536**

6	**1**	**0**	**3.414123**	**-0.814386**	**1.806831**
7	**1**	**0**	**1.909076**	**-1.609482**	**2.258735**
8	**6**	**0**	**-2.125393**	**1.151141**	**-1.855636**
9	**6**	**0**	**2.926937**	**0.383936**	**-0.823680**
10	**6**	**0**	**2.320924**	**0.872577**	**-2.152613**
11	**1**	**0**	**1.770169**	**0.077270**	**-2.661853**
12	**1**	**0**	**1.647454**	**1.721326**	**-2.018046**
13	**1**	**0**	**3.128557**	**1.197943**	**-2.816984**
14	**6**	**0**	**3.818684**	**-0.844052**	**-1.107083**
15	**1**	**0**	**4.591162**	**-0.557925**	**-1.828420**
16	**1**	**0**	**4.326609**	**-1.208330**	**-0.211174**
17	**1**	**0**	**3.241585**	**-1.666970**	**-1.535185**
18	**6**	**0**	**3.773850**	**1.502163**	**-0.186902**
19	**1**	**0**	**4.215705**	**1.206477**	**0.768775**
20	**1**	**0**	**4.600998**	**1.739545**	**-0.864942**
21	**1**	**0**	**3.203817**	**2.421868**	**-0.036990**
22	**6**	**0**	**-3.102656**	**-0.441427**	**0.495054**
23	**6**	**0**	**-2.721781**	**-0.961938**	**1.891896**
24	**1**	**0**	**-1.936721**	**-1.720788**	**1.842517**
25	**1**	**0**	**-2.386563**	**-0.154274**	**2.547367**
26	**1**	**0**	**-3.603211**	**-1.414583**	**2.358457**
27	**6**	**0**	**-3.682988**	**-1.601217**	**-0.343522**
28	**1**	**0**	**-4.588738**	**-1.980572**	**0.142065**
29	**1**	**0**	**-3.960149**	**-1.281935**	**-1.353014**
30	**1**	**0**	**-2.976478**	**-2.432405**	**-0.430146**
31	**6**	**0**	**-4.160277**	**0.669569**	**0.637007**
32	**1**	**0**	**-4.510314**	**1.037219**	**-0.330259**
33	**1**	**0**	**-5.029850**	**0.263255**	**1.165575**
34	**1**	**0**	**-3.795792**	**1.519944**	**1.219822**
35	**1**	**0**	**-3.112440**	**0.834979**	**-2.197128**
36	**1**	**0**	**-1.426650**	**0.980689**	**-2.678844**
37	**45**	**0**	**0.142722**	**-1.598256**	**-0.610689**
38	**1**	**0**	**1.292347**	**-2.731231**	**-0.602931**
39	**1**	**0**	**0.555918**	**-2.610487**	**0.483240**
40	**1**	**0**	**-1.453739**	**1.852963**	**1.330913**
41	**6**	**0**	**0.638354**	**1.018930**	**2.601830**
42	**1**	**0**	**0.403171**	**1.925817**	**3.166714**
43	**1**	**0**	**-0.129850**	**0.276935**	**2.844470**
44	**6**	**0**	**2.021139**	**0.460423**	**2.956346**
45	**1**	**0**	**2.050752**	**0.076654**	**3.979367**
46	**1**	**0**	**2.769832**	**1.256170**	**2.888869**
47	**6**	**0**	**-0.823400**	**2.772214**	**-0.511260**
48	**1**	**0**	**-0.806353**	**3.732255**	**0.012985**
49	**1**	**0**	**0.069111**	**2.743838**	**-1.144882**
50	**6**	**0**	**-2.070425**	**2.621113**	**-1.393605**
51	**1**	**0**	**-2.039594**	**3.298911**	**-2.251533**
52	**1**	**0**	**-2.966490**	**2.868049**	**-0.817472**
53	**1**	**0**	**1.251260**	**2.198113**	**0.919264**

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.787180	1.578621	0.446727
2	6	0	0.615453	1.312160	1.040277
3	15	0	-1.581117	0.088737	-0.402011
4	15	0	1.552955	-0.180704	0.346780
5	6	0	-2.142602	1.057204	-1.891429
6	1	0	-3.134583	0.746862	-2.224402
7	1	0	-1.442538	0.837528	-2.702286
8	6	0	2.277716	-0.692287	1.976753
9	6	0	-3.152257	-0.405643	0.530059
10	6	0	-2.776965	-0.867204	1.950374
11	1	0	-2.033313	-1.668121	1.936389
12	1	0	-2.389958	-0.045564	2.558701
13	1	0	-3.672823	-1.249014	2.451864
14	6	0	-3.758936	-1.595180	-0.245257
15	1	0	-4.661981	-1.940301	0.269853
16	1	0	-4.045823	-1.320750	-1.264682
17	1	0	-3.061162	-2.436035	-0.300523
18	6	0	-4.184290	0.732724	0.622516
19	1	0	-4.526208	1.064495	-0.360519
20	1	0	-5.063262	0.371747	1.168599
21	1	0	-3.798209	1.599294	1.165962
22	6	0	2.990500	0.363805	-0.761671
23	6	0	2.446254	0.884968	-2.105193
24	1	0	1.883608	0.120763	-2.647879
25	1	0	1.808017	1.762334	-1.982402
26	1	0	3.290235	1.182579	-2.736250
27	6	0	3.896825	-0.856982	-1.024612
28	1	0	4.717758	-0.546149	-1.679108
29	1	0	4.340450	-1.251741	-0.107057
30	1	0	3.352479	-1.664780	-1.516929
31	6	0	3.814838	1.469339	-0.071034
32	1	0	4.236057	1.143242	0.883161
33	1	0	4.654641	1.731670	-0.723385
34	1	0	3.238055	2.381481	0.096284
35	1	0	3.337780	-0.927932	1.877662
36	1	0	1.765661	-1.602048	2.292166
37	45	0	0.161039	-1.574533	-0.648516
38	1	0	-0.079557	-2.086750	0.752912
39	1	0	1.373742	-2.626647	-0.634905
40	6	0	0.628649	1.060167	2.566778
41	1	0	0.421349	1.992320	3.100337
42	1	0	-0.162861	0.352357	2.833091
43	6	0	-0.811999	2.705535	-0.617593
44	1	0	-0.774626	3.685153	-0.131734
45	1	0	0.078248	2.631472	-1.249601
46	6	0	1.991261	0.469221	2.949790
47	1	0	1.999638	0.116005	3.984083
48	1	0	2.766897	1.236124	2.863345
49	1	0	1.243461	2.187231	0.847435
50	6	0	-2.059746	2.544229	-1.494045
51	1	0	-2.011025	3.186108	-2.378567
52	1	0	-2.952827	2.833629	-0.933145
53	1	0	-1.446768	1.872904	1.268577

3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.598114	1.968174	1.501164
2	6	0	-1.160817	2.042893	0.350877
3	7	0	-0.688213	0.953903	-0.306415
4	6	0	-0.692154	-0.368664	0.281874
5	6	0	0.346463	-1.289872	-0.404174
6	1	0	0.102574	-1.376424	-1.467389
7	1	0	-0.417729	1.053289	-1.272781
8	6	0	1.774333	-0.814322	-0.237144
9	6	0	2.495872	-0.308717	-1.324435
10	6	0	2.405490	-0.879592	1.013106
11	6	0	3.813643	0.129187	-1.169131
12	1	0	2.028335	-0.262505	-2.302749
13	6	0	3.720108	-0.442532	1.173049

14	1	0	1.868162	-1.279712	1.867153
15	6	0	4.429038	0.065621	0.081158
16	1	0	4.355973	0.516164	-2.024569
17	1	0	4.192401	-0.503159	2.147206
18	1	0	5.451698	0.403567	0.204590
19	6	0	-1.114327	3.353672	-0.402830
20	1	0	-2.132241	3.738337	-0.499396
21	1	0	-0.541255	4.074750	0.183950
22	1	0	-0.670093	3.266214	-1.395148
23	6	0	-2.060792	-1.058853	0.266769
24	8	0	-2.344203	-1.954007	1.035108
25	8	0	-2.871328	-0.607442	-0.689877
26	6	0	-4.167356	-1.239542	-0.789626
27	1	0	-4.669794	-0.736356	-1.611864
28	1	0	-4.050368	-2.302367	-1.002061
29	1	0	-4.721091	-1.105030	0.139653
30	1	0	0.230710	-2.285208	0.032142
31	1	0	-0.437631	-0.268349	1.338054

6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.990403	-1.127851	0.258125
2	6	0	4.401975	0.355152	0.181400
3	15	0	2.184822	-1.414631	-0.232618
4	15	0	2.899790	1.492730	0.129154
5	6	0	1.849229	-2.635408	1.140990
6	1	0	1.278169	-3.494403	0.783857
7	1	0	1.242571	-2.125568	1.891762
8	6	0	3.571603	2.565231	-1.244724
9	6	0	2.133820	-2.439047	-1.831728
10	6	0	2.657260	-1.580697	-2.997446
11	1	0	2.116389	-0.633523	-3.074196
12	1	0	3.722749	-1.360315	-2.894361
13	1	0	2.526855	-2.128150	-3.937499
14	6	0	0.663898	-2.819482	-2.103541
15	1	0	0.613080	-3.405165	-3.028185
16	1	0	0.242064	-3.433531	-1.302663
17	1	0	0.031921	-1.937500	-2.222332
18	6	0	2.975720	-3.725709	-1.724863
19	1	0	2.612799	-4.396276	-0.942472
20	1	0	2.907698	-4.268341	-2.674487
21	1	0	4.034203	-3.522553	-1.543827
22	6	0	2.883045	2.605102	1.665009
23	6	0	2.651538	1.737663	2.916117
24	1	0	1.750637	1.125466	2.821842
25	1	0	3.498749	1.075945	3.115782
26	1	0	2.532812	2.387412	3.790473
27	6	0	1.697824	3.580387	1.497108
28	1	0	1.636113	4.230307	2.377076
29	1	0	1.813286	4.223946	0.620192
30	1	0	0.745976	3.048112	1.407995
31	6	0	4.186364	3.406366	1.835141
32	1	0	4.374089	4.079644	0.995545
33	1	0	4.107716	4.024447	2.736865
34	1	0	5.058345	2.759067	1.961345
35	1	0	3.368894	3.623240	-1.068777
36	1	0	3.052496	2.278370	-2.162436
37	45	0	0.984827	0.426000	-0.244868
38	8	0	-1.026638	-0.266846	-0.702798
39	6	0	-2.003144	-0.498761	0.039797
40	7	0	-3.229994	-0.545363	-0.521870
41	6	0	-1.866656	-0.709358	1.520613
42	1	0	-0.934446	-0.254673	1.854401
43	1	0	-2.710763	-0.287381	2.068837
44	1	0	-1.829902	-1.782583	1.726258
45	6	0	-4.458034	-0.884772	0.105485
46	6	0	-5.527315	-0.053871	0.134556
47	1	0	-6.428671	-0.495507	0.544239
48	6	0	-5.693099	1.324523	-0.321046
49	6	0	-7.012233	1.826666	-0.348573
50	6	0	-4.645450	2.187599	-0.708868
51	6	0	-7.280973	3.127881	-0.764625
52	1	0	-7.828993	1.181386	-0.042779
53	6	0	-4.916724	3.491660	-1.115082
54	1	0	-3.618952	1.852721	-0.678811
55	6	0	-6.231886	3.965945	-1.150944
56	1	0	-8.303383	3.488124	-0.783101
57	1	0	-4.098001	4.141391	-1.403653
58	1	0	-6.435140	4.981414	-1.472459
59	6	0	-4.551725	-2.290937	0.597141
60	8	0	-3.685737	-3.123518	0.403137
61	8	0	-5.678961	-2.539182	1.273424
62	6	0	-5.857047	-3.888066	1.752685
63	1	0	-6.816877	-3.885591	2.264337
64	1	0	-5.870344	-4.587488	0.915703
65	1	0	-5.054728	-4.151122	2.443182
66	6	0	5.227447	0.730527	-1.073678
67	1	0	6.274709	0.442407	-0.941233
68	1	0	4.851089	0.173630	-1.937049
69	6	0	5.074594	2.233535	-1.344810
70	1	0	5.471700	2.502458	-2.328091
71	1	0	5.637638	2.806864	-0.602730
72	6	0	4.104240	-1.753808	1.668008
73	1	0	5.150135	-1.972079	1.904418
74	1	0	3.749350	-1.036951	2.415471
75	6	0	3.227100	-3.011495	1.723620
76	1	0	3.129307	-3.384741	2.747166
77	1	0	3.682943	-3.810468	1.131588
78	1	0	4.988595	0.608432	1.069488
79	1	0	4.615568	-1.708286	-0.426654
80	1	0	-3.244835	-0.374016	-1.521198

