

SUPPORTING INFORMATION

Chalcogen Noncovalent Interactions between Diazines and Sulfur Oxides in Supramolecular Circular Chains

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Table S2. Cartesian coordinates of all systems under analysis together with ADF total bonding energy (in kcal mol⁻¹, in parentheses).

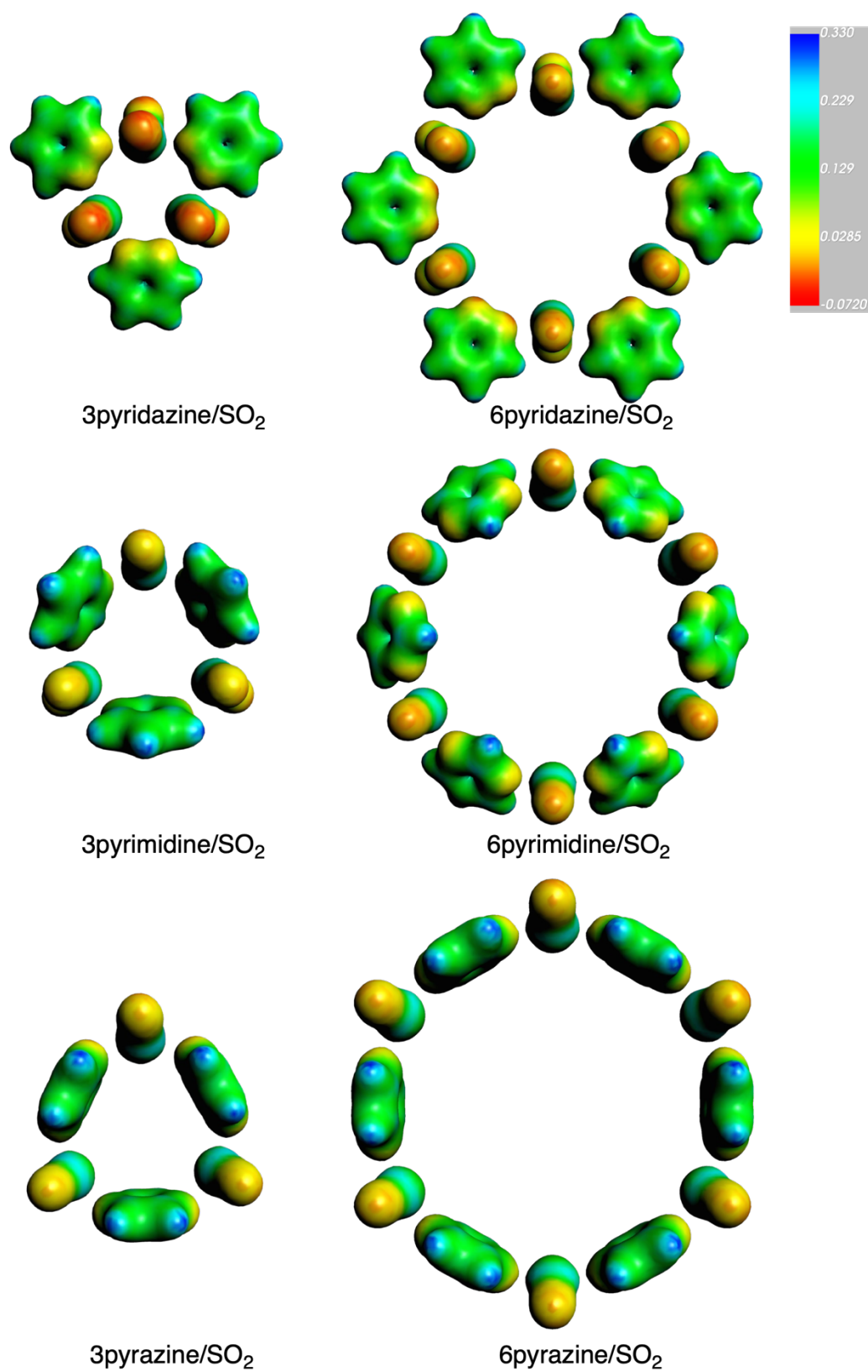


Figure S1. Molecular electrostatic potential isosurface (electronic density isovalue = 0.03 a.u.) of complexes of SO_2 with pyridazine, pyrimidine, pyrazine with 3 and 6 units.

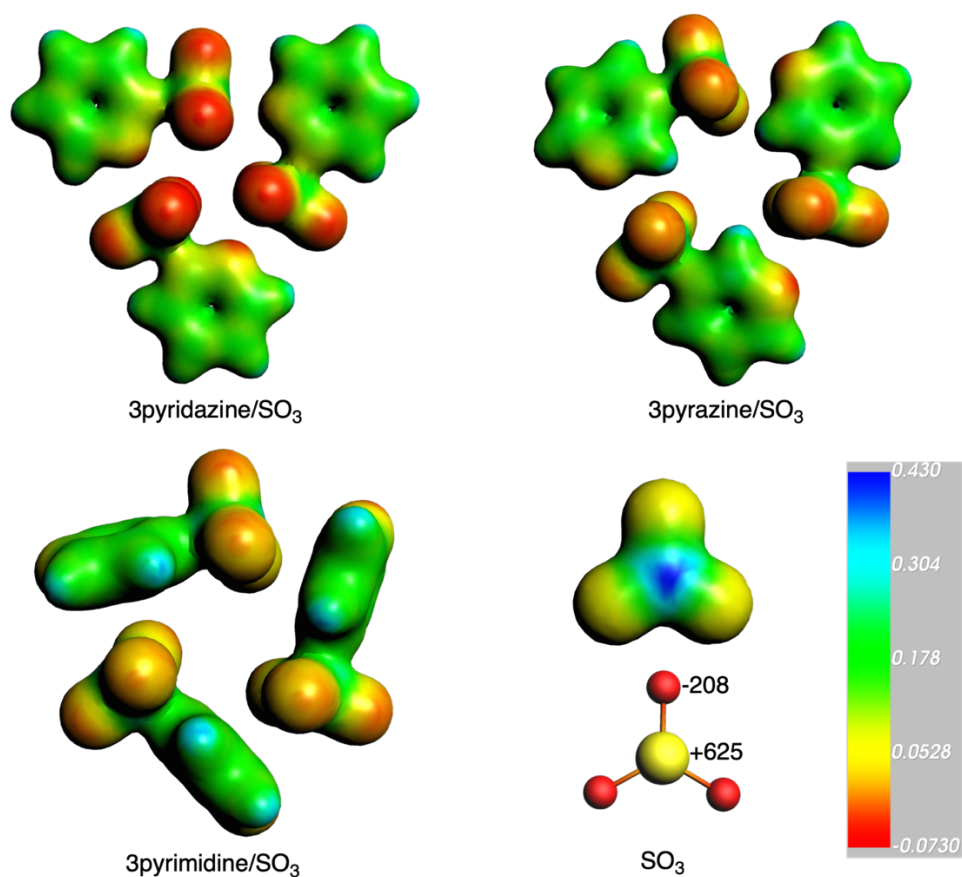


Figure S2. Molecular electrostatic potential isosurface (electronic density isovalue = 0.03 a.u.) of complexes of SO_3 with pyridazine, pyrimidine, pyrazine with 3units, together with SO_3 and its VDD charges (in milli-au).

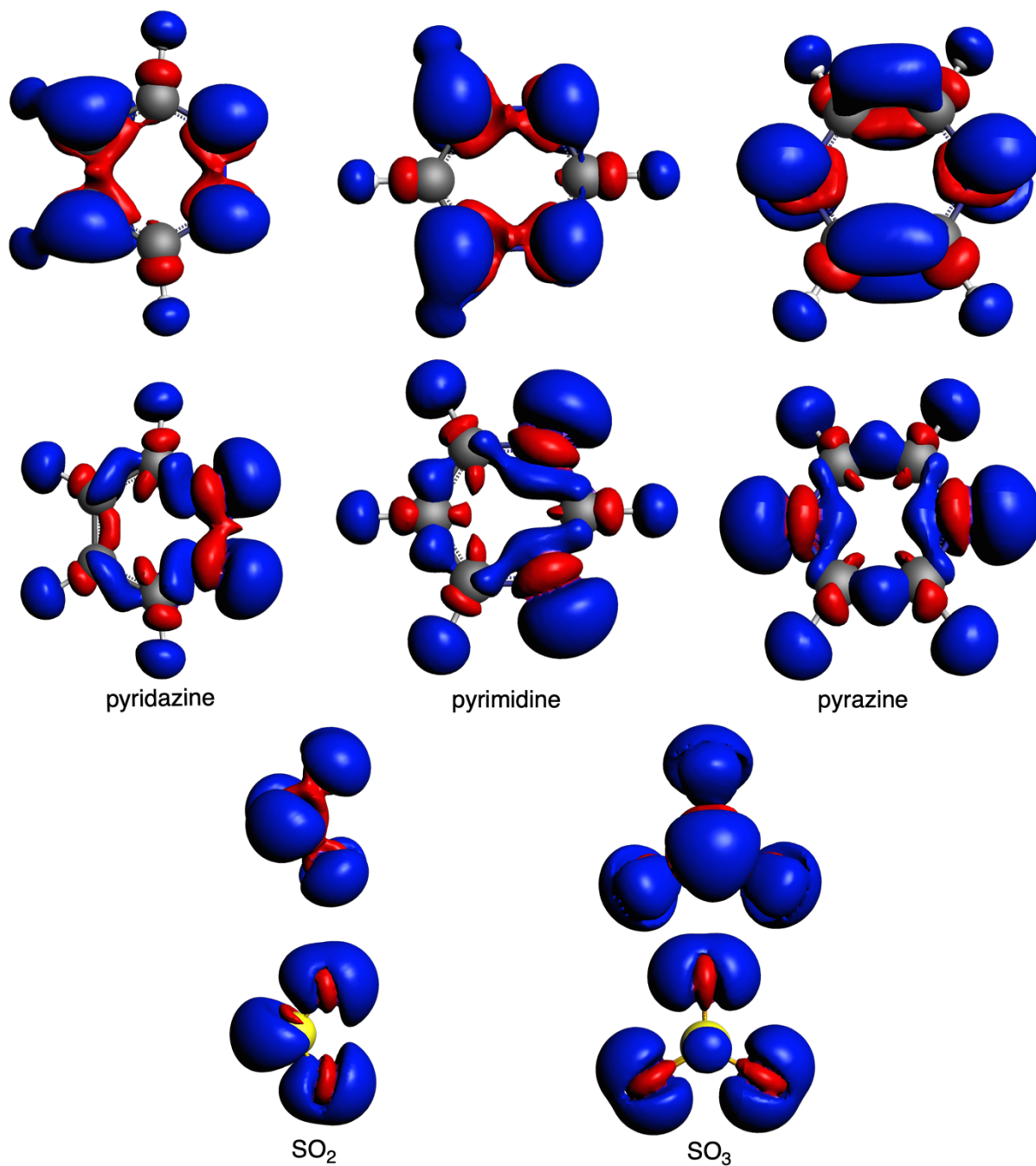


Figure S3. Fukui plus (top) and Fukui minus (bottom) functions of the diazines under analysis (isovalue = 0.003).

Table S1. Energy decomposition analysis (in kcal mol⁻¹) divided by the number of molecules for each system (2n) of the SO₂ complexes with pyridazine, pyrimidine and pyrazine.^a

	ΔE_{int}	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{oi}	ΔE_{disp}
pyridazine					
3	-8.1	19.4	-14.2	-9.2	-4.1
4	-8.1	17.9	-13.2	-8.7	-4.1
5	-7.5	14.4	-10.9	-7.0	-3.9
6	-6.9	12.7	-9.7	-5.9	-4.0
pyrimidine					
3	-6.5	14.4	-10.4	-6.6	-3.9
4	-7.1	16.4	-11.9	-7.7	-3.9
5	-7.5	17.8	-13.0	-8.4	-3.9
6	-7.7	18.5	-13.5	-8.7	-4.0
pyrazine					
3	-5.7	14.3	-9.7	-6.4	-3.8
4	-6.3	15.9	-11.2	-7.2	-3.8
5	-6.6	17.9	-12.6	-8.0	-3.9
6	-6.7	19.1	-13.4	-8.5	-3.9

^a Computed at BLYP-D3(BJ)/TZ2P level of theory. $\Delta E_{\text{int}} = \Delta E_{\text{Pauli}} + \Delta V_{\text{elstat}} + \Delta E_{\text{oi}} + \Delta E_{\text{disp}}$.

Table S2. Cartesian coordinates of all systems under analysis together with ADF total bonding energy (in kcal mol⁻¹, in parentheses).

