

Mechanism of the Paal-Knorr Reaction : The Importance of Water Mediated Hemiacetal Pathway

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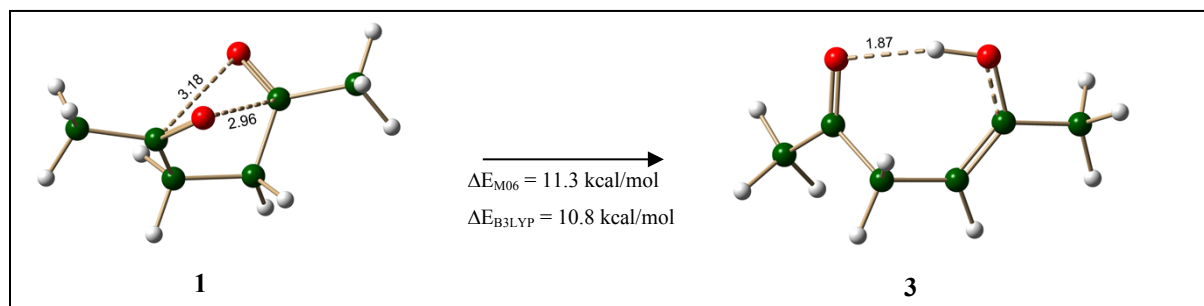
(i) Free Energy Change (ΔG) for pyrrole w.r.t. 1,4-diketone + amine.

The reaction between 1,4-diketones and amines lead to the synthesis of pyrroles (Paal-Knorr mechanism). Quantum chemical methods suggest that the Paal-Knorr synthesis of pyrrole is an exergonic process. The ΔG values for the pyrrole formation w.r.t. ketone-imine are given in the manuscript (Table 1) and the ΔG values w.r.t. starting material 1,4-diketone + amine are given in Table S1.

Table S1: The free energy change (ΔG) values of the Paal-Knorr reactions (under gas phase and implicit water conditions) leading to the formation pyrrole (w.r.t. 1,4-diketone + amine) estimated using various levels of quantum chemical analysis.

S. No.	Method	$\Delta G_{\text{pyrrole}}$ (kcal/mol)	
		Gas	Solvent
1	B3LYP*	-9.7	-11.6
2	M06*	-8.6	-11.6
3	G2MP2	-10.6	-13.4

(ii) Keto-enol tautomerism in 2,5-dimethylfuran.