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.028438	-1.998372	0.464031
2	6	0	-3.799091	-0.687934	0.717131
3	15	0	-1.183658	-1.744199	0.145531
4	15	0	-2.890062	0.856770	0.114162
5	6	0	-1.109179	-2.956139	-1.270008
6	1	0	-0.210894	-3.573668	-1.221448
7	1	0	-1.062110	-2.378658	-2.195902
8	6	0	-3.295563	1.865320	1.631502
9	6	0	-0.192695	-2.534170	1.557060
10	6	0	-0.370878	-1.679660	2.825936
11	1	0	-0.109030	-0.633250	2.645492
12	1	0	-1.395002	-1.718110	3.205517
13	1	0	0.283858	-2.064924	3.615249
14	6	0	1.296179	-2.529310	1.154087
15	1	0	1.882041	-2.971471	1.967562
16	1	0	1.482296	-3.124879	0.256037

17	1	0	1.667080	-1.519020	0.976382
18	6	0	-0.629881	-3.983199	1.843242
19	1	0	-0.473206	-4.639606	0.983819
20	1	0	-0.022410	-4.376024	2.666329
21	1	0	-1.675957	-4.056464	2.150263
22	6	0	-3.893168	1.643486	-1.295931
23	6	0	-3.828437	0.727649	-2.531874
24	1	0	-2.795464	0.509574	-2.816396
25	1	0	-4.349386	-0.218560	-2.366764
26	1	0	-4.317145	1.225228	-3.376777
27	6	0	-3.257867	3.004646	-1.648536
28	1	0	-3.864984	3.489420	-2.420616
29	1	0	-3.215230	3.682377	-0.791409
30	1	0	-2.247944	2.889921	-2.047194
31	6	0	-5.365636	1.871420	-0.901642
32	1	0	-5.469536	2.568298	-0.066499
33	1	0	-5.893767	2.307983	-1.756620
34	1	0	-5.880977	0.943102	-0.644128
35	1	0	-3.575471	2.888293	1.373607
36	1	0	-2.387388	1.916065	2.236614
37	45	0	-0.715686	0.477919	-0.307679
38	8	0	1.433211	0.227348	-0.680426
39	6	0	2.069929	0.117777	-1.738915
40	7	0	3.426420	0.057222	-1.734587
41	1	0	3.856975	-0.249637	-2.596799
42	6	0	1.410994	0.098408	-3.091549
43	1	0	2.067605	-0.285363	-3.873266
44	1	0	0.501624	-0.500468	-3.038676
45	1	0	1.121208	1.121665	-3.350414
46	6	0	4.247707	-0.053208	-0.585628
47	6	0	4.295079	0.815382	0.450802
48	1	0	4.924860	0.491773	1.271911
49	6	0	3.665018	2.118278	0.653686
50	6	0	3.623702	2.621861	1.969703
51	6	0	3.167867	2.928782	-0.386419
52	6	0	3.077233	3.874061	2.244206
53	1	0	4.023715	2.020201	2.779406
54	6	0	2.642061	4.188687	-0.113222
55	1	0	3.218997	2.588511	-1.412131
56	6	0	2.584435	4.663014	1.201754
57	1	0	3.046288	4.237029	3.265508
58	1	0	2.277141	4.804057	-0.928227
59	1	0	2.167697	5.642527	1.408936
60	6	0	5.132023	-1.251506	-0.645009
61	8	0	5.169920	-1.984218	-1.618801
62	8	0	5.886292	-1.424980	0.442895
63	6	0	6.785538	-2.553441	0.429509
64	1	0	7.293657	-2.525358	1.390739
65	1	0	6.224210	-3.482033	0.318825
66	1	0	7.502337	-2.453386	-0.386577
67	1	0	-0.378897	2.192840	-0.145894
68	1	0	-0.494655	2.101967	-0.958017
69	6	0	-4.097936	-0.401548	2.209127
70	1	0	-4.922604	-1.030688	2.557505
71	1	0	-3.222721	-0.657770	2.814467
72	6	0	-3.525028	-2.801623	-0.762581
73	1	0	-4.455743	-3.324039	-0.521774
74	1	0	-3.747509	-2.112828	-1.583303
75	6	0	-4.401092	1.092306	2.377072
76	1	0	-4.434072	1.377089	3.432626
77	1	0	-5.380100	1.325201	1.948979
78	6	0	-2.419528	-3.766822	-1.206600
79	1	0	-2.322967	-4.583829	-0.485789
80	1	0	-2.647199	-4.217047	-2.177034
81	1	0	-4.753065	-0.737690	0.184451
82	1	0	-3.124883	-2.633884	1.348738

TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	**6**	**0**	**-3.072058**	**-1.949073**	**0.502841**
2	**6**	**0**	**-3.800621**	**-0.607575**	**0.730434**
3	**15**	**0**	**-1.219269**	**-1.784480**	**0.170642**
4	**15**	**0**	**-2.887601**	**0.926851**	**0.096309**
5	**6**	**0**	**-1.219230**	**-3.011626**	**-1.235200**
6	**1**	**0**	**-0.342208**	**-3.660370**	**-1.200922**
7	**1**	**0**	**-1.167555**	**-2.442982**	**-2.167048**
8	**6**	**0**	**-3.332369**	**1.981143**	**1.566422**
9	**6**	**0**	**-0.264553**	**-2.616961**	**1.582651**
10	**6**	**0**	**-0.454430**	**-1.788742**	**2.866982**
11	**1**	**0**	**-0.179405**	**-0.741016**	**2.719334**
12	**1**	**0**	**-1.485102**	**-1.827421**	**3.229322**
13	**1**	**0**	**0.183743**	**-2.199262**	**3.657124**
14	**6**	**0**	**1.227607**	**-2.612316**	**1.192472**
15	**1**	**0**	**1.808233**	**-3.068628**	**2.001871**
16	**1**	**0**	**1.417052**	**-3.193261**	**0.285354**
17	**1**	**0**	**1.602056**	**-1.599715**	**1.032177**
18	**6**	**0**	**-0.719416**	**-4.066103**	**1.835660**
19	**1**	**0**	**-0.554783**	**-4.709364**	**0.967824**
20	**1**	**0**	**-0.131802**	**-4.480101**	**2.662949**
21	**1**	**0**	**-1.772096**	**-4.131191**	**2.122237**
22	**6**	**0**	**-3.829156**	**1.663494**	**-1.376813**
23	**6**	**0**	**-3.648478**	**0.743992**	**-2.599245**
24	**1**	**0**	**-2.592009**	**0.582579**	**-2.831139**
25	**1**	**0**	**-4.123295**	**-0.229313**	**-2.454600**
26	**1**	**0**	**-4.118279**	**1.208824**	**-3.472841**
27	**6**	**0**	**-3.221335**	**3.045762**	**-1.696565**
28	**1**	**0**	**-3.759192**	**3.478807**	**-2.546904**
29	**1**	**0**	**-3.312633**	**3.745163**	**-0.861135**
30	**1**	**0**	**-2.165964**	**2.970774**	**-1.966077**
31	**6**	**0**	**-5.330210**	**1.835461**	**-1.074704**
32	**1**	**0**	**-5.509560**	**2.511220**	**-0.234925**
33	**1**	**0**	**-5.817124**	**2.272774**	**-1.953318**
34	**1**	**0**	**-5.829049**	**0.885783**	**-0.868373**
35	**1**	**0**	**-3.639524**	**2.983048**	**1.262944**
36	**1**	**0**	**-2.431875**	**2.083188**	**2.175242**
37	**45**	**0**	**-0.708454**	**0.538871**	**-0.300891**
38	**8**	**0**	**1.442858**	**0.264416**	**-0.652589**
39	**6**	**0**	**2.057657**	**0.167951**	**-1.725008**
40	**7**	**0**	**3.412255**	**0.076144**	**-1.748931**
41	**1**	**0**	**3.818462**	**-0.220979**	**-2.626285**
42	**6**	**0**	**1.365936**	**0.187351**	**-3.060560**
43	**1**	**0**	**2.031104**	**-0.062062**	**-3.887474**
44	**1**	**0**	**0.529880**	**-0.513556**	**-3.036240**
45	**1**	**0**	**0.956086**	**1.188321**	**-3.224145**
46	**6**	**0**	**4.250795**	**-0.087824**	**-0.618867**
47	**6**	**0**	**4.339997**	**0.750370**	**0.439648**
48	**1**	**0**	**4.976330**	**0.388382**	**1.239455**
49	**6**	**0**	**3.748623**	**2.063373**	**0.688926**
50	**6**	**0**	**3.746050**	**2.533338**	**2.017961**
51	**6**	**0**	**3.252704**	**2.913210**	**-0.319916**
52	**6**	**0**	**3.238136**	**3.791638**	**2.335304**
53	**1**	**0**	**4.145452**	**1.900397**	**2.803770**
54	**6**	**0**	**2.765994**	**4.178779**	**-0.004100**
55	**1**	**0**	**3.273659**	**2.598159**	**-1.354647**
56	**6**	**0**	**2.746526**	**4.620102**	**1.323428**

57	1	0	3.236325	4.128409	3.366005
58	1	0	2.401037	4.824138	-0.795556
59	1	0	2.359682	5.604258	1.563904
60	6	0	5.101974	-1.306359	-0.728209
61	8	0	5.100472	-2.013747	-1.721332
62	8	0	5.874456	-1.527638	0.338041
63	6	0	6.743707	-2.677706	0.275586
64	1	0	7.277075	-2.684568	1.223428
65	1	0	6.155956	-3.589113	0.159217
66	1	0	7.441359	-2.577046	-0.556812
67	1	0	-0.431913	1.776642	0.593696
68	1	0	-0.496296	2.103785	-0.593554
69	1	0	-4.762659	-0.645615	0.211019
70	6	0	-4.081629	-0.281785	2.216766
71	1	0	-4.884755	-0.919943	2.597399
72	1	0	-3.189497	-0.495261	2.814521
73	6	0	-4.421666	1.208200	2.334902
74	1	0	-5.405365	1.402272	1.897031
75	1	0	-4.463884	1.529033	3.379469
76	6	0	-3.619391	-2.765301	-0.694693
77	1	0	-4.559991	-3.253018	-0.421405
78	1	0	-3.842342	-2.088320	-1.525075
79	6	0	-2.556229	-3.774218	-1.144013
80	1	0	-3.185759	-2.554368	1.407008
81	1	0	-2.477520	-4.586178	-0.415566
82	1	0	-2.816248	-4.226763	-2.105411