SO2 (-369.2)

1	S	0.00000000	0.00000000	-0.49332231
2	O	0.00000000	1.26307942	0.24666115
3	O	-0.00000000	-1.26307942	0.24666115

Pyridazine (-1447.6)

1	H	-0.00000000	-1.27268473	-1.73645540
2	N	0.00000000	0.67387623	1.60532402
3	N	-0.00000000	-0.67387623	1.60532402
4	C	-0.00000000	1.32920836	0.43232669
5	C	0.00000000	-1.32920836	0.43232669
6	C	0.00000000	-0.69386114	-0.81574004
7	C	-0.00000000	0.69386114	-0.81574004
8	H	-0.00000000	2.41535178	0.51454473
9	H	0.00000000	-2.41535178	0.51454473
10	H	0.00000000	1.27268473	-1.73645540

2pyridazine/SO2 (-3658.2)

1	C	3.73913148	-1.33557828	0.01061238
2	C	3.73913148	1.33557828	0.01061238
3	C	4.92694265	0.69391848	-0.36304399
4	C	4.92694265	-0.69391848	-0.36304399
5	H	3.65091638	-2.42033047	0.02984551
6	H	3.65091638	2.42033047	0.02984551
7	H	5.80454418	1.27125247	-0.64267315
8	H	5.80454418	-1.27125247	-0.64267315
9	O	0.00000000	2.75951409	1.60137260
10	O	0.00000000	2.39757529	-0.87551064
11	S	0.00000000	1.81226964	0.47550778
12	N	2.63220349	0.66904839	0.36457438
13	N	2.63220349	-0.66904839	0.36457438
14	S	-0.00000000	-1.81226964	0.47550778
15	O	-0.00000000	-2.75951409	1.60137260
16	O	-0.00000000	-2.39757529	-0.87551064
17	C	-3.73913148	-1.33557828	0.01061238
18	C	-3.73913148	1.33557828	0.01061238
19	C	-4.92694265	-0.69391848	-0.36304399
20	H	-3.65091638	-2.42033047	0.02984551
21	C	-4.92694265	0.69391848	-0.36304399
22	H	-3.65091638	2.42033047	0.02984551
23	H	-5.80454418	-1.27125247	-0.64267315
24	H	-5.80454418	1.27125247	-0.64267315
25	N	-2.63220349	-0.66904839	0.36457438
26	N	-2.63220349	0.66904839	0.36457438

3pyridazine/SO2 (-5496.3)

1	C	3.46164224	3.31657358	-0.11519200
2	C	1.14141585	4.65615691	-0.11519200
3	C	2.30995966	5.38990083	-0.35522464
4	C	3.51281121	4.69543416	-0.35522464
5	H	4.34773419	2.68358453	-0.11143104
6	H	0.15018529	5.10704053	-0.11143104
7	H	2.26418646	6.46070347	-0.53678879
8	H	4.46304010	5.19119472	-0.53678879
9	O	-1.46862382	-2.54373109	1.92491791
10	O	-1.90709116	-3.30317878	-0.41274945

11	N	1.15917828	3.33823632	0.11939038
12	N	2.31140831	2.67299600	0.11939038
13	O	2.93724765	-0.00000000	1.92491791
14	C	3.46164224	-3.31657358	-0.11519200
15	C	1.14141585	-4.65615691	-0.11519200
16	C	3.51281121	-4.69543416	-0.35522464
17	H	4.34773419	-2.68358453	-0.11143104
18	C	2.30995966	-5.38990083	-0.35522464
19	H	0.15018529	-5.10704053	-0.11143104
20	H	4.46304010	-5.19119472	-0.53678879
21	H	2.26418646	-6.46070347	-0.53678879
22	N	2.31140831	-2.67299600	0.11939038
23	N	1.15917828	-3.33823632	0.11939038
24	S	-1.31968864	2.28576777	0.48632370
25	O	-1.46862382	2.54373109	1.92491791
26	O	-1.90709116	3.30317878	-0.41274945
27	S	2.63937727	-0.00000000	0.48632370
28	S	-1.31968864	-2.28576777	0.48632370
29	C	-4.60305809	-1.33958333	-0.11519200
30	C	-5.82277087	-0.69446667	-0.35522464
31	H	-4.49791948	-2.42345599	-0.11143104
32	C	-4.60305809	1.33958333	-0.11519200
33	C	-5.82277087	0.69446667	-0.35522464
34	H	-6.72722656	-1.26950875	-0.53678879
35	H	-4.49791948	2.42345599	-0.11143104
36	H	-6.72722656	1.26950875	-0.53678879
37	N	-3.47058659	-0.66524032	0.11939038
38	N	-3.47058659	0.66524032	0.11939038
39	O	3.81418231	-0.00000000	-0.41274945

4pyridazine/SO2 (-7328.7)

1	C	5.69534913	-1.33784610	0.16113778
2	C	6.92531250	-0.69408554	0.34284090
3	H	5.59237430	-2.42146294	0.15367488
4	C	5.69534913	1.33784610	0.16113778
5	C	6.92531250	0.69408554	0.34284090
6	H	7.83699267	-1.27057475	0.47842380
7	H	5.59237430	2.42146294	0.15367488
8	H	7.83699267	1.27057475	0.47842380
9	C	1.33784610	5.69534913	0.16113778
10	C	0.69408554	6.92531250	0.34284090
11	H	2.42146294	5.59237430	0.15367488
12	C	-1.33784610	5.69534913	0.16113778
13	C	-0.69408554	6.92531250	0.34284090
14	H	1.27057475	7.83699267	0.47842380
15	H	-2.42146294	5.59237430	0.15367488
16	H	-1.27057475	7.83699267	0.47842380
17	C	-5.69534913	1.33784610	0.16113778
18	C	-5.69534913	-1.33784610	0.16113778
19	C	-6.92531250	0.69408554	0.34284090
20	H	-5.59237430	2.42146294	0.15367488
21	C	-6.92531250	-0.69408554	0.34284090
22	H	-5.59237430	-2.42146294	0.15367488
23	H	-7.83699267	1.27057475	0.47842380
24	H	-7.83699267	-1.27057475	0.47842380
25	C	-1.33784610	-5.69534913	0.16113778
26	C	-0.69408554	-6.92531250	0.34284090
27	H	-2.42146294	-5.59237430	0.15367488
28	C	1.33784610	-5.69534913	0.16113778
29	C	0.69408554	-6.92531250	0.34284090

30	H	-1.27057475	-7.83699267	0.47842380
31	H	2.42146294	-5.59237430	0.15367488
32	H	1.27057475	-7.83699267	0.47842380
33	N	0.66666112	-4.54871932	-0.01220674
34	N	-0.66666112	-4.54871932	-0.01220674
35	N	-4.54871932	-0.66666112	-0.01220674
36	N	-4.54871932	0.66666112	-0.01220674
37	N	-0.66666112	4.54871932	-0.01220674
38	N	0.66666112	4.54871932	-0.01220674
39	N	4.54871932	0.66666112	-0.01220674
40	N	4.54871932	-0.66666112	-0.01220674
41	O	3.54371151	3.54371151	0.15986669
42	O	2.58112968	2.58112968	-1.93702557
43	O	2.58112968	-2.58112968	-1.93702557
44	O	3.54371151	-3.54371151	0.15986669
45	O	-3.54371151	-3.54371151	0.15986669
46	O	-2.58112968	-2.58112968	-1.93702557
47	O	-2.58112968	2.58112968	-1.93702557
48	O	-3.54371151	3.54371151	0.15986669
49	S	2.59603160	2.59603160	-0.47058236
50	S	2.59603160	-2.59603160	-0.47058236
51	S	-2.59603160	-2.59603160	-0.47058236
52	S	-2.59603160	2.59603160	-0.47058236

5pyridazine/SO2 (-9155.7)

1	C	-6.96264136	1.33441967	-0.13053530
2	C	-6.96264136	-1.33441967	-0.13053530
3	C	-8.20672179	0.69332596	-0.10584665
4	H	-6.86772668	2.41811195	-0.14280983
5	C	-8.20672179	-0.69332596	-0.10584665
6	H	-6.86772668	-2.41811195	-0.14280983
7	H	-9.12655051	1.27261684	-0.08894971
8	H	-9.12655051	-1.27261684	-0.08894971
9	C	-0.88246599	7.03422379	-0.13053530
10	C	-1.87662433	8.01930574	-0.10584665
11	H	0.17751687	7.27883391	-0.14280983
12	C	-3.42068304	6.20950708	-0.13053530
13	C	-3.19540868	7.59080674	-0.10584665
14	H	-1.60992867	9.07312556	-0.08894971
15	H	-4.42200538	5.78435853	-0.14280983
16	H	-4.03058975	8.28660509	-0.08894971
17	C	6.41724739	3.01296972	-0.13053530
18	C	7.04690417	4.26287756	-0.10584665
19	H	6.97743815	2.08045480	-0.14280983
20	C	4.84854298	5.17210610	-0.13053530
21	C	6.23185063	5.38470253	-0.10584665
22	H	8.13155987	4.33488314	-0.08894971
23	H	4.13477706	5.99304212	-0.14280983
24	H	6.63550905	6.39402044	-0.08894971
25	C	4.84854298	-5.17210610	-0.13053530
26	C	6.23185063	-5.38470253	-0.10584665
27	H	4.13477706	-5.99304212	-0.14280983
28	C	6.41724739	-3.01296972	-0.13053530
29	C	7.04690417	-4.26287756	-0.10584665
30	H	6.63550905	-6.39402044	-0.08894971
31	H	6.97743815	-2.08045480	-0.14280983
32	H	8.13155987	-4.33488314	-0.08894971
33	C	-3.42068304	-6.20950708	-0.13053530
34	C	-0.88246599	-7.03422379	-0.13053530
35	C	-3.19540868	-7.59080674	-0.10584665

36	H	-4.42200538	-5.78435853	-0.14280983
37	C	-1.87662433	-8.01930574	-0.10584665
38	H	0.17751687	-7.27883391	-0.14280983
39	H	-4.03058975	-8.28660509	-0.08894971
40	H	-1.60992867	-9.07312556	-0.08894971
41	N	5.08475879	2.86798697	-0.14493571
42	N	4.29889457	3.94963627	-0.14493571
43	N	-1.15634081	5.72214970	-0.14493571
44	N	-2.42789583	5.30899642	-0.14493571
45	N	-5.79941672	0.66849603	-0.14493571
46	N	-5.79941672	-0.66849603	-0.14493571
47	N	-2.42789583	-5.30899642	-0.14493571
48	N	-1.15634081	-5.72214970	-0.14493571
49	N	4.29889457	-3.94963627	-0.14493571
50	N	5.08475879	-2.86798697	-0.14493571
51	S	1.49614704	-4.60466714	0.13633791
52	S	-3.91696383	-2.84584080	0.13633791
53	S	-3.91696383	2.84584080	0.13633791
54	S	1.49614704	4.60466714	0.13633791
55	S	4.84163355	0.00000000	0.13633791
56	O	-3.90913639	-2.84015383	1.60236757
57	O	-4.99215748	-3.62701472	-0.51255110
58	O	-4.99215748	3.62701472	-0.51255110
59	O	-3.90913639	2.84015383	1.60236757
60	O	1.90683448	5.86863309	-0.51255110
61	O	1.49315723	4.59546544	1.60236757
62	O	4.83195830	0.00000000	1.60236757
63	O	6.17064600	0.00000000	-0.51255110
64	O	1.49315723	-4.59546544	1.60236757
65	O	1.90683448	-5.86863309	-0.51255110

6pyridazine/SO2 (-10980.7)

1	C	-5.21930796	6.37372314	-0.06918853
2	C	-2.91015217	7.70691485	-0.06918853
3	C	-5.28353560	7.76508454	0.06746970
4	H	-6.11470256	5.75750173	-0.09405097
5	C	-4.08299268	8.45821833	0.06746970
6	H	-1.92879148	8.17423863	-0.09405097
7	H	-6.24276489	8.26698399	0.16699221
8	H	-4.03803571	9.53988498	0.16699221
9	C	-8.12946013	-1.33319171	-0.06918853
10	C	-9.36652828	-0.69313378	0.06746970
11	H	-8.04349404	-2.41673689	-0.09405097
12	C	-8.12946013	1.33319171	-0.06918853
13	C	-9.36652828	0.69313378	0.06746970
14	H	-10.28080060	-1.27290098	0.16699221
15	H	-8.04349404	2.41673689	-0.09405097
16	H	-10.28080060	1.27290098	0.16699221
17	C	-2.91015217	-7.70691485	-0.06918853
18	C	-4.08299268	-8.45821833	0.06746970
19	H	-1.92879148	-8.17423863	-0.09405097
20	C	-5.21930796	-6.37372314	-0.06918853
21	C	-5.28353560	-7.76508454	0.06746970
22	H	-4.03803571	-9.53988498	0.16699221
23	H	-6.11470256	-5.75750173	-0.09405097
24	H	-6.24276489	-8.26698399	0.16699221
25	C	5.21930796	-6.37372314	-0.06918853
26	C	5.28353560	-7.76508454	0.06746970
27	H	6.11470256	-5.75750173	-0.09405097
28	C	2.91015217	-7.70691485	-0.06918853