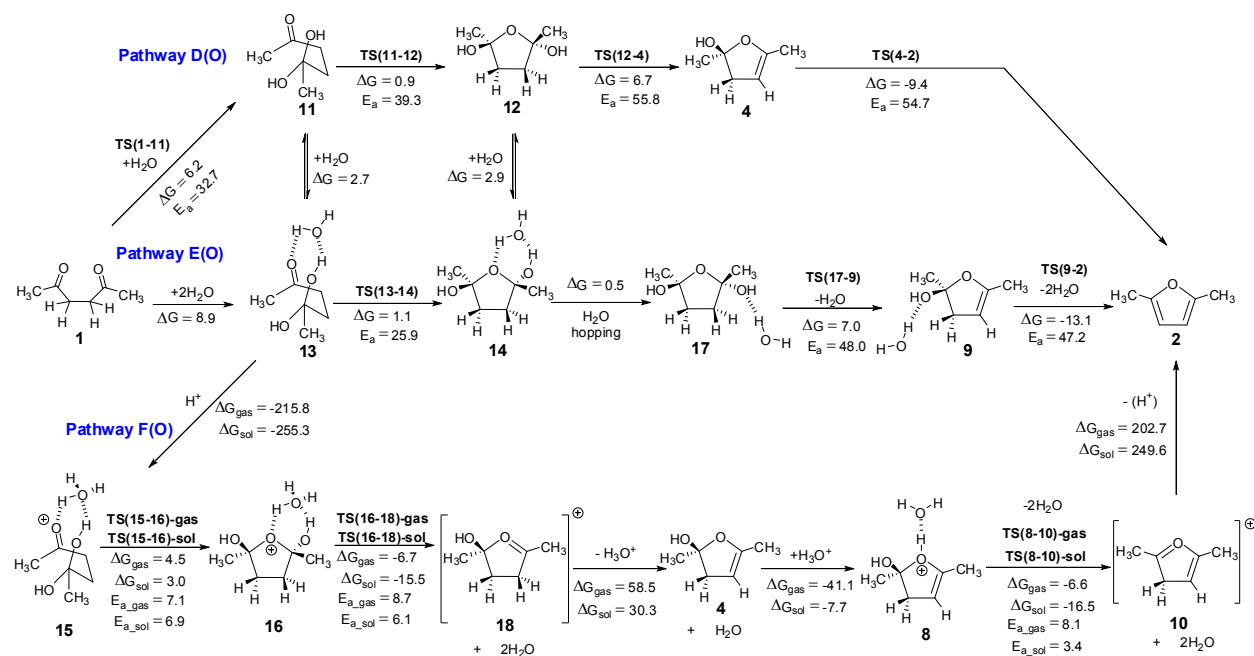
Fig

ure S1: Keto-enol tautomerism in 2,5-dimethylfuran. The distances are given in Å.

Energy difference for Keto-enol tautomers of 2,5-dimethylfuran and their 3D structures are given in Fig. S1. Compound 1 is characterised by two weak intramolecular electrostatic interactions with a distance of ~ 3.24 Å, between the oxygen atom at one carbonyl centre and the carbon atom at the other carbonyl centre. The monoenol tautomer 3 of compound 1 is characterized by intramolecular hydrogen bond interaction with a bond length of 1.87 Å. The monoenol tautomer is less stable than its keto tautomer by 11.3 kcal/mol and 10.8 kcal/mol, calculated at M06 and B3LYP levels respectively.

(iii) Schematic representation of energy profile for the Paal-Knorr furan synthesis hemiketal pathway (trans w.r.t. -OH groups) obtained using M06/6-311+G(2df,3pd) method and 3D structures of the transition states.

Scheme S1: Hemiketal pathways for the Paal-Knorr furan synthesis – (i) Pathway D(O) without explicit water, (ii) Pathway E(O) with explicit water and (iii) Pathway F(O) under proton catalysis condition. The energy values (kcal/mol) are obtained using M06 method. Structures **12**, **14**, **16** and **17** with trans arrangement of -OH groups are employed in the above scheme.