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.997566	-1.906502	0.726106
2	6	0	-3.699443	-0.540536	0.889787
3	15	0	-1.167625	-1.805959	0.246265
4	15	0	-2.886878	0.918419	0.000357
5	6	0	-1.307352	-3.112727	-1.078388
6	1	0	-0.434757	-3.768510	-1.089412
7	1	0	-1.336341	-2.594301	-2.040930
8	6	0	-3.275176	2.149136	1.341001
9	6	0	-0.133803	-2.590106	1.629227
10	6	0	-0.194150	-1.683197	2.872852
11	1	0	0.130478	-0.663745	2.649803
12	1	0	-1.199786	-1.639406	3.299440
13	1	0	0.469740	-2.086795	3.645228
14	6	0	1.321580	-2.655576	1.120588
15	1	0	1.958928	-3.068388	1.910570
16	1	0	1.421439	-3.306254	0.246837
17	1	0	1.703789	-1.667956	0.855096
18	6	0	-0.600875	-4.006755	2.011827
19	1	0	-0.521067	-4.708713	1.178440
20	1	0	0.039512	-4.384725	2.817070
21	1	0	-1.629420	-4.023239	2.381571
22	6	0	-3.899700	1.435837	-1.516937
23	6	0	-3.658075	0.435496	-2.663609
24	1	0	-2.604947	0.393678	-2.955224
25	1	0	-3.985387	-0.574470	-2.409367
26	1	0	-4.231574	0.753313	-3.540984
27	6	0	-3.419466	2.831478	-1.970035
28	1	0	-3.976467	3.117954	-2.868492
29	1	0	-3.599846	3.599875	-1.214206
30	1	0	-2.355080	2.833845	-2.213476
31	6	0	-5.404720	1.501510	-1.190442
32	1	0	-5.624132	2.198697	-0.377455
33	1	0	-5.941000	1.857054	-2.076997
34	1	0	-5.819433	0.524896	-0.930037
35	1	0	-3.704658	3.062777	0.928154
36	1	0	-2.331873	2.416469	1.819080
37	45	0	-0.729318	0.491342	-0.430368
38	8	0	1.436950	0.279365	-0.772962
39	6	0	2.091128	0.256497	-1.825108
40	7	0	3.449740	0.226173	-1.803993
41	1	0	3.897049	-0.019479	-2.677536
42	6	0	1.447001	0.299294	-3.184261
43	1	0	2.149478	0.106495	-3.995066
44	1	0	0.638455	-0.434559	-3.215480
45	1	0	1.003648	1.289542	-3.326781
46	6	0	4.260225	0.036749	-0.658718
47	6	0	4.258073	0.787990	0.467288
48	1	0	4.894349	0.402355	1.255992
49	6	0	3.575480	2.035396	0.803350
50	6	0	3.501945	2.390394	2.165691
51	6	0	3.059194	2.936300	-0.148958
52	6	0	2.906731	3.584793	2.567004
53	1	0	3.915361	1.718608	2.910929
54	6	0	2.485671	4.140020	0.251951
55	1	0	3.129961	2.709962	-1.204500
56	6	0	2.396725	4.465415	1.609668
57	1	0	2.851261	3.832285	3.621299
58	1	0	2.105741	4.826914	-0.496302
59	1	0	1.941465	5.400647	1.916487
60	6	0	5.206488	-1.101697	-0.835840
61	8	0	5.290188	-1.719474	-1.883973
62	8	0	5.960918	-1.355011	0.235680
63	6	0	6.918708	-2.427055	0.110097
64	1	0	7.420932	-2.475674	1.073591
65	1	0	6.407593	-3.366369	-0.104440
66	1	0	7.632069	-2.202479	-0.683853
67	1	0	-0.514382	0.935541	0.996019
68	1	0	-0.606999	2.052983	-0.760878
69	1	0	-4.717503	-0.627273	0.499189
70	6	0	-3.805947	-0.048489	2.351811
71	1	0	-4.520772	-0.665153	2.904869
72	1	0	-2.836570	-0.152998	2.850757
73	6	0	-4.212433	1.429715	2.332565
74	1	0	-5.252458	1.523327	2.004324
75	1	0	-4.145954	1.879692	3.326731
76	6	0	-3.651163	-2.811752	-0.349919
77	1	0	-4.559190	-3.275722	0.047161
78	1	0	-3.957786	-2.199774	-1.203409
79	6	0	-2.633955	-3.854808	-0.825935
80	1	0	-3.053358	-2.426448	1.687060
81	1	0	-2.497269	-4.622883	-0.059949
82	1	0	-2.979761	-4.362059	-1.731691

TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.283363	-0.507682	0.424806
2	6	0	-2.845999	-1.805709	-0.290178
3	15	0	-2.048494	0.926956	0.351345
4	15	0	-0.989533	-2.018909	-0.561864
5	6	0	-2.304217	1.412169	2.134204
6	1	0	-2.348418	2.496310	2.253328

7	1	0	-1.433104	1.058837	2.690373
8	6	0	-1.151304	-2.717372	-2.275893
9	6	0	-2.854362	2.314196	-0.663861
10	6	0	-3.047936	1.846020	-2.117804
11	1	0	-2.119258	1.471352	-2.555452
12	1	0	-3.808524	1.065473	-2.196907
13	1	0	-3.388422	2.692686	-2.723964
14	6	0	-1.873177	3.500520	-0.645786
15	1	0	-2.294191	4.331229	-1.222710
16	1	0	-1.680708	3.865251	0.366960
17	1	0	-0.920223	3.223998	-1.099775
18	6	0	-4.212813	2.769597	-0.098167
19	1	0	-4.125626	3.187366	0.907423
20	1	0	-4.616790	3.557903	-0.743378
21	1	0	-4.948503	1.961727	-0.075181
22	6	0	-0.348834	-3.429524	0.531966
23	6	0	-0.538904	-3.072692	2.017550
24	1	0	-0.077943	-2.117243	2.270544
25	1	0	-1.595531	-3.041975	2.293348
26	1	0	-0.069441	-3.851575	2.628250
27	6	0	1.150530	-3.637913	0.238810
28	1	0	1.507415	-4.488550	0.829273
29	1	0	1.338838	-3.865572	-0.814193
30	1	0	1.741609	-2.761941	0.509734
31	6	0	-1.107311	-4.739286	0.229174
32	1	0	-0.959565	-5.085788	-0.795784
33	1	0	-0.719671	-5.518107	0.894605
34	1	0	-2.179883	-4.658203	0.419916
35	1	0	-0.481817	-3.565580	-2.426032
36	1	0	-0.853963	-1.933775	-2.973012
37	45	0	0.072857	-0.073105	-0.361493
38	8	0	0.940769	-0.095469	1.744706
39	6	0	1.591338	0.809536	2.287737
40	7	0	2.200684	1.792071	1.581225
41	1	0	2.502671	2.611991	2.091167
42	6	0	1.768621	0.839222	3.782752
43	1	0	2.454552	0.036529	4.069504
44	1	0	2.173065	1.786802	4.139788
45	1	0	0.807988	0.642447	4.260590
46	6	0	2.152218	1.917023	0.170112
47	6	0	2.728925	1.036877	-0.707030
48	1	0	2.578413	1.299109	-1.747313
49	6	0	3.698346	-0.047216	-0.512790
50	6	0	4.160933	-0.691455	-1.679880
51	6	0	4.268121	-0.420660	0.719375
52	6	0	5.139696	-1.678418	-1.620935
53	1	0	3.740645	-0.410601	-2.639885
54	6	0	5.253854	-1.404835	0.776238
55	1	0	3.967011	0.064970	1.634997
56	6	0	5.689538	-2.042467	-0.388083
57	1	0	5.475318	-2.159681	-2.532733
58	1	0	5.683380	-1.672617	1.735205
59	1	0	6.452915	-2.810822	-0.335870
60	6	0	1.716860	3.273325	-0.271812
61	8	0	1.510481	4.172786	0.522595
62	8	0	1.661792	3.421542	-1.597944
63	6	0	1.432452	4.759655	-2.090512
64	1	0	1.403065	4.663553	-3.173396
65	1	0	0.487021	5.149688	-1.713784
66	1	0	2.251369	5.412403	-1.784966
67	1	0	-0.401622	0.078215	-1.811067
68	1	0	1.223249	-0.947072	-1.007102
69	1	0	-3.164707	-2.656516	0.320541
70	1	0	-4.200482	-0.159310	-0.059682
71	6	0	-3.582242	-0.690850	1.933329
72	1	0	-4.533849	-1.213861	2.070134
73	1	0	-2.806199	-1.313882	2.386988
74	6	0	-3.575273	0.683751	2.612033
75	1	0	-3.588999	0.589968	3.702025
76	1	0	-4.466550	1.248651	2.325372
77	6	0	-3.445209	-1.989281	-1.705850
78	1	0	-4.506777	-2.243392	-1.634310
79	1	0	-3.374071	-1.047185	-2.257053
80	6	0	-2.642842	-3.066682	-2.447123
81	1	0	-2.911028	-3.106402	-3.506293
82	1	0	-2.855819	-4.052259	-2.022969

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.166862	0.497549	0.613823
2	6	0	2.828991	1.760472	-0.201421
3	15	0	1.929776	-0.935094	0.482378
4	15	0	1.002112	1.990225	-0.594796
5	6	0	2.032241	-1.363894	2.294467
6	1	0	2.083988	-2.443009	2.447367
7	1	0	1.113154	-1.010459	2.763824
8	6	0	1.278048	2.530831	-2.349736
9	6	0	2.826911	-2.355672	-0.416174
10	6	0	3.050340	-1.981382	-1.892373
11	1	0	2.122786	-1.675967	-2.383332
12	1	0	3.783780	-1.180207	-2.005439
13	1	0	3.441215	-2.854594	-2.425700
14	6	0	1.929547	-3.603431	-0.348955
15	1	0	2.458106	-4.447935	-0.803767
16	1	0	1.674322	-3.887055	0.675011
17	1	0	1.007775	-3.452898	-0.906739
18	6	0	4.183561	-2.687145	0.236502
19	1	0	4.074526	-3.030375	1.267505
20	1	0	4.649280	-3.501678	-0.329095
21	1	0	4.880602	-1.846593	0.221965
22	6	0	0.349798	3.510616	0.331686
23	6	0	0.460915	3.293218	1.852298
24	1	0	-0.027923	2.372105	2.172335
25	1	0	1.501751	3.279047	2.184201
26	1	0	-0.026338	4.131771	2.361584
27	6	0	-1.129342	3.713496	-0.050120
28	1	0	-1.495524	4.624529	0.434916
29	1	0	-1.267565	3.837134	-1.128073
30	1	0	-1.751888	2.881558	0.282790
31	6	0	1.147457	4.773515	-0.054416
32	1	0	1.054476	5.022585	-1.113482
33	1	0	0.746971	5.618788	0.515216
34	1	0	2.208292	4.691741	0.193497
35	1	0	0.623661	3.361936	-2.617477
36	1	0	1.019423	1.687719	-2.991854
37	45	0	-0.190256	0.012047	-0.339384
38	8	0	-0.985826	0.271764	1.774590
39	6	0	-1.591070	-0.733346	2.204259
40	7	0	-1.889946	-1.752190	1.384773
41	1	0	-2.233976	-2.624998	1.762879
42	6	0	-2.019096	-0.825945	3.641809
43	1	0	-2.298505	-1.840390	3.928560
44	1	0	-1.212999	-0.467417	4.283229
45	1	0	-2.883254	-0.171462	3.790192
46	6	0	-1.655693	-1.700010	-0.030095

47	**6**	**0**	**-2.275212**	**-0.699855**	**-0.831263**
48	**1**	**0**	**-2.198117**	**-0.899751**	**-1.892938**
49	**6**	**0**	**-3.482966**	**0.117844**	**-0.491897**
50	**6**	**0**	**-3.783134**	**1.251419**	**-1.268494**
51	**6**	**0**	**-4.424542**	**-0.292040**	**0.465196**
52	**6**	**0**	**-4.963677**	**1.964883**	**-1.079715**
53	**1**	**0**	**-3.079043**	**1.579153**	**-2.026074**
54	**6**	**0**	**-5.609139**	**0.424633**	**0.658124**
55	**1**	**0**	**-4.257945**	**-1.185779**	**1.049985**
56	**6**	**0**	**-5.882239**	**1.558398**	**-0.106218**
57	**1**	**0**	**-5.166873**	**2.837052**	**-1.691522**
58	**1**	**0**	**-6.319930**	**0.084744**	**1.403528**
59	**1**	**0**	**-6.800241**	**2.114986**	**0.046725**
60	**6**	**0**	**-1.442472**	**-3.064411**	**-0.589172**
61	**8**	**0**	**-1.474743**	**-4.062218**	**0.108976**
62	**8**	**0**	**-1.295871**	**-3.089657**	**-1.916292**
63	**6**	**0**	**-1.258946**	**-4.392515**	**-2.537951**
64	**1**	**0**	**-1.139874**	**-4.197487**	**-3.601218**
65	**1**	**0**	**-0.417787**	**-4.973318**	**-2.158543**
66	**1**	**0**	**-2.192311**	**-4.923775**	**-2.346878**
67	**1**	**0**	**0.286766**	**-0.303513**	**-1.761216**
68	**1**	**0**	**-1.125636**	**1.024908**	**-1.091848**
69	**6**	**0**	**3.524754**	**1.841908**	**-1.583057**
70	**1**	**0**	**4.579651**	**2.101688**	**-1.456432**
71	**1**	**0**	**3.490189**	**0.863124**	**-2.069028**
72	**6**	**0**	**3.308747**	**0.746499**	**2.134806**
73	**1**	**0**	**4.239754**	**1.283109**	**2.341480**
74	**1**	**0**	**2.488996**	**1.380998**	**2.483587**
75	**6**	**0**	**2.780126**	**2.859343**	**-2.457257**
76	**1**	**0**	**3.113986**	**2.811052**	**-3.497235**
77	**1**	**0**	**2.974974**	**3.874967**	**-2.102199**
78	**6**	**0**	**3.244772**	**-0.599823**	**2.863647**
79	**1**	**0**	**3.145532**	**-0.464092**	**3.944405**
80	**1**	**0**	**4.165393**	**-1.164423**	**2.692815**
81	**1**	**0**	**3.134699**	**2.635076**	**0.381468**
82	**1**	**0**	**4.122777**	**0.113639**	**0.248172**

TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.219860	0.386402	0.572737
2	6	0	2.911901	1.649253	-0.256264
3	15	0	1.911764	-0.982823	0.500602
4	15	0	1.085727	1.943772	-0.609043
5	6	0	2.007620	-1.361307	2.322248
6	1	0	1.986685	-2.436420	2.507862
7	1	0	1.120836	-0.929234	2.788292
8	6	0	1.342148	2.462962	-2.374866
9	6	0	2.722164	-2.469791	-0.367030
10	6	0	2.980467	-2.133843	-1.846718
11	1	0	2.075394	-1.790432	-2.354033
12	1	0	3.754700	-1.372679	-1.964494
13	1	0	3.331965	-3.035255	-2.359991
14	6	0	1.747554	-3.656972	-0.285035
15	1	0	2.221635	-4.540390	-0.725912
16	1	0	1.473788	-3.907783	0.742952
17	1	0	0.837641	-3.454595	-0.845943
18	6	0	4.050902	-2.872411	0.302575
19	1	0	3.911899	-3.198758	1.335420
20	1	0	4.473937	-3.717815	-0.250950
21	1	0	4.794523	-2.072768	0.287078
22	6	0	0.521796	3.498326	0.319845
23	6	0	0.651588	3.286170	1.839740
24	1	0	0.125874	2.391735	2.177702
25	1	0	1.696495	3.225314	2.152610
26	1	0	0.214288	4.150350	2.351715
27	6	0	-0.954857	3.760586	-0.033241
28	1	0	-1.276838	4.684198	0.459327
29	1	0	-1.108254	3.891845	-1.108286
30	1	0	-1.602770	2.953159	0.311440
31	6	0	1.364293	4.723548	-0.090776
32	1	0	1.261296	4.967985	-1.150052
33	1	0	1.011143	5.589710	0.478998
34	1	0	2.425579	4.598386	0.136605
35	1	0	0.720804	3.322380	-2.632013
36	1	0	1.028767	1.629770	-3.005339
37	45	0	-0.160310	-0.003610	-0.313682
38	8	0	-0.965144	0.307531	1.782842
39	6	0	-1.644668	-0.658096	2.194994
40	7	0	-1.983924	-1.654054	1.365763
41	1	0	-2.400434	-2.500174	1.731048
42	6	0	-2.114205	-0.722664	3.620865
43	1	0	-2.476867	-1.713881	3.895262
44	1	0	-1.299112	-0.429181	4.283817
45	1	0	-2.929598	-0.004969	3.751336
46	6	0	-1.714772	-1.607357	-0.044950
47	6	0	-2.282228	-0.561057	-0.846468
48	1	0	-2.230255	-0.773078	-1.908019
49	6	0	-3.488089	0.261417	-0.487986
50	6	0	-3.710849	1.500908	-1.109749
51	6	0	-4.502250	-0.259165	0.330921
52	6	0	-4.892855	2.208991	-0.903291
53	1	0	-2.950441	1.917104	-1.761681
54	6	0	-5.687225	0.451058	0.542273
55	1	0	-4.389178	-1.231689	0.790482
56	6	0	-5.885885	1.689749	-0.067310
57	1	0	-5.037560	3.165007	-1.394462
58	1	0	-6.455590	0.026098	1.178869
59	1	0	-6.804287	2.241643	0.099578
60	6	0	-1.590169	-2.977467	-0.611331
61	8	0	-1.690173	-3.978181	0.076948
62	8	0	-1.431440	-3.001979	-1.938144
63	6	0	-1.451970	-4.301090	-2.567287
64	1	0	-1.310456	-4.106506	-3.627933
65	1	0	-0.644894	-4.924728	-2.181686
66	1	0	-2.412339	-4.787435	-2.390942
67	1	0	0.318264	-0.351138	-1.728686
68	1	0	-1.190776	0.928054	-1.074564
69	1	0	3.266773	2.519653	0.304251
70	6	0	3.575827	1.681967	-1.655009
71	1	0	4.644228	1.895727	-1.558292
72	1	0	3.485573	0.699987	-2.127472
73	6	0	2.855000	2.722050	-2.522511
74	1	0	3.160852	2.649067	-3.569704
75	1	0	3.102735	3.731334	-2.182824
76	6	0	3.416335	0.656205	2.084877
77	1	0	4.386199	1.132425	2.257776
78	1	0	2.650887	1.352670	2.437482
79	6	0	3.278710	-0.665192	2.849054
80	1	0	3.209961	-0.496202	3.927488
81	1	0	4.156415	-1.293100	2.675970
82	1	0	4.146785	-0.046875	0.186899

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.324026	0.139975	0.623325
2	6	0	-3.313447	-1.094527	-0.300382
3	15	0	-1.766850	1.213042	0.559324
4	15	0	-1.582625	-1.693718	-0.736102
5	6	0	-1.702995	1.516368	2.390578
6	1	0	-1.483158	2.561425	2.611854
7	1	0	-0.886735	0.913024	2.788287
8	6	0	-1.953612	-1.944388	-2.543013
9	6	0	-2.206271	2.876241	-0.238476
10	6	0	-2.575721	2.693130	-1.720572
11	1	0	-1.790215	2.180521	-2.280703
12	1	0	-3.511064	2.143577	-1.844300
13	1	0	-2.718067	3.680873	-2.171011
14	6	0	-0.983244	3.804514	-0.134758
15	1	0	-1.263889	4.798525	-0.498023
16	1	0	-0.623945	3.917081	0.891079
17	1	0	-0.164406	3.443406	-0.754215
18	6	0	-3.394683	3.529126	0.500853
19	1	0	-3.163773	3.760611	1.542763
20	1	0	-3.624996	4.476034	0.001765
21	1	0	-4.300399	2.919985	0.470636
22	6	0	-1.319033	-3.431138	-0.027323
23	6	0	-1.302679	-3.362587	1.510774
24	1	0	-0.578176	-2.633675	1.878248
25	1	0	-2.287191	-3.116230	1.917005
26	1	0	-1.028949	-4.346649	1.906903
27	6	0	0.048254	-3.936595	-0.531589
28	1	0	0.215595	-4.949719	-0.151159
29	1	0	0.099153	-3.981825	-1.622935
30	1	0	0.869137	-3.311309	-0.175996
31	6	0	-2.416451	-4.412283	-0.483593
32	1	0	-2.428715	-4.551896	-1.566761
33	1	0	-2.217053	-5.390309	-0.031844
34	1	0	-3.413805	-4.104084	-0.160649
35	1	0	-1.498833	-2.861531	-2.921141
36	1	0	-1.509791	-1.107978	-3.086492
37	45	0	-0.010582	0.001006	-0.218567
38	8	0	0.759508	-0.678661	1.783847
39	6	0	1.729138	0.018006	2.178170
40	7	0	2.264107	0.937510	1.375816
41	1	0	2.985755	1.554566	1.725812
42	6	0	2.298609	-0.175618	3.555122
43	1	0	3.074448	0.552543	3.792201
44	1	0	1.492145	-0.104480	4.288042
45	1	0	2.722417	-1.180843	3.623652
46	6	0	1.846460	1.081773	-0.001822
47	6	0	2.323225	-0.041941	-0.942705
48	1	0	2.356724	0.352034	-1.955401
49	6	0	3.636170	-0.720050	-0.596589
50	6	0	3.703055	-1.855722	0.218054
51	6	0	4.827340	-0.183678	-1.106981
52	6	0	4.933766	-2.443784	0.521960
53	1	0	2.792348	-2.289811	0.615774
54	6	0	6.058125	-0.768132	-0.803160
55	1	0	4.792615	0.689674	-1.750374
56	6	0	6.115476	-1.900823	0.013756
57	1	0	4.965619	-3.325933	1.152257
58	1	0	6.969304	-0.342314	-1.209343
59	1	0	7.070874	-2.357978	0.246747
60	6	0	2.145125	2.466234	-0.450380
61	8	0	2.497605	3.357922	0.305613
62	8	0	2.011413	2.643246	-1.773869
63	6	0	2.356489	3.944292	-2.289243
64	1	0	2.191260	3.880495	-3.362644
65	1	0	1.717822	4.711729	-1.849954
66	1	0	3.402318	4.169895	-2.075772
67	1	0	-0.403942	0.582314	-1.587929
68	1	0	1.556686	-0.889665	-1.011735
69	6	0	-4.008167	-0.878168	-1.668234
70	1	0	-5.094871	-0.922537	-1.551367
71	1	0	-3.766244	0.118903	-2.044757
72	6	0	-3.474551	-0.192732	2.127603
73	1	0	-4.502034	-0.500800	2.341379
74	1	0	-2.825089	-1.035184	2.383586
75	6	0	-3.490971	-1.921729	-2.666060
76	1	0	-3.795301	-1.678322	-3.687955
77	1	0	-3.905998	-2.906055	-2.432671
78	6	0	-3.056458	1.032187	2.950287
79	1	0	-2.967794	0.788122	4.012245
80	1	0	-3.809755	1.819608	2.860934
81	1	0	-4.161567	0.780919	0.332689
82	1	0	-3.820648	-1.912232	0.219432

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.993847	1.710752	0.422550
2	6	0	-3.686311	0.421721	-0.066190
3	15	0	-1.123435	1.772417	0.082574
4	15	0	-2.526135	-1.033681	-0.269132
5	6	0	-0.736402	2.569038	1.711977
6	1	0	0.288813	2.368415	2.018277
7	1	0	-0.864498	3.651454	1.622062
8	6	0	-3.232098	-1.605363	-1.891143
9	6	0	-0.834037	3.123524	-1.233590
10	6	0	-1.055486	2.546701	-2.643649
11	1	0	-0.405424	1.690577	-2.837836
12	1	0	-2.089600	2.231791	-2.801810
13	1	0	-0.832104	3.319914	-3.386789
14	6	0	0.622669	3.611357	-1.114865
15	1	0	0.792794	4.402506	-1.852603
16	1	0	0.846532	4.025847	-0.128581
17	1	0	1.333609	2.813949	-1.324887
18	6	0	-1.770860	4.332340	-1.029848
19	1	0	-1.704741	4.758142	-0.025714
20	1	0	-1.476671	5.118097	-1.733878
21	1	0	-2.816033	4.094352	-1.236430
22	6	0	-2.961345	-2.358649	1.015280
23	6	0	-2.601561	-1.825375	2.414203
24	1	0	-1.542435	-1.564366	2.485268
25	1	0	-3.194905	-0.948851	2.687003
26	1	0	-2.806910	-2.602502	3.158067
27	6	0	-2.127954	-3.621986	0.723436
28	1	0	-2.375997	-4.384888	1.469219
29	1	0	-2.346072	-4.041565	-0.262297
30	1	0	-1.056938	-3.424378	0.778677
31	6	0	-4.458493	-2.720975	0.966670
32	1	0	-4.751671	-3.141753	0.001850
33	1	0	-4.655917	-3.484508	1.727162
34	1	0	-5.108236	-1.870596	1.186639
35	45	0	-0.266526	-0.336766	-0.316103
36	8	0	0.281884	-2.281569	-1.024593