29	C	4.08299268	-8.45821833	0.06746970
30	H	6.24276489	-8.26698399	0.16699221
31	H	1.92879148	-8.17423863	-0.09405097
32	H	4.03803571	-9.53988498	0.16699221
33	C	8.12946013	1.33319171	-0.06918853
34	C	9.36652828	0.69313378	0.06746970
35	H	8.04349404	2.41673689	-0.09405097
36	C	8.12946013	-1.33319171	-0.06918853
37	C	9.36652828	-0.69313378	0.06746970
38	H	10.28080060	1.27290098	0.16699221
39	H	8.04349404	-2.41673689	-0.09405097
40	H	10.28080060	-1.27290098	0.16699221
41	C	2.91015217	7.70691485	-0.06918853
42	C	5.21930796	6.37372314	-0.06918853
43	C	4.08299268	8.45821833	0.06746970
44	H	1.92879148	8.17423863	-0.09405097
45	C	5.28353560	7.76508454	0.06746970
46	H	6.11470256	5.75750173	-0.09405097
47	H	4.03803571	9.53988498	0.16699221
48	H	6.24276489	8.26698399	0.16699221
49	O	5.42881880	-3.13433000	1.33582674
50	O	6.20907826	-3.58481301	-0.99662835
51	O	5.42881880	3.13433000	1.33582674
52	O	6.20907826	3.58481301	-0.99662835
53	O	-0.00000000	6.26865999	1.33582674
54	O	0.00000000	7.16962600	-0.99662835
55	O	-5.42881880	3.13433000	1.33582674
56	O	-6.20907826	3.58481301	-0.99662835
57	O	-6.20907826	-3.58481301	-0.99662835
58	O	-5.42881880	-3.13433000	1.33582674
59	O	0.00000000	-6.26865999	1.33582674
60	O	-0.00000000	-7.16962600	-0.99662835
61	S	-0.00000000	-5.99417107	-0.10578078
62	S	5.19110442	-2.99708553	-0.10578078
63	S	5.19110442	2.99708553	-0.10578078
64	S	0.00000000	5.99417107	-0.10578078
65	S	-5.19110442	2.99708553	-0.10578078
66	S	-5.19110442	-2.99708553	-0.10578078
67	N	4.06462502	-5.70179117	-0.18793120
68	N	2.90558350	-6.37096410	-0.18793120
69	N	-2.90558350	-6.37096410	-0.18793120
70	N	-4.06462502	-5.70179117	-0.18793120
71	N	-6.97020850	-0.66917293	-0.18793120
72	N	-6.97020850	0.66917293	-0.18793120
73	N	-4.06462502	5.70179117	-0.18793120
74	N	-2.90558350	6.37096410	-0.18793120
75	N	2.90558350	6.37096410	-0.18793120
76	N	4.06462502	5.70179117	-0.18793120
77	N	6.97020850	0.66917293	-0.18793120
78	N	6.97020850	-0.66917293	-0.18793120

Pyrimidine (-1468.4)

1	C	-3.58709353	3.83378711	0.00000000
2	C	-2.92257743	5.06205260	0.00000000
3	H	-4.67590648	3.77940341	0.00000000
4	C	-1.52661026	5.02340767	0.00000000
5	H	-3.46626797	6.00375223	0.00000000
6	H	-0.93510612	5.93915550	0.00000000
7	N	-2.92654729	2.66185100	0.00000000
8	C	-1.58474240	2.74485435	0.00000000

9	H	-1.03960952	1.80065651	0.00000000
10	N	-0.84195694	3.86538979	0.00000000

3pyrimidine/SO2 (-5550.2)

1	C	1.02019464	4.14754583	-0.65430123
2	C	2.17720683	3.77103283	-1.33825588
3	H	0.23050183	4.72928569	-1.12849577
4	C	3.08178274	2.95728739	-0.65430123
5	H	2.35161637	4.07311903	-2.36734523
6	H	3.98043064	2.56426329	-1.12849577
7	N	0.80495605	3.78088846	0.62098861
8	C	2.17720683	-3.77103283	-1.33825588
9	C	1.02019464	-4.14754583	-0.65430123
10	H	2.35161637	-4.07311903	-2.36734523
11	H	0.23050183	-4.72928569	-1.12849577
12	S	-1.97603367	3.42259071	0.99290515
13	S	-1.97603367	-3.42259071	0.99290515
14	C	1.74840919	3.02833354	1.20469107
15	H	1.58058680	2.73765664	2.24129771
16	N	2.87186743	2.58755662	0.62098861
17	S	3.95206734	0.00000000	0.99290515
18	O	-2.50490669	-4.33862567	2.00979296
19	O	-2.18950543	-3.79233465	-0.41946900
20	O	-2.50490669	4.33862567	2.00979296
21	O	-2.18950543	3.79233465	-0.41946900
22	O	5.00981340	-0.00000000	2.00979296
23	O	4.37901086	0.00000000	-0.41946900
24	C	-4.10197738	-1.19025844	-0.65430123
25	C	-3.49681836	0.00000000	1.20469107
26	C	-4.35441365	-0.00000000	-1.33825588
27	H	-4.21093247	-2.16502241	-1.12849577
28	H	-3.16117360	0.00000000	2.24129771
29	C	-4.10197738	1.19025844	-0.65430123
30	H	-4.70323274	-0.00000000	-2.36734523
31	H	-4.21093247	2.16502241	-1.12849577
32	N	-3.67682348	-1.19333184	0.62098861
33	N	-3.67682348	1.19333184	0.62098861
34	C	3.08178274	-2.95728739	-0.65430123
35	H	3.98043064	-2.56426329	-1.12849577
36	C	1.74840919	-3.02833354	1.20469107
37	H	1.58058680	-2.73765664	2.24129771
38	N	2.87186743	-2.58755662	0.62098861
39	N	0.80495605	-3.78088846	0.62098861

4pyrimidine/SO2 (-7405.0)

1	C	1.19054082	5.50476715	-0.63916226
2	C	-0.00000000	5.83529942	-1.28919984
3	H	2.16789788	5.67329901	-1.09094148
4	C	-1.19054082	5.50476715	-0.63916226
5	H	-0.00000000	6.30510157	-2.26907942
6	H	-2.16789788	5.67329901	-1.09094148
7	N	1.19214586	4.93082458	0.57601829
8	S	-3.63460618	3.63460618	0.95432116
9	S	3.63460618	3.63460618	0.95432116
10	C	-5.50476715	-1.19054082	-0.63916226
11	C	-5.83529942	-0.00000000	-1.28919984
12	H	-5.67329901	-2.16789788	-1.09094148
13	C	-5.50476715	1.19054082	-0.63916226
14	H	-6.30510157	-0.00000000	-2.26907942
15	H	-5.67329901	2.16789788	-1.09094148

16	N	-4.93082458	-1.19214586	0.57601829
17	C	1.19054082	-5.50476715	-0.63916226
18	C	-1.19054082	-5.50476715	-0.63916226
19	C	0.00000000	-5.83529942	-1.28919984
20	H	2.16789788	-5.67329901	-1.09094148
21	H	-2.16789788	-5.67329901	-1.09094148
22	H	0.00000000	-6.30510157	-2.26907942
23	N	-1.19214586	-4.93082458	0.57601829
24	C	5.50476715	1.19054082	-0.63916226
25	C	5.83529942	0.00000000	-1.28919984
26	H	5.67329901	2.16789788	-1.09094148
27	C	5.50476715	-1.19054082	-0.63916226
28	H	6.30510157	0.00000000	-2.26907942
29	H	5.67329901	-2.16789788	-1.09094148
30	N	4.93082458	1.19214586	0.57601829
31	S	-3.63460618	-3.63460618	0.95432116
32	S	3.63460618	-3.63460618	0.95432116
33	C	-4.68162312	0.00000000	1.13591981
34	C	0.00000000	4.68162312	1.13591981
35	C	4.68162312	-0.00000000	1.13591981
36	C	-0.00000000	-4.68162312	1.13591981
37	H	-0.00000000	-4.22878897	2.12678194
38	H	4.22878897	-0.00000000	2.12678194
39	H	-4.22878897	0.00000000	2.12678194
40	H	0.00000000	4.22878897	2.12678194
41	N	-1.19214586	4.93082458	0.57601829
42	N	-4.93082458	1.19214586	0.57601829
43	N	1.19214586	-4.93082458	0.57601829
44	N	4.93082458	-1.19214586	0.57601829
45	O	-4.31473819	-4.31473819	2.06252074
46	O	-4.03030167	-4.03030167	-0.41309347
47	O	4.03030167	4.03030167	-0.41309347
48	O	4.31473819	4.31473819	2.06252074
49	O	4.31473819	-4.31473819	2.06252074
50	O	4.03030167	-4.03030167	-0.41309347
51	O	-4.31473819	4.31473819	2.06252074
52	O	-4.03030167	4.03030167	-0.41309347

5pyrimidine/SO2 (-9259.4)

1	C	1.80316995	5.54958646	0.99189934
2	C	1.02434903	7.00572176	-0.59653419
3	C	3.28914415	6.26984522	-0.59653419
4	C	2.29371877	7.05934051	-1.17553742
5	H	0.17258068	7.55201043	-1.00177851
6	H	4.29933966	6.21114516	-1.00177851
7	H	2.49299185	7.67263997	-2.05016721
8	C	-4.72076021	3.42983305	0.99189934
9	C	-6.34629607	3.13910091	-0.59653419
10	C	-4.94657571	5.06565070	-0.59653419
11	C	-6.00503371	4.36291237	-1.17553742
12	H	-7.12905838	2.49783355	-1.00177851
13	H	-4.57858106	6.00826441	-1.00177851
14	H	-6.52673739	4.74195228	-2.05016721
15	C	-4.72076021	-3.42983305	0.99189934
16	C	-4.94657571	-5.06565070	-0.59653419
17	C	-6.34629607	-3.13910091	-0.59653419
18	C	-6.00503371	-4.36291237	-1.17553742
19	H	-4.57858106	-6.00826441	-1.00177851
20	H	-7.12905838	-2.49783355	-1.00177851
21	H	-6.52673739	-4.74195228	-2.05016721

22	C	1.80316995	-5.54958646	0.99189934
23	C	3.28914415	-6.26984522	-0.59653419
24	C	1.02434903	-7.00572176	-0.59653419
25	C	2.29371877	-7.05934051	-1.17553742
26	H	4.29933966	-6.21114516	-1.00177851
27	H	0.17258068	-7.55201043	-1.00177851
28	H	2.49299185	-7.67263997	-2.05016721
29	C	5.83518053	0.00000000	0.99189934
30	C	6.97937859	1.19067326	-0.59653419
31	C	6.97937859	-1.19067326	-0.59653419
32	C	7.42262987	0.00000000	-1.17553742
33	H	7.23571910	2.16956559	-1.00177851
34	H	7.23571910	-2.16956559	-1.00177851
35	H	8.06749109	-0.00000000	-2.05016721
36	N	6.18724010	-1.19105166	0.48889933
37	N	6.18724010	1.19105166	0.48889933
38	N	3.04471978	5.51635982	0.48889933
39	N	0.77920489	6.25247022	0.48889933
40	N	-4.30549979	4.60034952	0.48889933
41	N	-5.70566500	2.67318745	0.48889933
42	N	-4.30549979	-4.60034952	0.48889933
43	N	-5.70566500	-2.67318745	0.48889933
44	N	0.77920489	-6.25247022	0.48889933
45	N	3.04471978	-5.51635982	0.48889933
46	H	-4.20926906	-3.05821299	1.87907530
47	H	-4.20926906	3.05821299	1.87907530
48	H	1.60779771	-4.94829255	1.87907530
49	H	5.20294268	0.00000000	1.87907530
50	H	1.60779771	4.94829255	1.87907530
51	S	-6.28809282	-0.00000000	0.86273397
52	S	-1.94312754	-5.98033165	0.86273397
53	S	5.08717395	-3.69604823	0.86273397
54	S	5.08717395	3.69604823	0.86273397
55	S	-1.94312754	5.98033165	0.86273397
56	O	-2.18243964	-6.71685857	2.10936150
57	O	-2.18127016	-6.71325925	-0.39853875
58	O	5.71063941	-4.14902239	-0.39853875
59	O	5.71370117	-4.15124690	2.10936150
60	O	-2.18243964	6.71685857	2.10936150
61	O	-2.18127016	6.71325925	-0.39853875
62	O	-7.05873850	-0.00000000	-0.39853875
63	O	-7.06252305	-0.00000000	2.10936150
64	O	5.71063941	4.14902239	-0.39853875
65	O	5.71370117	4.15124690	2.10936150

6pyrimidine/SO2 (-11113.5)

1	C	8.89448788	-0.00000000	-1.05901529
2	C	8.36901722	-1.19080376	-0.55417119
3	C	6.99314446	-0.00000000	0.83896943
4	C	8.36901722	1.19080376	-0.55417119
5	H	9.66679796	0.00000000	-1.82321517
6	H	8.68958791	-2.17049192	-0.90836409
7	H	6.23366270	-0.00000000	1.61950111
8	H	8.68958791	2.17049192	-0.90836409
9	C	3.49657223	-6.05624076	0.83896943
10	C	5.21577491	-6.65237964	-0.55417119
11	H	3.11683135	-5.39851026	1.61950111
12	C	4.44724394	-7.70285245	-1.05901529
13	H	6.22449510	-6.44015792	-0.90836409
14	C	3.15324230	-7.84318340	-0.55417119

15	H	4.83339898	-8.37169260	-1.82321517
16	H	2.46509282	-8.61064985	-0.90836409
17	C	-3.15324230	-7.84318340	-0.55417119
18	C	-3.49657223	-6.05624076	0.83896943
19	C	-4.44724394	-7.70285245	-1.05901529
20	H	-2.46509282	-8.61064985	-0.90836409
21	H	-3.11683135	-5.39851026	1.61950111
22	C	-5.21577491	-6.65237964	-0.55417119
23	H	-4.83339898	-8.37169260	-1.82321517
24	H	-6.22449510	-6.44015792	-0.90836409
25	C	-6.99314446	0.00000000	0.83896943
26	C	-8.36901722	-1.19080376	-0.55417119
27	H	-6.23366270	0.00000000	1.61950111
28	C	-8.89448788	0.00000000	-1.05901529
29	H	-8.68958791	-2.17049192	-0.90836409
30	C	-8.36901722	1.19080376	-0.55417119
31	H	-9.66679796	-0.00000000	-1.82321517
32	H	-8.68958791	2.17049192	-0.90836409
33	C	-5.21577491	6.65237964	-0.55417119
34	C	-3.49657223	6.05624076	0.83896943
35	C	-4.44724394	7.70285245	-1.05901529
36	H	-6.22449510	6.44015792	-0.90836409
37	H	-3.11683135	5.39851026	1.61950111
38	C	-3.15324230	7.84318340	-0.55417119
39	H	-4.83339898	8.37169260	-1.82321517
40	H	-2.46509282	8.61064985	-0.90836409
41	C	3.49657223	6.05624076	0.83896943
42	C	3.15324230	7.84318340	-0.55417119
43	H	3.11683135	5.39851026	1.61950111
44	C	4.44724394	7.70285245	-1.05901529
45	H	2.46509282	8.61064985	-0.90836409
46	C	5.21577491	6.65237964	-0.55417119
47	H	4.83339898	8.37169260	-1.82321517
48	H	6.22449510	6.44015792	-0.90836409
49	N	7.41938399	1.19069790	0.39602128
50	N	7.41938399	-1.19069790	0.39602128
51	N	4.74086663	-5.83002607	0.39602128
52	N	2.67851736	-7.02072397	0.39602128
53	N	-2.67851736	-7.02072397	0.39602128
54	N	-4.74086663	-5.83002607	0.39602128
55	N	-7.41938399	-1.19069790	0.39602128
56	N	-7.41938399	1.19069790	0.39602128
57	N	-4.74086663	5.83002607	0.39602128
58	N	-2.67851736	7.02072397	0.39602128
59	N	2.67851736	7.02072397	0.39602128
60	N	4.74086663	5.83002607	0.39602128
61	S	6.49284130	3.74864367	0.79890708
62	O	7.03861200	4.06374453	2.12468889
63	O	7.28024869	4.20325355	-0.36680805
64	O	7.03861200	-4.06374453	2.12468889
65	O	7.28024869	-4.20325355	-0.36680805
66	S	6.49284130	-3.74864367	0.79890708
67	S	0.00000000	7.49728735	0.79890708
68	S	-6.49284130	3.74864367	0.79890708
69	S	-6.49284130	-3.74864367	0.79890708
70	S	-0.00000000	-7.49728735	0.79890708
71	O	0.00000000	8.40650710	-0.36680805
72	O	-7.03861200	4.06374453	2.12468889
73	O	-7.28024869	4.20325355	-0.36680805
74	O	-7.28024869	-4.20325355	-0.36680805

75	O	-7.03861200	-4.06374453	2.12468889
76	O	-0.00000000	-8.40650710	-0.36680805
77	O	-0.00000000	-8.12748907	2.12468889
78	O	0.00000000	8.12748907	2.12468889

Pyrazine (-1464.6)

1	C	-1.13901242	0.69994857	-3.91159836
2	C	1.13901242	0.69994857	-3.91159836
3	C	-1.13901242	-0.69994857	-3.91159836
4	H	-2.07486760	1.25919750	-3.91162673
5	C	1.13901242	-0.69994857	-3.91159836
6	H	2.07486760	1.25919750	-3.91162673
7	H	-2.07486760	-1.25919750	-3.91162673
8	H	2.07486760	-1.25919750	-3.91162673
9	N	0.00000000	1.41328857	-3.91254916
10	N	-0.00000000	-1.41328857	-3.91254915

3pyrazine/SO2 (-5534.7)

1	C	-0.69467095	-3.92253448	1.14575850
2	C	-0.69467095	-3.92253448	-1.14575850
3	C	0.70462621	-3.91850371	1.14576450
4	H	-1.26515895	-3.91190482	2.07413835
5	C	0.70462621	-3.91850371	-1.14576450
6	H	-1.26515895	-3.91190482	-2.07413835
7	H	1.27505434	-3.90463307	2.07413648
8	H	1.27505434	-3.90463307	-2.07413648
9	C	2.90107416	2.55964840	1.14599826
10	C	2.90107416	2.55964840	-1.14599826
11	C	3.53613003	1.31272162	1.14629439
12	H	2.63233791	3.06269576	2.07449292
13	C	3.53613003	1.31272162	-1.14629439
14	H	2.63233791	3.06269576	-2.07449292
15	H	3.78690808	0.79898379	2.07397683
16	H	3.78690808	0.79898379	-2.07397683
17	C	-3.53886418	1.29877140	-1.14628227
18	C	-3.53886418	1.29877140	1.14628227
19	C	-2.90663167	2.54713979	-1.14598830
20	H	-3.78853451	0.78451205	-2.07397486
21	C	-2.90663167	2.54713979	1.14598830
22	H	-3.78853451	0.78451205	2.07397486
23	H	-2.63912741	3.05082182	-2.07449435
24	H	-2.63912741	3.05082182	2.07449435
25	N	2.57336869	3.17728912	0.00000000
26	N	3.84273452	0.68569064	0.00000000
27	N	-2.58031141	3.16554006	0.00000000
28	N	-3.84406060	0.67102940	0.00000000
29	N	-1.39393707	-3.91145006	0.00000000
30	N	1.40380841	-3.90339232	0.00000000
31	S	-0.00567380	4.30253214	0.00000000
32	S	-3.52616943	-2.08918696	0.00000000
33	S	3.53009990	-2.07440157	0.00000000
34	O	-0.00742325	5.05760082	-1.25994257
35	O	-0.00742325	5.05760082	1.25994257
36	O	4.20365461	-2.41724482	-1.25989166
37	O	4.20365461	-2.41724482	1.25989166
38	O	-4.19903902	-2.43334978	-1.25989177
39	O	-4.19903902	-2.43334978	1.25989177

4pyrazine/SO2 (-7383.8)

1	C	-0.69974603	5.13406105	1.14668019
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2	C	-0.69974603	5.13406105	-1.14668019
3	C	0.69974603	5.13406105	1.14668019
4	H	-1.27305433	5.12861335	2.07327339
5	C	0.69974603	5.13406105	-1.14668019
6	H	-1.27305433	5.12861335	-2.07327339
7	H	1.27305433	5.12861335	2.07327339
8	H	1.27305433	5.12861335	-2.07327339
9	N	1.39615013	5.12373838	0.00000000
10	N	-1.39615013	5.12373838	0.00000000
11	C	-5.13406105	0.69974603	-1.14668019
12	C	-5.13406105	0.69974603	1.14668019
13	C	-5.13406105	-0.69974603	-1.14668019
14	H	-5.12861335	1.27305433	-2.07327339
15	C	-5.13406105	-0.69974603	1.14668019
16	H	-5.12861335	1.27305433	2.07327339
17	H	-5.12861335	-1.27305433	-2.07327339
18	H	-5.12861335	-1.27305433	2.07327339
19	N	-5.12373838	1.39615013	0.00000000
20	N	-5.12373838	-1.39615013	0.00000000
21	C	0.69974603	-5.13406105	-1.14668019
22	C	0.69974603	-5.13406105	1.14668019
23	C	-0.69974603	-5.13406105	-1.14668019
24	H	1.27305433	-5.12861335	-2.07327339
25	C	-0.69974603	-5.13406105	1.14668019
26	H	1.27305433	-5.12861335	2.07327339
27	H	-1.27305433	-5.12861335	-2.07327339
28	H	-1.27305433	-5.12861335	2.07327339
29	N	1.39615013	-5.12373838	0.00000000
30	N	-1.39615013	-5.12373838	0.00000000
31	C	5.13406105	0.69974603	1.14668019
32	C	5.13406105	0.69974603	-1.14668019
33	C	5.13406105	-0.69974603	1.14668019
34	H	5.12861335	1.27305433	2.07327339
35	C	5.13406105	-0.69974603	-1.14668019
36	H	5.12861335	1.27305433	-2.07327339
37	H	5.12861335	-1.27305433	2.07327339
38	H	5.12861335	-1.27305433	-2.07327339
39	N	5.12373838	1.39615013	0.00000000
40	N	5.12373838	-1.39615013	0.00000000
41	S	3.86790744	3.86790744	0.00000000
42	S	-3.86790744	3.86790744	0.00000000
43	S	3.86790744	-3.86790744	0.00000000
44	S	-3.86790744	-3.86790744	0.00000000
45	O	-4.40381842	4.40381842	-1.25945824
46	O	-4.40381842	-4.40381842	-1.25945824
47	O	4.40381842	4.40381842	-1.25945824
48	O	4.40381842	-4.40381842	-1.25945824
49	O	-4.40381842	-4.40381842	1.25945824
50	O	4.40381842	-4.40381842	1.25945824
51	O	4.40381842	4.40381842	1.25945824
52	O	-4.40381842	4.40381842	1.25945824

5pyrazine/SO2 (-9232.7)

1	C	-4.79334378	-4.34759291	-1.14766616
2	C	-4.79334378	-4.34759291	1.14766616
3	C	-5.61603126	-3.21526074	-1.14766616
4	H	-4.45376249	-4.81072546	-2.07343227
5	C	-5.61603126	-3.21526074	1.14766616
6	H	-4.45376249	-4.81072546	2.07343227
7	H	-5.95156009	-2.74918391	-2.07343227