37	6	0	1.510406	-2.430829	-1.230770
38	7	0	2.361701	-1.440105	-0.966473
39	1	0	3.350998	-1.593588	-1.116160
40	6	0	2.035296	-3.720501	-1.791111
41	1	0	1.389815	-4.046109	-2.608163
42	1	0	3.062354	-3.631202	-2.145726
43	1	0	1.998351	-4.482387	-1.007162
44	6	0	1.973872	-0.243948	-0.239796
45	6	0	2.971587	0.899581	-0.564092
46	1	0	2.715076	1.755860	0.056905
47	6	0	4.431652	0.526200	-0.357559
48	6	0	5.215252	0.122628	-1.449744
49	6	0	5.032750	0.580334	0.909949
50	6	0	6.556398	-0.234139	-1.280985
51	1	0	4.778885	0.102816	-2.444069
52	6	0	6.372024	0.226119	1.081198
53	1	0	4.453999	0.912739	1.763798
54	6	0	7.137813	-0.187165	-0.012809
55	1	0	7.143536	-0.540467	-2.139958
56	1	0	6.818685	0.278927	2.068314
57	1	0	8.178522	-0.460898	0.121740
58	6	0	1.872777	-0.564058	1.248265
59	8	0	1.817668	-1.693151	1.700906
60	8	0	1.907405	0.533259	2.020354
61	6	0	1.851867	0.310859	3.445062
62	1	0	1.894716	1.301310	3.893179
63	1	0	0.922828	-0.192592	3.714867
64	1	0	2.703082	-0.290848	3.766276
65	1	0	0.826231	0.368181	-1.195835
66	1	0	2.834177	1.191185	-1.607250
67	1	0	-4.455014	0.138881	0.657154
68	1	0	-3.439778	2.533078	-0.136131
69	6	0	-3.146932	2.041188	1.943263
70	1	0	-3.548125	3.054806	2.033008
71	1	0	-3.875314	1.375405	2.413192
72	6	0	-1.787794	1.983455	2.665673
73	1	0	-1.818754	2.540348	3.606325
74	1	0	-1.527446	0.950871	2.914804
75	6	0	-4.361202	0.561151	-1.455017
76	6	0	-4.560987	-0.835731	-2.056846
77	1	0	-3.349317	-2.689838	-1.919246
78	1	0	-2.522473	-1.330107	-2.674274
79	1	0	-5.365471	-1.357996	-1.530973
80	1	0	-4.847724	-0.778682	-3.110512
81	1	0	-5.304043	1.107910	-1.362670
82	1	0	-3.716066	1.147241	-2.116938

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.149838	-0.278650	-0.198364
2	8	0	0.633953	-2.074467	-1.282223
3	6	0	1.529123	-2.786061	-0.764115
4	7	0	2.084320	-2.403022	0.382753
5	6	0	1.673141	-1.191313	1.052898
6	6	0	2.281338	0.029068	0.728842
7	1	0	2.192388	0.775966	1.508609
8	1	0	2.807149	-2.968599	0.807131
9	15	0	-2.043024	-0.516046	-1.003456
10	15	0	-0.582454	1.764195	0.631554
11	6	0	3.408346	0.246477	-0.205345
12	6	0	4.523397	0.953858	0.286436
13	6	0	3.440006	-0.196825	-1.538861
14	6	0	5.642912	1.178287	-0.512972
15	1	0	4.512202	1.320919	1.307526
16	6	0	4.558183	0.035797	-2.341229
17	1	0	2.577089	-0.690568	-1.965983
18	6	0	5.666017	0.717484	-1.832450
19	1	0	6.492726	1.716585	-0.107522
20	1	0	4.557206	-0.309176	-3.369545
21	1	0	6.532433	0.897474	-2.459272
22	6	0	1.983689	-4.050368	-1.429415
23	1	0	1.128113	-4.722783	-1.527339
24	1	0	2.337178	-3.812241	-2.435251
25	1	0	2.776776	-4.551905	-0.875563
26	6	0	1.087722	-1.386032	2.421102
27	8	0	1.085337	-0.539877	3.293747
28	8	0	0.604923	-2.624402	2.585928
29	6	0	0.060200	-2.932451	3.885531
30	1	0	-0.247503	-3.974171	3.828417
31	1	0	0.822064	-2.798558	4.654593
32	1	0	-0.796076	-2.290897	4.097994
33	6	0	0.242219	3.323903	-0.103353
34	6	0	-0.468858	4.615165	0.350142
35	1	0	0.052247	5.468746	-0.097234
36	1	0	-1.509601	4.670553	0.026110
37	1	0	-0.434718	4.748832	1.434103
38	6	0	0.214683	3.231250	-1.640336
39	1	0	0.776623	4.071434	-2.062643
40	1	0	0.671829	2.304265	-1.997062
41	1	0	-0.801121	3.289556	-2.036144
42	6	0	1.709786	3.404410	0.359594
43	1	0	1.810458	3.399103	1.448351
44	1	0	2.311660	2.597043	-0.052961
45	1	0	2.137170	4.346695	0.000077
46	6	0	-0.675617	2.070754	2.465936
47	1	0	0.109640	2.754012	2.794489
48	1	0	-0.500049	1.115448	2.961315
49	6	0	-3.003998	-2.038009	-0.383059
50	6	0	-2.254139	-3.316103	-0.805151
51	1	0	-1.278625	-3.384875	-0.325252
52	1	0	-2.846309	-4.185543	-0.499917
53	1	0	-2.108830	-3.377823	-1.886723
54	6	0	-4.428752	-2.082106	-0.970641
55	1	0	-4.944670	-2.956119	-0.557964
56	1	0	-5.023322	-1.203734	-0.710034
57	1	0	-4.426774	-2.191757	-2.057564
58	6	0	-3.085558	-1.990742	1.153269
59	1	0	-2.094399	-1.911710	1.605790
60	1	0	-3.698534	-1.158916	1.508258
61	1	0	-3.551713	-2.913965	1.514026
62	6	0	-2.292475	-0.470798	-2.848436
63	1	0	-2.464214	-1.468429	-3.256431
64	1	0	-1.369011	-0.090469	-3.291123
65	6	0	-2.450666	1.970615	0.361855
66	6	0	-3.084777	1.006747	-0.658291
67	6	0	-3.049148	1.883929	1.784985
68	1	0	-4.052462	2.320702	1.799134
69	1	0	-3.151365	0.835889	2.082710
70	6	0	-3.347601	1.628749	-2.054217
71	1	0	-4.245171	2.253532	-2.026178
72	1	0	-2.513825	2.281910	-2.325574
73	6	0	-3.461140	0.505552	-3.094135
74	1	0	-3.429604	0.903095	-4.112568
75	1	0	-4.416147	-0.014303	-2.981042
76	6	0	-2.097991	2.592728	2.755028

77	1	0	-2.146890	3.674448	2.601203
78	1	0	-2.374418	2.402915	3.796163
79	1	0	-4.040637	0.661523	-0.256184
80	1	0	-2.603698	2.990230	0.001421

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.220716	-0.020177	-0.526466
2	8	0	1.009968	-1.726146	-1.594302
3	6	0	1.752691	-2.473987	-0.909057
4	7	0	1.992306	-2.176576	0.364490
5	6	0	1.547042	-0.934401	0.958114
6	6	0	2.123794	0.303733	0.480230
7	1	0	1.998884	1.088479	1.218727
8	1	0	2.535108	-2.816230	0.928409
9	15	0	-2.023417	-0.905270	-0.853398
10	15	0	-0.863819	1.800192	0.429889
11	6	0	3.443475	0.429283	-0.215019
12	6	0	4.499108	1.004879	0.518985
13	6	0	3.705843	0.036256	-1.536446
14	6	0	5.770037	1.158744	-0.036055
15	1	0	4.319574	1.333404	1.537880
16	6	0	4.978062	0.186396	-2.093817
17	1	0	2.908369	-0.364777	-2.148007
18	6	0	6.017864	0.744477	-1.347313
19	1	0	6.562950	1.604934	0.554901
20	1	0	5.150324	-0.124225	-3.118981
21	1	0	7.003267	0.865164	-1.783916
22	6	0	2.376112	-3.694029	-1.519608
23	1	0	1.635351	-4.205806	-2.135298
24	1	0	3.197415	-3.380581	-2.170242
25	1	0	2.767571	-4.377263	-0.765645
26	6	0	1.211032	-1.069954	2.404033
27	8	0	1.165949	-0.150202	3.199111
28	8	0	1.002940	-2.349796	2.755676
29	6	0	0.725661	-2.598228	4.149602
30	1	0	0.608377	-3.676532	4.231207
31	1	0	1.557422	-2.254620	4.765842
32	1	0	-0.191176	-2.088687	4.448194
33	6	0	-0.263319	3.526942	-0.144091
34	6	0	-1.173923	4.644340	0.411696
35	1	0	-0.743652	5.606902	0.116838
36	1	0	-2.182716	4.602846	-0.004150
37	1	0	-1.243518	4.644828	1.500645
38	6	0	-0.264712	3.646415	-1.680544
39	1	0	-0.029728	4.682107	-1.946277
40	1	0	0.490876	3.017126	-2.149910
41	1	0	-1.236671	3.410905	-2.122512
42	6	0	1.171341	3.743724	0.377648
43	1	0	1.237062	3.663503	1.466389
44	1	0	1.874739	3.037989	-0.066855
45	1	0	1.497531	4.752994	0.104847
46	6	0	-1.049818	1.927782	2.273086
47	1	0	-0.737102	2.925486	2.587115
48	1	0	-0.400266	1.211917	2.771061
49	6	0	-2.601679	-2.546054	-0.091162
50	6	0	-1.780240	-3.684614	-0.726784
51	1	0	-0.715117	-3.579138	-0.516973
52	1	0	-2.109528	-4.641407	-0.307375
53	1	0	-1.913850	-3.736050	-1.810955
54	6	0	-4.101422	-2.811319	-0.327951
55	1	0	-4.361348	-3.771285	0.131797
56	1	0	-4.736620	-2.051003	0.132424
57	1	0	-4.357318	-2.881486	-1.387423
58	6	0	-2.333720	-2.503045	1.423761
59	1	0	-1.280482	-2.324469	1.643392
60	1	0	-2.927171	-1.733006	1.924401
61	1	0	-2.611506	-3.466190	1.865739
62	6	0	-2.560015	-0.960573	-2.640434
63	1	0	-3.135835	-1.869814	-2.826541
64	1	0	-1.690786	-0.979358	-3.299509
65	6	0	-2.718157	1.755703	0.076021
66	6	0	-3.298647	0.377380	-0.341936
67	1	0	0.681951	0.982395	-1.889873
68	1	0	-0.085635	0.735627	-2.106721
69	6	0	-4.260813	0.484981	-1.554979
70	1	0	-5.018245	-0.301417	-1.491416
71	1	0	-4.792919	1.440924	-1.548982
72	6	0	-3.361761	2.263178	1.392967
73	1	0	-3.341718	3.354075	1.429698
74	1	0	-4.412675	1.964135	1.444102
75	6	0	-3.438281	0.291867	-2.839438
76	1	0	-2.805165	1.167891	-3.015811
77	1	0	-4.081718	0.184551	-3.717103
78	6	0	-2.547210	1.694061	2.566674
79	1	0	-2.832790	2.158877	3.514062
80	1	0	-2.736003	0.621100	2.669579
81	1	0	-2.896058	2.463468	-0.736990
82	1	0	-3.830195	-0.032599	0.519416

TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.149707	0.156055	-0.549654
2	8	0	1.052062	-1.350227	-1.882479
3	6	0	1.813545	-2.196164	-1.360031
4	7	0	2.117552	-2.128349	-0.058416
5	6	0	1.652497	-1.068860	0.787735
6	6	0	2.162293	0.250247	0.587765
7	1	0	1.949803	0.899013	1.430719
8	1	0	2.664397	-2.871456	0.354315
9	15	0	-1.976102	-0.934297	-0.778584
10	15	0	-0.964371	1.862631	0.483154
11	6	0	3.505312	0.533512	-0.022148
12	6	0	4.511914	0.947021	0.866616
13	6	0	3.820372	0.398121	-1.379931
14	6	0	5.807092	1.196388	0.410864
15	1	0	4.280377	1.072850	1.919293
16	6	0	5.116293	0.649466	-1.835759
17	1	0	3.048609	0.124662	-2.088377
18	6	0	6.115094	1.044855	-0.943342
19	1	0	6.569878	1.515215	1.112792
20	1	0	5.340278	0.543703	-2.891673
21	1	0	7.119474	1.243564	-1.300691
22	6	0	2.406527	-3.300277	-2.187002
23	1	0	1.610460	-3.784023	-2.756037
24	1	0	3.112613	-2.866936	-2.900269
25	1	0	2.927369	-4.041091	-1.579972
26	6	0	1.207848	-1.467811	2.140153
27	8	0	0.976224	-0.702470	3.060209
28	8	0	1.140963	-2.806173	2.266263

29	6	0	0.828571	-3.315304	3.578531
30	1	0	0.827706	-4.397965	3.472870
31	1	0	1.589041	-3.000545	4.294488
32	1	0	-0.151118	-2.962045	3.901600
33	6	0	-0.686292	3.613583	-0.202673
34	6	0	-1.482697	4.649675	0.620517
35	1	0	-1.318462	5.637859	0.178856
36	1	0	-2.559034	4.463828	0.604425
37	1	0	-1.152536	4.701576	1.659709
38	6	0	-1.129147	3.709523	-1.673478
39	1	0	-0.899017	4.714065	-2.043372
40	1	0	-0.605895	2.993089	-2.310041
41	1	0	-2.205329	3.560230	-1.790180
42	6	0	0.815286	3.950945	-0.102092
43	1	0	1.192684	3.872985	0.921198
44	1	0	1.420929	3.308000	-0.743822
45	1	0	0.965278	4.984654	-0.430379
46	6	0	-0.787939	2.019476	2.323632
47	1	0	-0.131052	2.848832	2.591549
48	1	0	-0.324619	1.101136	2.688273
49	6	0	-2.462112	-2.573761	0.041044
50	6	0	-1.408461	-3.620910	-0.374086
51	1	0	-0.415836	-3.363355	-0.001517
52	1	0	-1.682248	-4.591146	0.054110
53	1	0	-1.351980	-3.744691	-1.459090
54	6	0	-3.858296	-3.052141	-0.403499
55	1	0	-4.087878	-3.987622	0.118848
56	1	0	-4.645116	-2.337853	-0.148497
57	1	0	-3.909671	-3.259055	-1.474645
58	6	0	-2.453933	-2.413976	1.571087
59	1	0	-1.532903	-1.953905	1.933828
60	1	0	-3.298488	-1.815167	1.918610
61	1	0	-2.542838	-3.400905	2.037011
62	6	0	-2.445100	-1.128940	-2.571423
63	1	0	-2.495611	-2.178761	-2.862314
64	1	0	-1.659234	-0.660784	-3.166688
65	6	0	-2.818716	1.506272	0.519127
66	6	0	-3.288759	0.367591	-0.408516
67	1	0	1.373670	1.167055	-0.702279
68	1	0	-0.418390	0.944911	-1.762770
69	1	0	-3.319701	2.428125	0.208545
70	1	0	-4.130048	-0.138316	0.075472
71	6	0	-3.129580	1.271261	2.018275
72	1	0	-4.189715	1.456359	2.213745
73	1	0	-2.934634	0.226412	2.270480
74	6	0	-2.222512	2.165158	2.872748
75	1	0	-2.260901	1.874756	3.926305
76	1	0	-2.552347	3.205199	2.812681
77	6	0	-3.753022	0.833459	-1.809343
78	1	0	-4.727611	1.325740	-1.738929
79	1	0	-3.047954	1.571000	-2.204210
80	6	0	-3.785354	-0.382550	-2.742451
81	1	0	-3.935186	-0.084274	-3.783799
82	1	0	-4.618120	-1.038136	-2.471259

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.032153	0.141642	-0.597063
2	8	0	1.048155	-1.183198	-1.920824
3	6	0	1.985140	-1.843780	-1.395926
4	7	0	2.288057	-1.676310	-0.111692
5	6	0	1.676493	-0.638838	0.687418
6	6	0	2.160006	0.771288	0.378605
7	1	0	1.987399	1.384476	1.262754
8	1	0	3.013108	-2.254412	0.292434
9	15	0	-1.892184	-1.148477	-0.727073
10	15	0	-1.318586	1.717223	0.464876
11	6	0	3.591002	0.913881	-0.109624
12	6	0	4.641949	0.812968	0.813998
13	6	0	3.892661	1.140844	-1.455930
14	6	0	5.967358	0.933298	0.394760
15	1	0	4.422929	0.645590	1.863785
16	6	0	5.220382	1.261593	-1.878230
17	1	0	3.088987	1.229289	-2.180498
18	6	0	6.261287	1.157034	-0.954263
19	1	0	6.769202	0.856880	1.121340
20	1	0	5.436926	1.439253	-2.926098
21	1	0	7.291633	1.252271	-1.278998
22	6	0	2.768486	-2.820629	-2.223221
23	1	0	2.076534	-3.435181	-2.801513
24	1	0	3.395132	-2.265824	-2.926971
25	1	0	3.407218	-3.459451	-1.612575
26	6	0	1.548411	-0.978557	2.106627
27	8	0	1.359786	-0.179326	3.014627
28	8	0	1.661660	-2.309287	2.333228
29	6	0	1.551920	-2.739238	3.701775
30	1	0	1.675971	-3.820229	3.675692
31	1	0	2.333656	-2.281228	4.309818
32	1	0	0.573266	-2.479448	4.108277
33	6	0	-1.279024	3.463964	-0.288562
34	6	0	-2.112696	4.440887	0.567912
35	1	0	-2.069702	5.429721	0.099679
36	1	0	-3.165920	4.155803	0.622812
37	1	0	-1.725139	4.546663	1.582762
38	6	0	-1.842358	3.462846	-1.720047
39	1	0	-1.748746	4.472587	-2.133123
40	1	0	-1.299308	2.781619	-2.377983
41	1	0	-2.902823	3.200756	-1.743961
42	6	0	0.185372	3.947921	-0.318368
43	1	0	0.648769	3.942468	0.672116
44	1	0	0.799301	3.349390	-0.995023
45	1	0	0.207821	4.980011	-0.682898
46	6	0	-1.109077	1.944929	2.292864
47	1	0	-0.553934	2.856343	2.521136
48	1	0	-0.517238	1.104788	2.660959
49	6	0	-1.985809	-2.809950	0.177126
50	6	0	-0.795015	-3.677020	-0.277052
51	1	0	0.154687	-3.261467	0.058902
52	1	0	-0.897597	-4.671441	0.169461
53	1	0	-0.760217	-3.805891	-1.361846
54	6	0	-3.303381	-3.536583	-0.169903
55	1	0	-3.328264	-4.476660	0.391198
56	1	0	-4.189742	-2.966273	0.117456
57	1	0	-3.378522	-3.789873	-1.229383
58	6	0	-1.915046	-2.599281	1.699381
59	1	0	-1.061907	-1.984705	1.990713
60	1	0	-2.827139	-2.143486	2.090273
61	1	0	-1.807492	-3.574176	2.185706
62	6	0	-2.377642	-1.495305	-2.485617
63	1	0	-2.244538	-2.547049	-2.739849
64	1	0	-1.716076	-0.911773	-3.126700
65	6	0	-3.101980	1.124373	0.564565
66	6	0	-3.399015	-0.103961	-0.318568
67	1	0	1.542831	1.284978	-0.443156
68	1	0	-0.724249	0.856738	-1.813199

69	1	0	-4.100956	-0.751965	0.213906
70	1	0	-3.737188	1.950054	0.231532
71	6	0	-4.002021	0.217748	-1.708119
72	1	0	-5.049519	0.513687	-1.602150
73	1	0	-3.469993	1.063150	-2.153741
74	6	0	-3.840475	-1.014651	-2.608755
75	1	0	-4.082939	-0.783165	-3.649077
76	1	0	-4.523618	-1.805055	-2.284884
77	6	0	-3.346248	0.898311	2.077816
78	1	0	-4.415941	0.955661	2.297778
79	1	0	-3.014392	-0.105634	2.352242
80	6	0	-2.535821	1.924351	2.881105
81	1	0	-2.509863	1.662407	3.942426
82	1	0	-2.996343	2.912731	2.804257

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.149707	0.156055	-0.549654
2	8	0	1.052062	-1.350227	-1.882479
3	6	0	1.813545	-2.196164	-1.360031
4	7	0	2.117552	-2.128349	-0.058416
5	6	0	1.652497	-1.068860	0.787735
6	6	0	2.162293	0.250247	0.587765
7	1	0	1.949803	0.899013	1.430719
8	1	0	2.664397	-2.871456	0.354315
9	15	0	-1.976102	-0.934297	-0.778584
10	15	0	-0.964371	1.862631	0.483154
11	6	0	3.505312	0.533512	-0.022148
12	6	0	4.511914	0.947021	0.866616
13	6	0	3.820372	0.398121	-1.379931
14	6	0	5.807092	1.196388	0.410864
15	1	0	4.280377	1.072850	1.919293
16	6	0	5.116293	0.649466	-1.835759
17	1	0	3.048609	0.124662	-2.088377
18	6	0	6.115094	1.044855	-0.943342
19	1	0	6.569878	1.515215	1.112792
20	1	0	5.340278	0.543703	-2.891673
21	1	0	7.119474	1.243564	-1.300691
22	6	0	2.406527	-3.300277	-2.187002
23	1	0	1.610460	-3.784023	-2.756037
24	1	0	3.112613	-2.866936	-2.900269
25	1	0	2.927369	-4.041091	-1.579972
26	6	0	1.207848	-1.467811	2.140153
27	8	0	0.976224	-0.702470	3.060209
28	8	0	1.140963	-2.806173	2.266263
29	6	0	0.828571	-3.315304	3.578531
30	1	0	0.827706	-4.397965	3.472870
31	1	0	1.589041	-3.000545	4.294488
32	1	0	-0.151118	-2.962045	3.901600
33	6	0	-0.686292	3.613583	-0.202673
34	6	0	-1.482697	4.649675	0.620517
35	1	0	-1.318462	5.637859	0.178856
36	1	0	-2.559034	4.463828	0.604425
37	1	0	-1.152536	4.701576	1.659709
38	6	0	-1.129147	3.709523	-1.673478
39	1	0	-0.899017	4.714065	-2.043372
40	1	0	-0.605895	2.993089	-2.310041
41	1	0	-2.205329	3.560230	-1.790180
42	6	0	0.815286	3.950945	-0.102092
43	1	0	1.192684	3.872985	0.921198
44	1	0	1.420929	3.308000	-0.743822
45	1	0	0.965278	4.984654	-0.430379
46	6	0	-0.787939	2.019476	2.323632
47	1	0	-0.131052	2.848832	2.591549
48	1	0	-0.324619	1.101136	2.688273
49	6	0	-2.462112	-2.573761	0.041044
50	6	0	-1.408461	-3.620910	-0.374086
51	1	0	-0.415836	-3.363355	-0.001517
52	1	0	-1.682248	-4.591146	0.054110
53	1	0	-1.351980	-3.744691	-1.459090
54	6	0	-3.858296	-3.052141	-0.403499
55	1	0	-4.087878	-3.987622	0.118848
56	1	0	-4.645116	-2.337853	-0.148497
57	1	0	-3.909671	-3.259055	-1.474645
58	6	0	-2.453933	-2.413976	1.571087
59	1	0	-1.532903	-1.953905	1.933828
60	1	0	-3.298488	-1.815167	1.918610
61	1	0	-2.542838	-3.400905	2.037011
62	6	0	-2.445100	-1.128940	-2.571423
63	1	0	-2.495611	-2.178761	-2.862314
64	1	0	-1.659234	-0.660784	-3.166688
65	6	0	-2.818716	1.506272	0.519127
66	6	0	-3.288759	0.367591	-0.408516
67	1	0	1.373670	1.167055	-0.702279
68	1	0	-0.418390	0.944911	-1.762770
69	1	0	-3.319701	2.428125	0.208545
70	1	0	-4.130048	-0.138316	0.075472
71	6	0	-3.129580	1.271261	2.018275
72	1	0	-4.189715	1.456359	2.213745
73	1	0	-2.934634	0.226412	2.270480
74	6	0	-2.222512	2.165158	2.872748
75	1	0	-2.260901	1.874756	3.926305
76	1	0	-2.552347	3.205199	2.812681
77	6	0	-3.753022	0.833459	-1.809343
78	1	0	-4.727611	1.325740	-1.738929
79	1	0	-3.047954	1.571000	-2.204210
80	6	0	-3.785354	-0.382550	-2.742451
81	1	0	-3.935186	-0.084274	-3.783799
82	1	0	-4.618120	-1.038136	-2.471259