8	H	-5.95156009	-2.74918391	2.07343227
9	C	2.65358189	-5.90222093	-1.14766616
10	C	2.65358189	-5.90222093	1.14766616
11	C	1.32244558	-6.33473333	-1.14766616
12	H	3.19898350	-5.72237576	-2.07343227
13	C	1.32244558	-6.33473333	1.14766616
14	H	3.19898350	-5.72237576	2.07343227
15	H	0.77549607	-6.50981456	-2.07343227
16	H	0.77549607	-6.50981456	2.07343227
17	C	6.43334758	0.69981977	-1.14766616
18	C	6.43334758	0.69981977	1.14766616
19	C	6.43334758	-0.69981977	-1.14766616
20	H	6.43084302	1.27410274	-2.07343227
21	C	6.43334758	-0.69981977	1.14766616
22	H	6.43084302	1.27410274	2.07343227
23	H	6.43084302	-1.27410274	-2.07343227
24	H	6.43084302	-1.27410274	2.07343227
25	C	1.32244558	6.33473333	1.14766616
26	C	1.32244558	6.33473333	-1.14766616
27	C	2.65358189	5.90222093	1.14766616
28	H	0.77549607	6.50981456	2.07343227
29	C	2.65358189	5.90222093	-1.14766616
30	H	0.77549607	6.50981456	-2.07343227
31	H	3.19898350	5.72237576	2.07343227
32	H	3.19898350	5.72237576	-2.07343227
33	C	-5.61603126	3.21526074	-1.14766616
34	C	-5.61603126	3.21526074	1.14766616
35	C	-4.79334378	4.34759291	-1.14766616
36	H	-5.95156009	2.74918391	-2.07343227
37	C	-4.79334378	4.34759291	1.14766616
38	H	-5.95156009	2.74918391	2.07343227
39	H	-4.45376249	4.81072546	-2.07343227
40	H	-4.45376249	4.81072546	2.07343227
41	O	-2.30956353	-7.10810564	1.25957451
42	O	-2.30956353	-7.10810564	-1.25957451
43	O	-7.47390456	-0.00000000	-1.25957451
44	O	-7.47390456	-0.00000000	1.25957451
45	O	-2.30956353	7.10810564	-1.25957451
46	O	-2.30956353	7.10810564	1.25957451
47	O	6.04651580	4.39305088	1.25957451
48	O	6.04651580	4.39305088	-1.25957451
49	O	6.04651580	-4.39305088	1.25957451
50	O	6.04651580	-4.39305088	-1.25957451
51	N	-6.01523569	-2.64789232	0.00000000
52	N	-4.37710530	-4.90258538	0.00000000
53	N	0.65948519	-6.53907283	0.00000000
54	N	3.31003585	-5.67785671	0.00000000
55	N	6.42281996	-1.39347694	0.00000000
56	N	6.42281996	1.39347694	0.00000000
57	N	3.31003585	5.67785671	0.00000000
58	N	0.65948519	6.53907283	0.00000000
59	N	-6.01523569	2.64789232	0.00000000
60	N	-4.37710530	4.90258538	0.00000000
61	S	5.43231410	-3.94680721	0.00000000
62	S	5.43231410	3.94680721	0.00000000
63	S	-2.07495935	6.38606822	0.00000000
64	S	-6.71470950	-0.00000000	0.00000000
65	S	-2.07495935	-6.38606822	0.00000000

6pyrazine/SO2 (-11081.2)

1	C	3.25794127	7.04258698	1.14821048
2	C	3.25794127	7.04258698	-1.14821048
3	C	4.47008859	6.34275339	1.14821048
4	H	2.75962300	7.33055119	2.07318372
5	C	4.47008859	6.34275339	-1.14821048
6	H	2.75962300	7.33055119	-2.07318372
7	H	4.96863206	6.05517922	2.07318372
8	H	4.96863206	6.05517922	-2.07318372
9	C	-4.47008859	6.34275339	-1.14821048
10	C	-4.47008859	6.34275339	1.14821048
11	C	-3.25794127	7.04258698	-1.14821048
12	H	-4.96863206	6.05517922	-2.07318372
13	C	-3.25794127	7.04258698	1.14821048
14	H	-4.96863206	6.05517922	2.07318372
15	H	-2.75962300	7.33055119	-2.07318372
16	H	-2.75962300	7.33055119	2.07318372
17	C	-7.72802986	-0.69983359	-1.14821048
18	C	-7.72802986	-0.69983359	1.14821048
19	C	-7.72802986	0.69983359	-1.14821048
20	H	-7.72825506	-1.27537198	-2.07318372
21	C	-7.72802986	0.69983359	1.14821048
22	H	-7.72825506	-1.27537198	2.07318372
23	H	-7.72825506	1.27537198	-2.07318372
24	H	-7.72825506	1.27537198	2.07318372
25	C	-3.25794127	-7.04258698	-1.14821048
26	C	-3.25794127	-7.04258698	1.14821048
27	C	-4.47008859	-6.34275339	-1.14821048
28	H	-2.75962300	-7.33055119	-2.07318372
29	C	-4.47008859	-6.34275339	1.14821048
30	H	-2.75962300	-7.33055119	2.07318372
31	H	-4.96863206	-6.05517922	-2.07318372
32	H	-4.96863206	-6.05517922	2.07318372
33	C	4.47008859	-6.34275339	-1.14821048
34	C	4.47008859	-6.34275339	1.14821048
35	C	3.25794127	-7.04258698	-1.14821048
36	H	4.96863206	-6.05517922	-2.07318372
37	C	3.25794127	-7.04258698	1.14821048
38	H	4.96863206	-6.05517922	2.07318372
39	H	2.75962300	-7.33055119	-2.07318372
40	H	2.75962300	-7.33055119	2.07318372
41	C	7.72802986	0.69983359	-1.14821048
42	C	7.72802986	0.69983359	1.14821048
43	C	7.72802986	-0.69983359	-1.14821048
44	H	7.72825506	1.27537198	-2.07318372
45	C	7.72802986	-0.69983359	1.14821048
46	H	7.72825506	1.27537198	2.07318372
47	H	7.72825506	-1.27537198	-2.07318372
48	H	7.72825506	-1.27537198	2.07318372
49	N	-7.71698122	1.39184419	0.00000000
50	N	-7.71698122	-1.39184419	0.00000000
51	N	-5.06386303	5.98717968	0.00000000
52	N	-2.65311818	7.37902387	0.00000000
53	N	2.65311818	7.37902387	0.00000000
54	N	5.06386303	5.98717968	0.00000000
55	N	7.71698122	1.39184419	0.00000000
56	N	7.71698122	-1.39184419	0.00000000
57	N	5.06386303	-5.98717968	0.00000000
58	N	2.65311818	-7.37902387	0.00000000
59	N	-2.65311818	-7.37902387	0.00000000
60	N	-5.06386303	-5.98717968	0.00000000

61	O	7.56918342	4.37007008	1.25975865
62	O	7.56918342	4.37007008	-1.25975865
63	O	0.00000000	8.74014017	-1.25975865
64	O	0.00000000	8.74014017	1.25975865
65	O	-7.56918342	4.37007008	-1.25975865
66	O	-7.56918342	4.37007008	1.25975865
67	O	-7.56918342	-4.37007008	1.25975865
68	O	-7.56918342	-4.37007008	-1.25975865
69	O	-0.00000000	-8.74014017	1.25975865
70	O	-0.00000000	-8.74014017	-1.25975865
71	O	7.56918342	-4.37007008	-1.25975865
72	O	7.56918342	-4.37007008	1.25975865
73	S	6.91112806	3.99014165	0.00000000
74	S	6.91112806	-3.99014165	0.00000000
75	S	-0.00000000	-7.98028329	0.00000000
76	S	-6.91112806	-3.99014165	0.00000000
77	S	-6.91112806	3.99014165	0.00000000
78	S	0.00000000	7.98028329	0.00000000

SO3 (-495.6)

1	O	1.06725512	-1.50542382	1.25751340
2	O	2.04412642	-3.45182255	0.00000000
3	O	1.06725512	-1.50542382	-1.25751340
4	S	1.39252909	-2.15412182	0.00000000

3pyridazine/SO3 (-5898.9)

1	C	4.54867614	0.86457335	0.00000000
2	C	4.54739360	-1.82341557	0.00000000
3	C	5.78856593	-1.17864057	0.00000000
4	C	5.78909400	0.20993352	0.00000000
5	H	4.45511222	1.94866752	0.00000000
6	H	4.41514997	-2.90184602	0.00000000
7	H	6.70765225	-1.75788716	0.00000000
8	H	6.71363467	0.78139048	0.00000000
9	O	-3.99965142	-0.00362413	0.00000000
10	O	-1.84933756	-0.12985029	-1.26259986
11	N	3.41389396	-1.11418868	0.00000000
12	N	3.38214811	0.20991897	0.00000000
13	O	0.81221513	1.66649845	1.26259986
14	C	-0.69457259	4.84986617	0.00000000
15	C	-3.02308055	3.50698241	0.00000000
16	C	-1.87355029	5.60236543	0.00000000
17	H	0.30549739	5.27455504	0.00000000
18	C	-3.07635476	4.90853571	0.00000000
19	H	-3.91515170	2.88390660	0.00000000
20	H	-1.83145119	6.68794082	0.00000000
21	H	-4.03352134	5.42348293	0.00000000
22	N	-0.74203129	3.51361324	0.00000000
23	N	-1.87286922	2.82406670	0.00000000
24	S	1.49395660	-2.08150802	0.00000000
25	O	1.03712243	-1.53664816	1.26259986
26	O	2.00296429	-3.46198768	0.00000000
27	S	1.05566052	2.33455839	0.00000000
28	S	-2.54961713	-0.25305036	0.00000000
29	C	-3.85282101	-3.02645059	0.00000000
30	C	-3.91501564	-4.42372486	0.00000000
31	H	-4.72064735	-2.37270902	0.00000000
32	C	-1.52559558	-4.37155576	0.00000000
33	C	-2.71273923	-5.11846923	0.00000000
34	H	-4.87620106	-4.93005367	0.00000000

35	H	-0.53996053	-4.83257412	0.00000000
36	H	-2.68011333	-6.20487341	0.00000000
37	N	-2.67186267	-2.39942456	0.00000000
38	N	-1.50927889	-3.03398566	0.00000000
39	O	1.99668713	3.46561179	0.00000000
40	O	1.03712243	-1.53664816	-1.26259986
41	O	-1.84933756	-0.12985029	1.26259986
42	O	0.81221513	1.66649845	-1.26259986

4pyridazine/SO3 (-7870.9)

1	C	-6.24972544	6.39780335	0.00000000
2	C	-6.85590401	7.66285384	0.00000000
3	H	-6.81530654	5.46887009	0.00000000
4	C	-4.65257171	8.56202405	0.00000000
5	C	-6.03291926	8.78035072	0.00000000
6	H	-7.93921311	7.75069419	0.00000000
7	H	-3.90362299	9.34813564	0.00000000
8	H	-6.42744358	9.79258639	0.00000000
9	C	1.41358797	8.20522987	0.00000000
10	C	2.68388694	8.80029702	0.00000000
11	H	0.48831201	8.77687577	0.00000000
12	C	3.56437029	6.58893236	0.00000000
13	C	3.79420561	7.96743005	0.00000000
14	H	2.78154911	9.88276137	0.00000000
15	H	4.34388367	5.83310474	0.00000000
16	H	4.80976215	8.35329258	0.00000000
17	C	3.07446591	0.50345856	0.00000000
18	C	1.49604745	-1.67465897	0.00000000
19	C	3.69155466	-0.75628823	0.00000000
20	H	3.63256669	1.43712049	0.00000000
21	C	2.87821150	-1.88089117	0.00000000
22	H	0.75387454	-2.46714953	0.00000000
23	H	4.77558353	-0.83478570	0.00000000
24	H	3.28158749	-2.88963568	0.00000000
25	C	-4.56983452	-1.31082954	0.00000000
26	C	-5.84533405	-1.89434434	0.00000000
27	H	-3.65028460	-1.89153297	0.00000000
28	C	-6.70497529	0.32495960	0.00000000
29	C	-6.94784896	-1.05126467	0.00000000
30	H	-5.95274945	-2.97588804	0.00000000
31	H	-7.47759106	1.08780719	0.00000000
32	H	-7.96697977	-1.42761307	0.00000000
33	N	-5.45029953	0.79023899	0.00000000
34	N	-4.37720041	0.01494692	0.00000000
35	N	0.99783108	-0.43271424	0.00000000
36	N	1.74393577	0.66111690	0.00000000
37	N	2.31385707	6.11279920	0.00000000
38	N	1.23362113	6.87785916	0.00000000
39	N	-4.16510999	7.31593086	0.00000000
40	N	-4.92071387	6.22852907	0.00000000
41	O	-1.98248862	6.29466047	1.26102761
42	O	-1.98248862	6.29466047	-1.26102761
43	O	-4.39144107	2.95752646	-1.26098768
44	O	-4.39144107	2.95752646	1.26098768
45	O	-1.19250089	0.57045892	1.26110782
46	O	-1.19250089	0.57045892	-1.26110782
47	O	1.26607455	3.94542861	-1.26086606
48	O	1.26607455	3.94542861	1.26086606
49	S	-2.07612503	7.00383385	0.00000000
50	S	-5.10200430	2.87506519	0.00000000

51	S	-1.09265599	-0.13773230	0.00000000
52	S	1.97650439	4.03216864	0.00000000
53	O	-1.43589424	-1.57152149	0.00000000
54	O	3.40212414	3.65614532	0.00000000
55	O	-1.72154235	8.43485962	0.00000000
56	O	-6.52714463	3.25249375	0.00000000

5pyridazine/SO3 (-9834.4)