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.032153	0.141642	-0.597063
2	8	0	1.048155	-1.183198	-1.920824
3	6	0	1.985140	-1.843780	-1.395926
4	7	0	2.288057	-1.676310	-0.111692
5	6	0	1.676493	-0.638838	0.687418
6	6	0	2.160006	0.771288	0.378605
7	1	0	1.987399	1.384476	1.262754
8	1	0	3.013108	-2.254412	0.292434
9	15	0	-1.892184	-1.148477	-0.727073
10	15	0	-1.318586	1.717223	0.464876
11	6	0	3.591002	0.913881	-0.109624
12	6	0	4.641949	0.812968	0.813998
13	6	0	3.892661	1.140844	-1.455930
14	6	0	5.967358	0.933298	0.394760
15	1	0	4.422929	0.645590	1.863785
16	6	0	5.220382	1.261593	-1.878230
17	1	0	3.088987	1.229289	-2.180498
18	6	0	6.261287	1.157034	-0.954263

19	1	0	6.769202	0.856880	1.121340
20	1	0	5.436926	1.439253	-2.926098
21	1	0	7.291633	1.252271	-1.278998
22	6	0	2.768486	-2.820629	-2.223221
23	1	0	2.076534	-3.435181	-2.801513
24	1	0	3.395132	-2.265824	-2.926971
25	1	0	3.407218	-3.459451	-1.612575
26	6	0	1.548411	-0.978557	2.106627
27	8	0	1.359786	-0.179326	3.014627
28	8	0	1.661660	-2.309287	2.333228
29	6	0	1.551920	-2.739238	3.701775
30	1	0	1.675971	-3.820229	3.675692
31	1	0	2.333656	-2.281228	4.309818
32	1	0	0.573266	-2.479448	4.108277
33	6	0	-1.279024	3.463964	-0.288562
34	6	0	-2.112696	4.440887	0.567912
35	1	0	-2.069702	5.429721	0.099679
36	1	0	-3.165920	4.155803	0.622812
37	1	0	-1.725139	4.546663	1.582762
38	6	0	-1.842358	3.462846	-1.720047
39	1	0	-1.748746	4.472587	-2.133123
40	1	0	-1.299308	2.781619	-2.377983
41	1	0	-2.902823	3.200756	-1.743961
42	6	0	0.185372	3.947921	-0.318368
43	1	0	0.648769	3.942468	0.672116
44	1	0	0.799301	3.349390	-0.995023
45	1	0	0.207821	4.980011	-0.682898
46	6	0	-1.109077	1.944929	2.292864
47	1	0	-0.553934	2.856343	2.521136
48	1	0	-0.517238	1.104788	2.660959
49	6	0	-1.985809	-2.809950	0.177126
50	6	0	-0.795015	-3.677020	-0.277052
51	1	0	0.154687	-3.261467	0.058902
52	1	0	-0.897597	-4.671441	0.169461
53	1	0	-0.760217	-3.805891	-1.361846
54	6	0	-3.303381	-3.536583	-0.169903
55	1	0	-3.328264	-4.476660	0.391198
56	1	0	-4.189742	-2.966273	0.117456
57	1	0	-3.378522	-3.789873	-1.229383
58	6	0	-1.915046	-2.599281	1.699381
59	1	0	-1.061907	-1.984705	1.990713
60	1	0	-2.827139	-2.143486	2.090273
61	1	0	-1.807492	-3.574176	2.185706
62	6	0	-2.377642	-1.495305	-2.485617
63	1	0	-2.244538	-2.547049	-2.739849
64	1	0	-1.716076	-0.911773	-3.126700
65	6	0	-3.101980	1.124373	0.564565
66	6	0	-3.399015	-0.103961	-0.318568
67	1	0	1.542831	1.284978	-0.443156
68	1	0	-0.724249	0.856738	-1.813199
69	1	0	-4.100956	-0.751965	0.213906
70	1	0	-3.737188	1.950054	0.231532
71	6	0	-4.002021	0.217748	-1.708119
72	1	0	-5.049519	0.513687	-1.602150
73	1	0	-3.469993	1.063150	-2.153741
74	6	0	-3.840475	-1.014651	-2.608755
75	1	0	-4.082939	-0.783165	-3.649077
76	1	0	-4.523618	-1.805055	-2.284884
77	6	0	-3.346248	0.898311	2.077816
78	1	0	-4.415941	0.955661	2.297778
79	1	0	-3.014392	-0.105634	2.352242
80	6	0	-2.535821	1.924351	2.881105
81	1	0	-2.509863	1.662407	3.942426
82	1	0	-2.996343	2.912731	2.804257

TS8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.261134	-0.264309	-0.338440
2	8	0	0.321456	-2.141426	-1.182589
3	6	0	1.557743	-2.278138	-1.347919
4	7	0	2.396904	-1.315001	-0.971372
5	6	0	1.984109	-0.136559	-0.227544
6	6	0	2.969762	1.025757	-0.524144
7	1	0	2.707393	1.850550	0.135877
8	1	0	3.390281	-1.448871	-1.113532
9	15	0	-2.519097	-0.965942	-0.397264
10	15	0	-1.128828	1.788695	0.273286
11	6	0	4.434687	0.662699	-0.336074
12	6	0	5.038107	0.678732	0.932058
13	6	0	5.221654	0.312901	-1.444284
14	6	0	6.383924	0.341747	1.086076
15	1	0	4.452739	0.963925	1.798414
16	6	0	6.569335	-0.026911	-1.292111
17	1	0	4.782314	0.321982	-2.437448
18	6	0	7.153757	-0.016429	-0.024526
19	1	0	6.832751	0.364887	2.073442
20	1	0	7.159124	-0.291203	-2.163172
21	1	0	8.199630	-0.276278	0.097233
22	6	0	2.106181	-3.528689	-1.970716
23	1	0	1.508545	-3.784929	-2.846837
24	1	0	3.153298	-3.426586	-2.255841
25	1	0	2.015191	-4.346240	-1.249761
26	6	0	1.889633	-0.383397	1.273267
27	8	0	1.959071	0.498863	2.109545
28	8	0	1.781597	-1.684259	1.589203
29	6	0	1.710116	-1.995788	2.995222
30	1	0	1.617133	-3.078444	3.045619
31	1	0	2.618343	-1.665313	3.500969
32	1	0	0.841877	-1.514630	3.447552
33	6	0	-0.848379	3.284300	-0.873085
34	6	0	-1.742122	4.479870	-0.482688
35	1	0	-1.471166	5.332681	-1.114220
36	1	0	-2.803675	4.286093	-0.646646
37	1	0	-1.603406	4.790212	0.555607
38	6	0	-1.139463	2.888363	-2.332761
39	1	0	-0.891605	3.729780	-2.988985
40	1	0	-0.545236	2.026286	-2.645541
41	1	0	-2.193893	2.652080	-2.494246
42	6	0	0.623757	3.722932	-0.759669
43	1	0	0.908897	3.975969	0.264930
44	1	0	1.301369	2.956159	-1.131175
45	1	0	0.774938	4.616177	-1.374929
46	6	0	-0.725739	2.354118	1.990070
47	1	0	0.289839	2.063356	2.254641
48	1	0	-0.812006	3.442525	2.051386
49	6	0	-2.971077	-2.439566	0.710356
50	6	0	-2.137342	-3.662261	0.280191
51	1	0	-1.066414	-3.474405	0.362116
52	1	0	-2.390992	-4.505289	0.932046
53	1	0	-2.351521	-3.966166	-0.748031
54	6	0	-4.468083	-2.789097	0.601612
55	1	0	-4.677586	-3.631434	1.270090
56	1	0	-5.118096	-1.965357	0.905260
57	1	0	-4.748044	-3.099245	-0.407907
58	6	0	-2.629951	-2.077810	2.167468

59	1	0	-1.571699	-1.830648	2.285737
60	1	0	-3.225221	-1.237269	2.533455
61	1	0	-2.847452	-2.936518	2.811499
62	6	0	-3.213375	-1.331793	-2.081097
63	6	0	-2.999787	1.685877	0.597668
64	6	0	-3.687474	0.449756	-0.020691
65	1	0	2.822341	1.355747	-1.554329
66	1	0	0.834839	0.513676	-1.150826
67	1	0	-4.442952	0.081679	0.677916
68	1	0	-3.450421	2.557652	0.124043
69	6	0	-3.151024	1.858121	2.143757
70	1	0	-3.513806	2.871262	2.340502
71	1	0	-3.907188	1.174061	2.538082
72	6	0	-1.797903	1.674248	2.855671
73	1	0	-1.821238	2.102199	3.861831
74	1	0	-1.560866	0.611863	2.965230
75	6	0	-4.385700	0.737562	-1.376604
76	1	0	-5.340663	1.243589	-1.208100
77	1	0	-3.764775	1.418032	-1.966982
78	6	0	-4.558752	-0.578664	-2.145318
79	1	0	-4.853192	-0.397772	-3.182823
80	1	0	-5.348185	-1.180188	-1.686005
81	1	0	-2.510382	-0.939215	-2.818812
82	1	0	-3.304147	-2.405511	-2.252625