1	C	-11.43618661	-0.15716880	0.00000000
2	C	-11.00401999	-2.80943766	0.00000000
3	C	-12.55566590	-0.98889513	0.00000000
4	H	-11.48567901	0.92743409	0.00000000
5	C	-12.33025441	-2.36025189	0.00000000
6	H	-10.74232533	-3.86298545	0.00000000
7	H	-13.55572175	-0.56472071	0.00000000
8	H	-13.15032316	-3.07341050	0.00000000
9	C	-5.35476993	5.44403596	0.00000000
10	C	-6.50535577	6.23206438	0.00000000
11	H	-4.34505946	5.84308928	0.00000000
12	C	-7.72252793	4.17265351	0.00000000
13	C	-7.72894119	5.57290256	0.00000000
14	H	-6.42936716	7.31567834	0.00000000
15	H	-8.63331895	3.58185338	0.00000000
16	H	-8.66994142	6.11665379	0.00000000
17	C	1.84285689	1.32527731	0.00000000
18	C	2.26163656	2.65564883	0.00000000
19	H	2.51874922	0.47558865	0.00000000
20	C	-0.06284261	3.22060707	0.00000000
21	C	1.27488138	3.63448362	0.00000000
22	H	3.32041502	2.89860651	0.00000000
23	H	-0.89332308	3.91984251	0.00000000
24	H	1.52120246	4.69301366	0.00000000
25	C	0.18804144	-6.79338365	0.00000000
26	C	1.58170002	-6.74061767	0.00000000
27	H	-0.38471081	-7.71576883	0.00000000
28	C	1.33173034	-4.36141525	0.00000000
29	C	2.17125373	-5.48215465	0.00000000
30	H	2.16647054	-7.65607912	0.00000000
31	H	1.71203951	-3.34470413	0.00000000
32	H	3.25091280	-5.35781066	0.00000000
33	C	-8.07178343	-7.74174032	0.00000000
34	C	-5.41271779	-8.13031793	0.00000000
35	C	-7.61673235	-9.06010958	0.00000000
36	H	-9.12073312	-7.46144947	0.00000000
37	C	-6.24136316	-9.25916944	0.00000000
38	H	-4.32929815	-8.19942921	0.00000000
39	H	-8.32309239	-9.88535379	0.00000000
40	H	-5.80891232	-10.25621527	0.00000000
41	N	0.53717502	1.02510571	0.00000000
42	N	-0.42518273	1.92832451	0.00000000
43	N	-5.44784034	4.10744020	0.00000000
44	N	-6.59210242	3.44914262	0.00000000
45	N	-10.20224934	-0.67906546	0.00000000
46	N	-9.95230602	-1.97531363	0.00000000
47	N	-7.20165648	-6.72308715	0.00000000
48	N	-5.89010496	-6.87584471	0.00000000
49	N	-0.53397366	-5.66483729	0.00000000
50	N	-0.00738846	-4.45400907	0.00000000
51	S	-2.64183937	-5.86123763	0.00000000
52	S	-8.00192151	-4.76314641	0.00000000

53	S	-8.57342765	0.67851428	0.00000000
54	S	-3.64455745	3.00921344	0.00000000
55	S	0.00444211	-1.02189898	0.00000000
56	O	-8.77143183	-4.90294141	1.23951360
57	O	-8.77143183	-4.90294141	-1.23951360
58	O	-8.94183304	1.36763098	-1.23984427
59	O	-8.94183304	1.36763098	1.23984427
60	O	-3.10852639	3.57885773	-1.23958618
61	O	-3.10852639	3.57885773	1.23958618
62	O	0.70429614	-1.37076334	1.23956245
63	O	0.70429614	-1.37076334	-1.23956245
64	O	-2.73214449	-6.63799569	1.23962255
65	O	-2.73214449	-6.63799569	-1.23962255
66	O	-4.19874178	1.67634558	0.00000000
67	O	-1.43139327	-0.87338900	0.00000000
68	O	-2.99167120	-4.46073476	0.00000000
69	O	-6.76325105	-4.02198135	0.00000000
70	O	-7.49142444	-0.27694768	0.00000000

6pyridazine/SO3 (-11802.5)

1	C	-5.66028534	4.20228319	0.00000000
2	C	-3.04173895	3.58601596	0.00000000
3	C	-4.75207772	5.26066798	0.00000000
4	H	-6.73890445	4.32531009	0.00000000
5	C	-3.39999702	4.94051750	0.00000000
6	H	-2.00647038	3.25854749	0.00000000
7	H	-5.10636051	6.28748529	0.00000000
8	H	-2.63145452	5.70879538	0.00000000
9	C	-12.28780327	-1.23536801	0.00000000
10	C	-12.65845128	0.10931214	0.00000000
11	H	-12.99236151	-2.06137224	0.00000000
12	C	-10.31404296	0.59270897	0.00000000
13	C	-11.63780245	1.05210364	0.00000000
14	H	-13.70808184	0.38895541	0.00000000
15	H	-9.46577812	1.27062514	0.00000000
16	H	-11.84553917	2.11873280	0.00000000
17	C	-10.90113583	-9.66898352	0.00000000
18	C	-12.27422748	-9.42504314	0.00000000
19	H	-10.45906305	-10.66054669	0.00000000
20	C	-11.70159919	-7.10116762	0.00000000
21	C	-12.68603875	-8.09789750	0.00000000
22	H	-12.97844882	-10.25203813	0.00000000
23	H	-11.94531495	-6.04319213	0.00000000
24	H	-13.73835024	-7.82670436	0.00000000
25	C	-2.87219667	-12.46548972	0.00000000
26	C	-3.78045871	-13.52382736	0.00000000
27	H	-1.79358402	-12.58857066	0.00000000
28	C	-5.49071887	-11.84909209	0.00000000
29	C	-5.13252458	-13.20360992	0.00000000
30	H	-3.42622967	-14.55066323	0.00000000
31	H	-6.52596388	-11.52156271	0.00000000
32	H	-5.90110230	-13.97185300	0.00000000
33	C	3.75546509	-7.02796381	0.00000000
34	C	4.12614466	-8.37263401	0.00000000
35	H	4.46000101	-6.20194079	0.00000000
36	C	1.78174696	-8.85609354	0.00000000
37	C	3.10551817	-9.31545251	0.00000000
38	H	5.17578180	-8.65225257	0.00000000
39	H	0.93349548	-9.53402675	0.00000000
40	H	3.31328365	-10.38207616	0.00000000

41	C	2.36868165	1.40560808	0.00000000
42	C	3.16897991	-1.16219985	0.00000000
43	C	3.74177652	1.16158607	0.00000000
44	H	1.92667214	2.39719978	0.00000000
45	C	4.15352314	-0.16558594	0.00000000
46	H	3.41264913	-2.22018539	0.00000000
47	H	4.44604408	1.98854204	0.00000000
48	H	5.20581317	-0.43686274	0.00000000
49	O	-1.20108386	-10.08237526	1.23900838
50	O	-1.20108386	-10.08237526	-1.23900838
51	O	2.70068434	-4.30752192	1.23914562
52	O	2.70068434	-4.30752192	-1.23914562
53	O	-0.53698592	1.63366213	1.23901794
54	O	-0.53698592	1.63366213	-1.23901794
55	O	-7.33127644	1.81907123	1.23901178
56	O	-7.33127644	1.81907123	-1.23901178
57	O	-11.23311577	-3.95584080	-1.23916417
58	O	-11.23311577	-3.95584080	1.23916417
59	O	-7.99550986	-9.89690173	1.23901826
60	O	-7.99550986	-9.89690173	-1.23901826
61	S	-7.99740554	-9.11336115	0.00000000
62	S	-1.87778589	-9.68740367	0.00000000
63	S	1.99689053	-4.65195667	0.00000000
64	S	-0.53511482	0.85012122	0.00000000
65	S	-6.65455125	1.42413717	0.00000000
66	S	-10.52930882	-3.61143139	0.00000000
67	N	-3.31133891	-11.19982404	0.00000000
68	N	-4.58653478	-10.85723536	0.00000000
69	N	-10.03397877	-8.64776192	0.00000000
70	N	-10.38770443	-7.37568877	0.00000000
71	N	-10.99282278	-1.57779854	0.00000000
72	N	-9.99641440	-0.71124104	0.00000000
73	N	-5.22108228	2.93664066	0.00000000
74	N	-3.94586864	2.59410930	0.00000000
75	N	1.50144372	0.38444129	0.00000000
76	N	1.85511695	-0.88763777	0.00000000
77	N	2.46047409	-6.68556977	0.00000000
78	N	1.46408957	-7.55215103	0.00000000
79	O	-9.08737189	-3.51811706	0.00000000
80	O	-7.45442795	-7.77441332	0.00000000
81	O	-2.75259216	-8.53707666	0.00000000
82	O	0.55495756	-4.74533369	0.00000000
83	O	-1.07813477	-0.48880958	0.00000000
84	O	-5.77968083	0.27385918	0.00000000

3pyrimidine/SO3 (-5968.8)

1	N	-3.93393602	-1.44363609	0.31177751
2	C	-4.87222541	1.08132542	-0.29277779
3	C	-5.74004918	-0.00224869	-0.36075694
4	C	-5.21599411	-1.26014235	-0.04681762
5	O	-1.09459743	-2.26932797	-0.97389038
6	H	-5.14957638	2.10913979	-0.50897847
7	H	-6.77925529	0.13039434	-0.64639601
8	H	-5.83886290	-2.15322796	-0.08150681
9	O	4.68842235	1.05576706	-0.08688485
10	O	2.51259439	0.18671480	-0.97389038
11	N	-3.59222076	0.88023734	0.06438572
12	C	-3.15676939	-0.36196128	0.35555005
13	O	-1.06551982	-2.66879506	1.48730376
14	C	1.49965741	-4.76013369	-0.29277779

15	N	3.21719353	-2.68507049	0.31177751
16	C	2.87197202	-4.96990407	-0.36075694
17	H	0.74821956	-5.51423385	-0.50897847
18	C	3.69931234	-3.88711223	-0.04681762
19	O	2.84400424	0.41163030	1.48730376
20	H	3.27670283	-5.93620447	-0.64639601
21	H	4.78418157	-3.97998962	-0.08150681
22	N	1.03380248	-3.55107309	0.06438572
23	C	1.89185236	-2.55286185	0.35555005
24	S	-2.27948423	2.47434453	0.13512680
25	O	-1.77848441	2.25716477	1.48730376
26	O	-3.25853227	3.53240933	-0.08688485
27	S	-1.00310310	-3.21126352	0.13512680
28	S	3.28258734	0.73691899	0.13512680
29	C	3.37256799	3.67880827	-0.29277779
30	C	2.86807717	4.97215276	-0.36075694
31	H	4.40135682	3.40509407	-0.50897847
32	N	0.71674248	4.12870657	0.31177751
33	C	1.51668177	5.14725458	-0.04681762
34	H	3.50255246	5.80581013	-0.64639601
35	O	-1.41799696	2.08261317	-0.97389038
36	H	1.05468133	6.13321758	-0.08150681
37	N	2.55841828	2.67083575	0.06438572
38	C	1.26491703	2.91482313	0.35555005
39	O	-1.42989009	-4.58817640	-0.08688485
40	H	0.65039190	2.06799579	0.64386504
41	H	1.46574094	-1.59725381	0.64386504
42	H	-2.11613284	-0.47074198	0.64386504

4pyrimidine/SO3 (-7973.7)

1	N	-3.37852444	-3.96273944	1.57909800
2	C	-3.09101158	-4.78389057	0.55035695
3	O	5.21985098	0.23443446	0.01878420
4	C	-3.11262067	-2.96681435	-0.98756927
5	C	-2.94486340	-4.32696919	-0.76075314
6	H	-2.95979906	-5.83626361	0.79329837
7	H	-3.00680709	-2.48402725	-1.95358250
8	H	-2.67865271	-4.99564738	-1.57220986
9	N	-3.96273944	3.37852444	1.57909800
10	C	-4.78389057	3.09101158	0.55035695
11	O	-5.21985098	-0.23443446	0.01878420
12	C	-2.96681435	3.11262067	-0.98756927
13	C	-4.32696919	2.94486340	-0.76075314
14	H	-5.83626361	2.95979906	0.79329837
15	H	-2.48402725	3.00680709	-1.95358250
16	H	-4.99564738	2.67865271	-1.57220986
17	N	3.37852444	3.96273944	1.57909800
18	C	3.11262067	2.96681435	-0.98756927
19	C	3.09101158	4.78389057	0.55035695
20	O	0.23443446	-5.21985098	0.01878420
21	C	2.94486340	4.32696919	-0.76075314
22	H	3.00680709	2.48402725	-1.95358250
23	H	2.95979906	5.83626361	0.79329837
24	H	2.67865271	4.99564738	-1.57220986
25	N	3.96273944	-3.37852444	1.57909800
26	C	4.78389057	-3.09101158	0.55035695
27	O	-0.23443446	5.21985098	0.01878420
28	C	2.96681435	-3.11262067	-0.98756927
29	C	4.32696919	-2.94486340	-0.76075314
30	H	5.83626361	-2.95979906	0.79329837