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.828425	1.485781	0.294366
2	6	0	-3.200405	-0.012432	0.183444
3	15	0	-1.019210	1.826164	-0.086801
4	15	0	-1.775853	-1.264492	0.113544
5	6	0	-0.616859	2.537140	1.588297
6	1	0	0.338089	2.153956	1.946316
7	1	0	-0.525563	3.621165	1.496395
8	6	0	-2.557772	-2.312967	-1.218206
9	6	0	-0.967246	3.319398	-1.269823
10	6	0	-1.298606	2.855805	-2.700586
11	1	0	-0.555226	2.154720	-3.084203
12	1	0	-2.287379	2.391829	-2.767332
13	1	0	-1.304734	3.726547	-3.364929
14	6	0	0.452056	3.922843	-1.239587
15	1	0	0.490850	4.765642	-1.938589
16	1	0	0.714851	4.308609	-0.251255
17	1	0	1.205914	3.196460	-1.542940
18	6	0	-1.980304	4.403469	-0.848530
19	1	0	-1.802297	4.779983	0.161222
20	1	0	-1.877618	5.253692	-1.531591
21	1	0	-3.015523	4.061026	-0.913611
22	6	0	-1.918734	-2.342034	1.686519
23	6	0	-1.541153	-1.523010	2.932482
24	1	0	-0.564396	-1.043567	2.845831
25	1	0	-2.287034	-0.754944	3.146241
26	1	0	-1.508753	-2.191187	3.799305
27	6	0	-0.992532	-3.563839	1.558203
28	1	0	-1.133586	-4.197649	2.440496
29	1	0	-1.229965	-4.171512	0.681340
30	1	0	0.060502	-3.300755	1.503858
31	6	0	-3.360689	-2.867095	1.864565
32	1	0	-3.668375	-3.526421	1.051060
33	1	0	-3.386534	-3.458795	2.785890
34	1	0	-4.102750	-2.074710	1.973953
35	1	0	-2.475760	-3.373441	-0.977292
36	1	0	-2.007611	-2.151515	-2.144927
37	45	0	0.131317	-0.172918	-0.713165
38	8	0	1.648350	0.928548	-1.806951
39	6	0	2.770010	0.369205	-1.890626
40	7	0	2.956880	-0.809962	-1.301947
41	1	0	3.878001	-1.227903	-1.328344
42	6	0	3.891694	1.019836	-2.642778
43	1	0	4.157752	1.956606	-2.146969
44	1	0	4.773671	0.382761	-2.704155
45	1	0	3.544393	1.262543	-3.649319
46	6	0	1.918355	-1.431574	-0.509040
47	6	0	1.543996	-0.813224	0.755314
48	1	0	1.067251	-1.535979	1.404949
49	6	0	2.392765	0.107684	1.569666
50	6	0	2.878563	1.360259	1.158793
51	6	0	2.741258	-0.335023	2.861534
52	6	0	3.701575	2.122092	1.990793
53	1	0	2.586815	1.769820	0.202494
54	6	0	3.562704	0.424318	3.694688
55	1	0	2.370530	-1.293049	3.211588
56	6	0	4.052988	1.658241	3.259968
57	1	0	4.058687	3.086785	1.646232
58	1	0	3.816183	0.052277	4.681657
59	1	0	4.690040	2.253711	3.904669
60	6	0	1.951573	-2.923090	-0.609603
61	8	0	1.915937	-3.650328	0.366638
62	8	0	2.088467	-3.527909	-1.808538
63	6	0	1.905335	-2.886155	-3.084155
64	1	0	1.580995	-3.676903	-3.759532
65	1	0	1.141878	-2.112588	-3.030915
66	1	0	2.847183	-2.466485	-3.438159
67	1	0	-0.835789	0.036327	-2.389127
68	1	0	-0.413049	-0.616079	-2.502231
69	1	0	-3.803453	-0.282680	1.052839
70	6	0	-4.028496	-0.319478	-1.090547
71	1	0	-5.044966	0.067983	-0.974213
72	1	0	-3.587939	0.203127	-1.946636
73	6	0	-3.084310	2.157370	1.671043
74	1	0	-3.397193	3.190776	1.496784
75	1	0	-3.906670	1.665339	2.198437
76	1	0	-3.419146	2.007549	-0.460836
77	6	0	-4.016292	-1.827936	-1.356042
78	1	0	-4.403873	-2.058307	-2.352068
79	1	0	-4.657939	-2.340852	-0.635377
80	6	0	-1.793664	2.161805	2.508548
81	1	0	-1.870852	2.866386	3.341386
82	1	0	-1.617435	1.178828	2.945120

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Standard orientation:

Center Number	**Atomic Number**	**Atomic Type**	**Coordinates (Angstroms) X**	**Y**	**Z**
1	**6**	**0**	**-2.311877**	**2.115608**	**-0.001770**
2	**6**	**0**	**-3.096504**	**0.781065**	**0.019643**
3	**15**	**0**	**-0.456062**	**1.923041**	**-0.240612**
4	**15**	**0**	**-2.114615**	**-0.835033**	**0.080579**
5	**6**	**0**	**0.010347**	**2.715471**	**1.379641**
6	**1**	**0**	**0.803405**	**2.152726**	**1.869575**
7	**1**	**0**	**0.390950**	**3.719492**	**1.181977**
8	**6**	**0**	**-3.200914**	**-1.726135**	**-1.147007**

9	6	0	0.048091	3.187223	-1.571732
10	6	0	-0.356786	2.661274	-2.962116
11	1	0	0.155048	1.730593	-3.209472
12	1	0	-1.435442	2.497320	-3.043039
13	1	0	-0.083742	3.408133	-3.715578
14	6	0	1.577893	3.376067	-1.515294
15	1	0	1.873259	4.090575	-2.291445
16	1	0	1.908826	3.782615	-0.555920
17	1	0	2.106574	2.441298	-1.700711
18	6	0	-0.630301	4.553062	-1.338397
19	1	0	-0.382659	4.989322	-0.368414
20	1	0	-0.274092	5.248969	-2.105643
21	1	0	-1.717599	4.502693	-1.429236
22	6	0	-2.528104	-1.672704	1.745994
23	6	0	-1.963319	-0.858666	2.922535
24	1	0	-0.900922	-0.635001	2.815568
25	1	0	-2.501695	0.082074	3.053566
26	1	0	-2.090584	-1.434610	3.844871
27	6	0	-1.933238	-3.090782	1.752831
28	1	0	-2.255140	-3.598399	2.668595
29	1	0	-2.281794	-3.692225	0.908959
30	1	0	-0.846268	-3.087794	1.742137
31	6	0	-4.057438	-1.793041	1.931102
32	1	0	-4.522039	-2.438492	1.183588
33	1	0	-4.236741	-2.251877	2.909317
34	1	0	-4.571127	-0.829768	1.931690
35	1	0	-3.431383	-2.736214	-0.806692
36	1	0	-2.646000	-1.815322	-2.079781
37	45	0	0.029702	-0.412414	-0.768557
38	8	0	1.743527	0.096407	-2.010147
39	6	0	2.743660	-0.650287	-1.907120
40	7	0	2.738297	-1.640617	-1.012807
41	1	0	3.563680	-2.218526	-0.915557
42	6	0	3.949042	-0.435854	-2.773447
43	1	0	4.681137	-1.236494	-2.670592
44	1	0	3.624543	-0.365447	-3.813324
45	1	0	4.418547	0.513808	-2.504458
46	6	0	1.626263	-1.859428	-0.118311
47	6	0	1.411772	-0.978771	0.979665
48	1	0	0.747041	-1.423279	1.708740
49	6	0	2.362471	-0.042204	1.624291
50	6	0	2.354141	-0.023091	3.035083
51	6	0	3.278869	0.803071	0.972514
52	6	0	3.228429	0.784782	3.760810
53	1	0	1.656955	-0.660449	3.568884
54	6	0	4.157046	1.609011	1.697207
55	1	0	3.294734	0.874812	-0.103815
56	6	0	4.140795	1.605272	3.093981
57	1	0	3.195287	0.770793	4.844851
58	1	0	4.849176	2.251519	1.163659
59	1	0	4.822452	2.237264	3.652231
60	6	0	1.303200	-3.321587	0.056586
61	8	0	1.103935	-3.799607	1.157366
62	8	0	1.304323	-4.171404	-0.983642
63	6	0	1.336649	-3.816971	-2.381298
64	1	0	0.881417	-4.662575	-2.894914
65	1	0	0.761163	-2.913510	-2.574256
66	1	0	2.366629	-3.697613	-2.716691
67	1	0	-0.846663	-0.165898	-2.075384
68	1	0	-0.407377	-1.363380	-1.977030
69	6	0	-2.464359	3.008112	1.259657
70	1	0	-2.463381	4.056053	0.946506
71	1	0	-3.424739	2.828153	1.751271
72	6	0	-4.001854	0.616103	-1.228158
73	1	0	-4.850017	1.304304	-1.166459
74	1	0	-3.430678	0.890580	-2.122186
75	6	0	-4.451546	-0.843925	-1.338679
76	1	0	-5.199394	-1.065709	-0.573492
77	1	0	-4.915131	-1.044308	-2.308448
78	6	0	-1.282697	2.771706	2.215370
79	1	0	-1.410312	1.831818	2.754007
80	1	0	-1.221225	3.562093	2.968720
81	1	0	-3.734806	0.771759	0.906356
82	1	0	-2.677050	2.671495	-0.867420

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.953601	1.290305	0.550176
2	6	0	-3.419453	-0.182500	0.502953
3	15	0	-1.292944	1.635239	-0.292564
4	15	0	-2.067383	-1.468262	0.186510
5	6	0	-0.656032	2.701639	1.098497
6	1	0	-0.111876	3.569289	0.720598
7	1	0	0.052847	2.100554	1.673638
8	6	0	-3.119529	-2.532831	-0.917840
9	6	0	-1.599434	2.828197	-1.735255
10	6	0	-2.413648	2.104976	-2.824393
11	1	0	-1.928028	1.182401	-3.151919
12	1	0	-3.424444	1.861397	-2.486551
13	1	0	-2.511524	2.761683	-3.695769
14	6	0	-0.218245	3.210376	-2.306790
15	1	0	-0.357400	3.874094	-3.167501
16	1	0	0.393850	3.746373	-1.575428
17	1	0	0.337858	2.331073	-2.636619
18	6	0	-2.343583	4.109123	-1.313896
19	1	0	-1.778891	4.693691	-0.583849
20	1	0	-2.485362	4.741874	-2.197509
21	1	0	-3.334177	3.902432	-0.900782
22	6	0	-1.744483	-2.481048	1.753875
23	6	0	-1.038820	-1.596984	2.798884
24	1	0	-0.121566	-1.150649	2.405889
25	1	0	-1.684083	-0.794225	3.162092
26	1	0	-0.767009	-2.211599	3.663680
27	6	0	-0.820029	-3.660833	1.387677
28	1	0	-0.644006	-4.260387	2.287046
29	1	0	-1.263723	-4.318754	0.635676
30	1	0	0.144782	-3.316238	1.012978
31	6	0	-3.055293	-3.034884	2.345749
32	1	0	-3.574691	-3.701832	1.653507
33	1	0	-2.814706	-3.618917	3.240718
34	1	0	-3.745843	-2.245732	2.651464
35	1	0	-3.015860	-3.589652	-0.667730
36	1	0	-2.757454	-2.400230	-1.938263
37	45	0	-0.249799	-0.529410	-0.721462
38	8	0	1.524259	0.275302	-1.781397
39	6	0	2.727510	0.103895	-2.012976
40	7	0	3.561993	-0.611724	-1.220624
41	1	0	4.518989	-0.694749	-1.536661
42	6	0	3.342551	0.719229	-3.245202
43	1	0	3.168856	1.797392	-3.221290
44	1	0	4.412463	0.528818	-3.331621
45	1	0	2.831890	0.320267	-4.124969
46	6	0	3.223297	-1.259037	0.001829
47	6	0	3.022532	-0.596435	1.167112
48	1	0	2.752198	-1.249633	1.989970

49	6	0	3.130761	0.810849	1.542355
50	6	0	2.698712	1.146241	2.844006
51	6	0	3.686245	1.834171	0.745504
52	6	0	2.796172	2.448776	3.326498
53	1	0	2.286726	0.369135	3.479046
54	6	0	3.790847	3.134119	1.232999
55	1	0	4.060786	1.617657	-0.243855
56	6	0	3.342573	3.449709	2.519961
57	1	0	2.453990	2.679756	4.328982
58	1	0	4.228217	3.904179	0.607366
59	1	0	3.425923	4.465076	2.891271
60	6	0	3.206853	-2.760226	0.068054
61	8	0	3.238824	-3.339377	1.139188
62	8	0	3.244253	-3.525958	-1.036001
63	6	0	2.803947	-3.154622	-2.361095
64	1	0	2.529717	-4.097042	-2.833988
65	1	0	1.930156	-2.506473	-2.315704
66	1	0	3.617651	-2.693108	-2.919437
67	1	0	-1.016160	-0.702456	-2.011308
68	1	0	0.221296	-2.023580	-1.021373
69	1	0	-3.870557	-0.427430	1.469153
70	6	0	-4.470403	-0.485282	-0.592177
71	1	0	-5.434414	-0.045617	-0.319526
72	1	0	-4.162340	-0.025184	-1.536823
73	6	0	-4.561123	-2.005442	-0.774872
74	1	0	-5.159720	-2.269239	-1.651019
75	1	0	-5.046879	-2.457311	0.095446
76	6	0	-2.797990	1.845379	1.989253
77	1	0	-3.779773	2.078275	2.413014
78	1	0	-2.351402	1.079116	2.629500
79	6	0	-1.876473	3.069923	1.965555
80	1	0	-1.568826	3.354654	2.976336
81	1	0	-2.401320	3.927378	1.536056
82	1	0	-3.706122	1.893879	0.034079