31	H	2.48402725	-3.00680709	-1.95358250
32	H	4.99564738	-2.67865271	-1.57220986
33	N	2.16522174	-3.40819566	0.04946629
34	C	2.67347668	-3.51722659	1.29542847
35	N	3.40819566	2.16522174	0.04946629
36	C	3.51722659	2.67347668	1.29542847
37	N	-2.16522174	3.40819566	0.04946629
38	C	-2.67347668	3.51722659	1.29542847
39	N	-3.40819566	-2.16522174	0.04946629
40	C	-3.51722659	-2.67347668	1.29542847
41	O	-2.91964841	0.34326384	0.78142938
42	O	-3.35719905	-0.11725253	-1.63843043
43	O	0.11725253	-3.35719905	-1.63843043
44	O	-0.34326384	-2.91964841	0.78142938
45	O	2.91964841	-0.34326384	0.78142938
46	O	3.35719905	0.11725253	-1.63843043
47	O	-0.11725253	3.35719905	-1.63843043
48	O	0.34326384	2.91964841	0.78142938
49	S	-3.78208236	-0.22947905	-0.24498785
50	S	0.22947905	-3.78208236	-0.24498785
51	S	3.78208236	0.22947905	-0.24498785
52	S	-0.22947905	3.78208236	-0.24498785
53	H	-3.73403043	-1.96428289	2.08967138
54	H	1.96428289	-3.73403043	2.08967138
55	H	3.73403043	1.96428289	2.08967138
56	H	-1.96428289	3.73403043	2.08967138

5pyrimidine/SO3 (-9965.1)

1	C	2.13193925	-4.98396464	-0.99009441
2	N	3.04584778	-5.50795129	1.56712413
3	C	3.48432226	-5.21721006	-0.78339371
4	H	1.68256267	-4.76095928	-1.95259533
5	C	3.89881942	-5.48331295	0.52466386
6	O	3.40336235	-2.18963158	0.78270498
7	H	4.18830856	-5.16599057	-1.60682124
8	H	4.94669168	-5.66474660	0.75095529
9	C	-4.08122659	-3.56772449	-0.99009441
10	C	-3.88514683	-4.92599395	-0.78339371
11	H	-4.00800089	-3.07142952	-1.95259533
12	N	-4.29715424	-4.59882394	1.56712413
13	C	-4.01013905	-5.40243451	0.52466386
14	H	-3.61889046	-5.57969703	-1.60682124
15	O	-1.03076657	-3.91342331	0.78270498
16	H	-3.85888238	-6.45508633	0.75095529
17	C	-4.65427599	2.77898964	-0.99009441
18	C	-5.88547504	2.17277837	-0.78339371
19	H	-4.15964345	2.86271144	-1.95259533
20	N	-5.70163516	2.66572179	1.56712413
21	C	-6.37722166	2.14442480	0.52466386
22	H	-6.42490587	1.71754815	-1.60682124
23	O	-4.04041113	-0.22899704	0.78270498
24	H	-7.33161214	1.67528385	0.75095529
25	C	1.20472583	5.28523454	-0.99009441
26	C	0.24772321	6.26884483	-0.78339371
27	H	1.43719986	4.84068249	-1.95259533
28	N	0.77334991	6.24633061	1.56712413
29	C	0.06879931	6.72776192	0.52466386
30	H	-0.35191974	6.64120017	-1.60682124
31	O	-1.46634484	3.77189535	0.78270498
32	H	-0.67230313	7.49046869	0.75095529

33	C	5.39883751	0.48746495	-0.99009441
34	N	6.17959169	1.19472283	1.56712413
35	C	6.03857642	1.70158081	-0.78339371
36	H	5.04788181	0.12899486	-1.95259533
37	C	6.41974197	2.01356074	0.52466386
38	O	3.13416018	2.56015658	0.78270498
39	H	6.20740751	2.38693928	-1.60682124
40	H	6.91610596	2.95408039	0.75095529
41	N	-3.99932370	3.30439605	0.06080591
42	C	-4.52583785	3.22280274	1.30166257
43	N	-4.37852639	-2.78246832	0.06080591
44	C	-4.46362835	-3.30842677	1.30166257
45	N	1.29324557	-5.02405605	0.06080591
46	C	1.76716382	-5.26752293	1.30166257
47	N	5.17779610	-0.32256908	0.06080591
48	C	5.55579566	0.05291856	1.30166257
49	N	1.90680841	4.82469739	0.06080591
50	C	1.66650673	5.30022839	1.30166257
51	S	3.43983653	3.57322269	-0.21920196
52	S	4.46130467	-2.16729241	-0.21920196
53	S	-0.68259861	-4.91268307	-0.21920196
54	S	-4.88317382	-0.86891270	-0.21920196
55	S	-2.33536878	4.37566548	-0.21920196
56	O	5.68218737	-2.91580036	0.08135717
57	O	4.07630372	-2.05381162	-1.62364128
58	O	-0.69364381	-4.51145791	-1.62364128
59	O	-1.01719846	-6.30511319	0.08135717
60	O	-4.50499916	-0.73442270	-1.62364128
61	O	-6.31085060	-0.98097389	0.08135717
62	O	-2.88312170	5.69883798	0.08135717
63	O	-2.09059880	4.05755972	-1.62364128
64	O	4.52898339	4.50304947	0.08135717
65	O	3.21293806	3.24213251	-1.62364128
66	H	-4.68913146	-2.61350617	2.10647402
67	H	-3.93461339	3.65201121	2.10647402
68	H	2.25740665	4.87057322	2.10647402
69	H	5.32976742	-0.64183140	2.10647402
70	H	1.03657077	-5.26724685	2.10647402

6pyrimidine/SO3 (-11955.7)

1	C	-5.92536132	3.19252686	-0.96601103
2	N	-6.54397261	4.24602721	1.51637645
3	C	-5.87438059	4.56631996	-0.77509126
4	H	-5.69038095	2.68855863	-1.89843787
5	C	-6.19170015	5.05356752	0.49604935
6	O	-2.82460638	-4.99976135	0.94953896
7	H	-5.57125179	5.22930290	-1.57793307
8	H	-6.14514894	6.11861448	0.70984659
9	C	-5.72749002	-3.53525000	-0.96601103
10	C	-6.89173938	-2.80420285	-0.77509126
11	H	-5.17355055	-3.58373514	-1.89843787
12	N	-6.94915373	-3.54423292	1.51637645
13	C	-7.47236793	-2.83538586	0.49604935
14	H	-7.31433505	-2.21019412	-1.57793307
15	O	2.91761715	-4.94606155	0.94953896
16	H	-8.37145005	-2.26254784	0.70984659
17	C	0.19787129	-6.72777685	-0.96601103
18	C	-1.01735879	-7.37052280	-0.77509126
19	H	0.51683040	-6.27229378	-1.89843787
20	N	-0.40518111	-7.79026013	1.51637645

21	C	-1.28066778	-7.88895338	0.49604935
22	H	-1.74308326	-7.43949702	-1.57793307
23	O	5.74222353	0.05369979	0.94953896
24	H	-2.22630111	-8.38116233	0.70984659
25	C	5.92536132	-3.19252686	-0.96601103
26	C	5.87438059	-4.56631996	-0.77509126
27	H	5.69038095	-2.68855863	-1.89843787
28	N	6.54397261	-4.24602721	1.51637645
29	C	6.19170015	-5.05356752	0.49604935
30	H	5.57125179	-5.22930290	-1.57793307
31	O	2.82460638	4.99976135	0.94953896
32	H	6.14514894	-6.11861448	0.70984659
33	C	5.72749002	3.53525000	-0.96601103
34	C	6.89173938	2.80420285	-0.77509126
35	H	5.17355055	3.58373514	-1.89843787
36	N	6.94915373	3.54423292	1.51637645
37	C	7.47236793	2.83538586	0.49604935
38	H	7.31433505	2.21019412	-1.57793307
39	O	-2.91761715	4.94606155	0.94953896
40	H	8.37145005	2.26254784	0.70984659
41	C	-0.19787129	6.72777685	-0.96601103
42	N	0.40518111	7.79026013	1.51637645
43	C	1.01735879	7.37052280	-0.77509126
44	H	-0.51683040	6.27229378	-1.89843787
45	C	1.28066778	7.88895338	0.49604935
46	O	-5.74222353	-0.05369979	0.94953896
47	H	1.74308326	7.43949702	-1.57793307
48	H	2.22630111	8.38116233	0.70984659
49	O	7.95737652	-0.34916857	-0.11946078
50	O	5.89467841	-0.30865953	-1.52375969
51	O	4.28107712	6.71670593	-0.11946078
52	O	3.21464619	4.95061149	-1.52375969
53	O	-3.67629941	7.06587450	-0.11946078
54	O	-2.68003222	5.25927101	-1.52375969
55	O	-7.95737652	0.34916857	-0.11946078
56	O	-5.89467841	0.30865953	-1.52375969
57	O	-3.21464619	-4.95061149	-1.52375969
58	O	-4.28107712	-6.71670593	-0.11946078
59	O	3.67629941	-7.06587450	-0.11946078
60	O	2.68003222	-5.25927101	-1.52375969
61	S	2.87749836	-5.84306192	-0.19895642
62	S	6.49898924	-0.42954428	-0.19895642
63	S	3.62149088	5.41351763	-0.19895642
64	S	-2.87749836	5.84306192	-0.19895642
65	S	-6.49898924	0.42954428	-0.19895642
66	S	-3.62149088	-5.41351763	-0.19895642
67	N	6.28134559	-2.40218706	0.06365669
68	C	6.57337145	-2.94193623	1.26703408
69	N	1.06031778	-6.64089839	0.06365669
70	C	0.73889422	-7.16367478	1.26703408
71	N	-5.22102782	-4.23871132	0.06365669
72	C	-5.83447724	-4.22173856	1.26703408
73	N	-6.28134559	2.40218706	0.06365669
74	C	-6.57337145	2.94193623	1.26703408
75	N	-1.06031778	6.64089839	0.06365669
76	C	-0.73889422	7.16367478	1.26703408
77	N	5.22102782	4.23871132	0.06365669
78	C	5.83447724	4.22173856	1.26703408
79	H	-6.84314403	2.24578475	2.05714798
80	H	-1.47666537	7.04922894	2.05714798

81	H	5.36647865	4.80344420	2.05714798
82	H	6.84314403	-2.24578475	2.05714798
83	H	1.47666537	-7.04922894	2.05714798
84	H	-5.36647865	-4.80344420	2.05714798

3pyrazine/SO3 (-5967.2)

1	C	-4.11765915	-1.11661771	0.95449361
2	C	-3.49257655	0.42756222	-1.16484037
3	C	-4.35043737	-0.66351467	-1.27452906
4	N	-4.67938943	-1.42829718	-0.21987782
5	O	-1.41287601	-1.91151620	-0.89321308
6	H	-3.20923357	1.06345527	-1.99705656
7	H	-4.78332447	-0.92536262	-2.23760508
8	H	1.59243625	2.27722232	2.03939237
9	O	4.38033444	0.85839454	0.04677165
10	O	2.36185959	-0.26782841	-0.89321308
11	N	-2.97388488	0.72672451	0.03817203
12	C	-3.24847561	-0.03141958	1.10629933
13	O	-1.20061632	-2.25544528	1.57169993
14	C	1.37600853	-3.23844113	-1.16484037
15	C	3.02584888	-3.00768858	0.95449361
16	C	2.74983924	-3.43583195	-1.27452906
17	H	0.68363750	-3.31100542	-1.99705656
18	N	3.57663636	-3.33832153	-0.21987782
19	O	2.55358107	0.08795841	1.57169993
20	H	3.19304977	-3.67979919	-2.23760508
21	H	-2.76835050	0.24047908	2.03939237
22	N	0.85758055	-2.93882211	0.03817203
23	C	1.65144797	-2.79755261	1.10629933
24	S	-1.87000942	2.38427724	0.22138099
25	O	-1.35296475	2.16748688	1.57169993
26	O	-2.93355869	3.36428363	0.04677165
27	S	-1.12983995	-2.81161428	0.22138099
28	S	2.99984936	0.42733704	0.22138099
29	C	2.11656802	2.81087891	-1.16484037
30	C	1.60059813	4.09934662	-1.27452906
31	H	2.52559607	2.24755015	-1.99705656
32	C	1.09181028	4.12430628	0.95449361
33	N	1.10275308	4.76661871	-0.21987782
34	H	1.59027470	4.60516181	-2.23760508
35	O	-0.94898358	2.17934461	-0.89321308
36	H	1.17591426	-2.51770140	2.03939237
37	N	2.11630433	2.21209759	0.03817203
38	C	1.59702765	2.82897220	1.10629933
39	O	-1.44677574	-4.22267817	0.04677165
40	H	3.68901993	-2.89468061	1.80891208
41	H	0.66235699	4.64212529	1.80891208
42	H	-4.35137692	-1.74744467	1.80891208

4pyrazine/SO3 (-7952.0)

1	C	-2.18375029	-4.53019325	-0.47339364
2	N	-3.08253964	-5.19299450	-1.22060607
3	O	5.50273387	0.90628336	0.47164164
4	C	-4.69572122	-3.53606307	-0.58309787
5	C	-4.32800072	-4.69268511	-1.27002329
6	H	-2.81441513	1.79418100	0.82738336
7	H	-5.68960884	-3.09977275	-0.60400144
8	H	-5.05969626	-5.22560854	-1.87488871
9	C	-4.53019325	2.18375029	-0.47339364

10	N	-5.19299450	3.08253964	-1.22060607
11	O	-5.50273387	-0.90628336	0.47164164
12	C	-3.53606307	4.69572122	-0.58309787
13	C	-4.69268511	4.32800072	-1.27002329
14	H	-1.79418100	-2.81441513	0.82738336
15	H	-3.09977275	5.68960884	-0.60400144
16	H	-5.22560854	5.05969626	-1.87488871
17	C	2.18375029	4.53019325	-0.47339364
18	C	4.69572122	3.53606307	-0.58309787
19	N	3.08253964	5.19299450	-1.22060607
20	O	0.90628336	-5.50273387	0.47164164
21	C	4.32800072	4.69268511	-1.27002329
22	H	5.68960884	3.09977275	-0.60400144
23	H	2.81441513	-1.79418100	0.82738336
24	H	5.05969626	5.22560854	-1.87488871
25	C	4.53019325	-2.18375029	-0.47339364
26	N	5.19299450	-3.08253964	-1.22060607
27	O	-0.90628336	5.50273387	0.47164164
28	C	3.53606307	-4.69572122	-0.58309787
29	C	4.69268511	-4.32800072	-1.27002329
30	H	1.79418100	2.81441513	0.82738336
31	H	3.09977275	-5.68960884	-0.60400144
32	H	5.22560854	-5.05969626	-1.87488871
33	N	2.89798203	-3.76972345	0.15256277
34	C	3.36487947	-2.51348365	0.22937882
35	N	3.76972345	2.89798203	0.15256277
36	C	2.51348365	3.36487947	0.22937882
37	N	-2.89798203	3.76972345	0.15256277
38	C	-3.36487947	2.51348365	0.22937882
39	N	-3.76972345	-2.89798203	0.15256277
40	C	-2.51348365	-3.36487947	0.22937882
41	O	-4.47767812	-1.91631247	2.52147817
42	O	-3.10894353	-0.46400722	1.01157099
43	O	0.46400722	-3.10894353	1.01157099
44	O	1.91631247	-4.47767812	2.52147817
45	O	4.47767812	1.91631247	2.52147817
46	O	3.10894353	0.46400722	1.01157099
47	O	-0.46400722	3.10894353	1.01157099
48	O	-1.91631247	4.47767812	2.52147817
49	S	-4.30541537	-1.27385839	1.22979301
50	S	1.27385839	-4.30541537	1.22979301
51	S	4.30541537	1.27385839	1.22979301
52	S	-1.27385839	4.30541537	1.22979301
53	H	-4.92835577	1.17353136	-0.41779773
54	H	-1.17353136	-4.92835577	-0.41779773
55	H	4.92835577	-1.17353136	-0.41779773
56	H	1.17353136	4.92835577	-0.41779773

5pyrazine/SO3 (-9938.5)

1	C	1.75259399	-6.61743604	-0.63910662
2	C	3.72378310	-4.77323970	-0.52032182
3	C	2.91304611	-6.72641012	-1.40485135
4	H	0.93955351	-7.33663879	-0.64887734
5	N	3.89845893	-5.81572019	-1.34982747
6	O	5.46258868	-1.14030633	2.64368459
7	H	3.04899291	-7.57288982	-2.07588884
8	H	0.26794989	4.47419698	0.91851229
9	C	-5.75197434	-3.71171613	-0.63910662
10	C	-5.49701542	-4.84904653	-1.40485135
11	H	-6.68722012	-3.16071456	-0.64887734

12	C	-3.38890847	-5.01654037	-0.52032182
13	N	-4.32638852	-5.50481114	-1.34982747
14	H	-6.26005559	-5.23991623	-2.07588884
15	O	0.60353697	-5.54760460	2.64368459
16	H	4.33801526	1.12776742	0.91851229
17	C	-5.30750964	4.32346932	-0.63910662
18	C	-6.31038848	3.72953455	-1.40485135
19	H	-5.07248284	5.38320976	-0.64887734
20	C	-5.81824372	1.67284725	-0.52032182
21	N	-6.57231408	2.41355980	-1.34982747
22	H	-6.91792004	4.33444350	-2.07588884
23	O	-5.08958232	-2.28830186	2.64368459
24	H	2.41309099	-3.77719839	0.91851229
25	C	2.47175299	6.38376712	-0.63910662
26	C	1.59698085	7.15402564	-1.40485135
27	H	3.55225332	6.48772116	-0.64887734
28	C	-0.20696391	6.05041683	-0.52032182
29	N	0.26447504	6.99647313	-1.34982747
30	H	1.98454588	7.91874964	-2.07588884
31	O	-3.74907183	4.13335627	2.64368459
32	H	-2.84664301	-3.46220440	0.91851229
33	C	6.83513700	-0.37808426	-0.63910662
34	C	5.69033299	2.06651599	-0.52032182
35	C	7.29737692	0.69189645	-1.40485135
36	H	7.26789613	-1.37357757	-0.64887734
37	N	6.73576864	1.91049840	-1.34982747
38	O	2.77252850	4.84285653	2.64368459
39	H	8.14443684	0.55961292	-2.07588884
40	H	-4.17241313	1.63743839	0.91851229
41	N	-4.56924668	3.55094940	0.17574710
42	C	-4.79568880	2.23026010	0.25599619
43	N	-4.78912845	-3.24830811	0.17574710
44	C	-3.60305273	-3.87178281	0.25599619
45	N	1.60940252	-5.55851422	0.17574710
46	C	2.56887975	-4.62315347	0.25599619
47	N	5.78379390	-0.18704260	0.17574710
48	C	5.19070773	1.01451684	0.25599619
49	N	1.96517869	5.44291553	0.17574710
50	C	0.63915406	5.25015935	0.25599619
51	S	3.21507700	4.35368255	1.34970055
52	S	5.13411159	-1.71235805	1.34970055
53	S	-0.04202154	-5.41197802	1.34970055
54	S	-5.16008234	-1.63242832	1.34970055
55	S	-3.14708472	4.40308183	1.34970055
56	O	5.99927000	-2.76349797	0.81065112
57	O	3.73408075	-1.73307897	0.93241625
58	O	-0.49436164	-4.08687269	0.93241625
59	O	-0.77436637	-6.55961266	0.81065112
60	O	-4.03961304	-0.79274725	0.93241625
61	O	-6.47785473	-1.29056561	0.81065112
62	O	-3.22916803	5.76199924	0.81065112
63	O	-2.00225652	3.59692794	0.93241625
64	O	4.48211913	4.85167699	0.81065112
65	O	2.80215046	3.01577097	0.93241625
66	H	-6.03224539	0.61034212	-0.44783459
67	H	-1.28359649	5.92561237	-0.44783459
68	H	5.23893913	3.05188773	-0.44783459
69	H	4.52143894	-4.03944202	-0.44783459
70	H	-2.44453619	-5.54840020	-0.44783459

6pyrazine/SO3 (-11924.4)

1	C	-7.49575012	2.94460671	-0.37536104
2	C	-5.43337344	4.66725160	-0.64617674
3	C	-7.62348904	4.14625239	-1.07287151
4	H	-8.29950402	2.22908152	-0.23219907
5	N	-6.60235700	5.00677404	-1.21346067
6	O	-4.08742822	-4.20082505	2.47464844
7	H	-8.57520632	4.41780564	-1.52643795
8	H	-4.32070139	3.18071032	0.50981398
9	C	-6.29797927	-5.01920667	-0.37536104
10	C	-7.40250443	-4.52900898	-1.07287151
11	H	-6.08019324	-6.07304057	-0.23219907
12	C	-6.75864516	-2.37181363	-0.64617674
13	N	-7.63717201	-3.21442187	-1.21346067
14	H	-8.11353507	-5.21744368	-1.52643795
15	O	1.59430710	-5.64022921	2.47464844
16	H	0.59422524	5.33219233	0.50981398
17	C	1.19777084	-7.96381338	-0.37536104
18	C	0.22098462	-8.67526138	-1.07287151
19	H	2.21931080	-8.30212207	-0.23219907
20	C	-1.32527172	-7.03906523	-0.64617674
21	N	-1.03481501	-8.22119591	-1.21346067
22	H	0.46167124	-9.63524932	-1.52643795
23	O	5.68173533	-1.43940415	2.47464844
24	H	4.91492663	2.15148201	0.50981398
25	C	7.49575012	-2.94460671	-0.37536104
26	C	7.62348904	-4.14625239	-1.07287151
27	H	8.29950402	-2.22908152	-0.23219907
28	C	5.43337344	-4.66725160	-0.64617674
29	N	6.60235700	-5.00677404	-1.21346067
30	H	8.57520632	-4.41780564	-1.52643795
31	O	4.08742822	4.20082505	2.47464844
32	H	4.32070139	-3.18071032	0.50981398
33	C	6.29797927	5.01920667	-0.37536104
34	C	7.40250443	4.52900898	-1.07287151
35	H	6.08019324	6.07304057	-0.23219907
36	C	6.75864516	2.37181363	-0.64617674
37	N	7.63717201	3.21442187	-1.21346067
38	H	8.11353507	5.21744368	-1.52643795
39	O	-1.59430710	5.64022921	2.47464844
40	H	-0.59422524	-5.33219233	0.50981398
41	C	-1.19777084	7.96381338	-0.37536104
42	C	1.32527172	7.03906523	-0.64617674
43	C	-0.22098462	8.67526138	-1.07287151
44	H	-2.21931080	8.30212207	-0.23219907
45	N	1.03481501	8.22119591	-1.21346067
46	O	-5.68173533	1.43940415	2.47464844
47	H	-0.46167124	9.63524932	-1.52643795
48	H	-4.91492663	-2.15148201	0.50981398
49	O	7.45618953	-0.39017878	1.04369525
50	O	5.06774368	-0.27014350	0.34895141
51	O	4.06599949	6.26216016	1.04369525
52	O	2.76782298	4.25372301	0.34895141
53	O	-3.39019004	6.65233894	1.04369525
54	O	-2.29992070	4.52386652	0.34895141
55	O	-7.45618953	0.39017878	1.04369525
56	O	-5.06774368	0.27014350	0.34895141
57	O	-2.76782298	-4.25372301	0.34895141
58	O	-4.06599949	-6.26216016	1.04369525
59	O	3.39019004	-6.65233894	1.04369525

60	O	2.29992070	-4.52386652	0.34895141
61	S	2.27545629	-5.71672262	1.19467706
62	S	6.08855515	-0.88775836	1.19467706
63	S	3.81309886	4.82896425	1.19467706
64	S	-2.27545629	5.71672262	1.19467706
65	S	-6.08855515	0.88775836	1.19467706
66	S	-3.81309886	-4.82896425	1.19467706
67	N	6.30783141	-2.63303964	0.16822456
68	C	5.26310672	-3.46758096	0.05340407
69	N	0.87363648	-6.77926207	0.16822456
70	C	-0.37145984	-6.29177460	0.05340407
71	N	-5.43419493	-4.14622242	0.16822456
72	C	-5.63456656	-2.82419364	0.05340407
73	N	-6.30783141	2.63303964	0.16822456
74	C	-5.26310672	3.46758096	0.05340407
75	N	-0.87363648	6.77926207	0.16822456
76	C	0.37145984	6.29177460	0.05340407
77	N	5.43419493	4.14622242	0.16822456
78	C	5.63456656	2.82419364	0.05340407
79	H	2.34267187	6.67064768	-0.72690786
80	H	6.94828629	1.30651048	-0.72690786
81	H	4.60561441	-5.36413719	-0.72690786
82	H	-2.34267187	-6.67064768	-0.72690786
83	H	-6.94828629	-1.30651048	-0.72690786
84	H	-4.60561441	5.36413719	-0.72690786