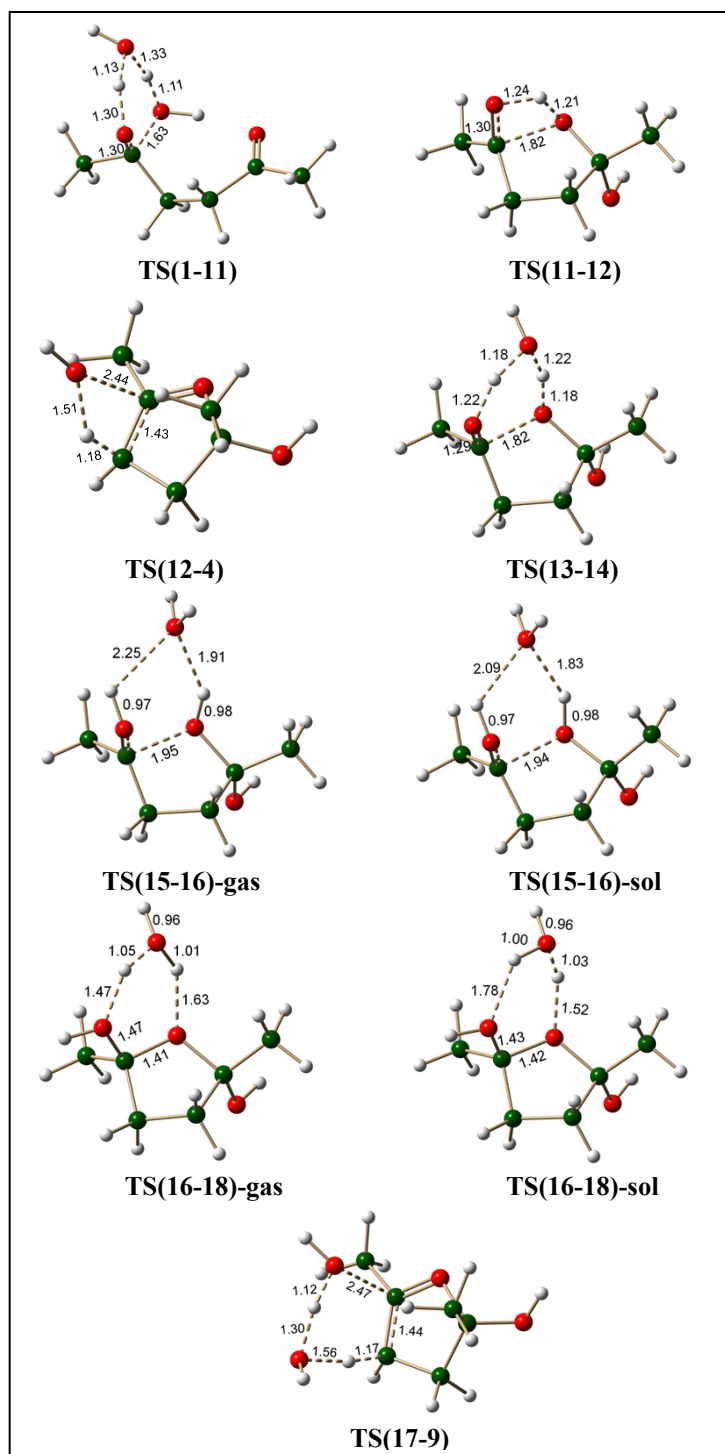
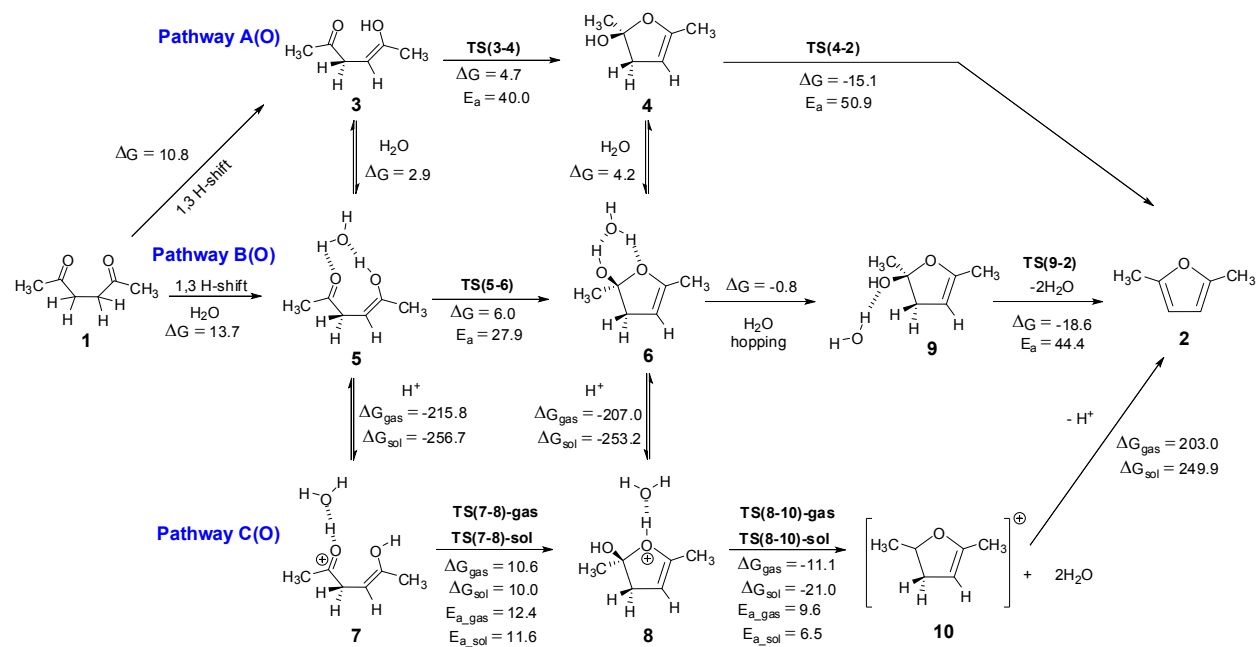


Figure S2: The 3D structures of the transition states on the potential energy surface of the hemiketal pathways (referring to trans position of -OH group) for the Paal-Knorr synthesis of furan. The distances are given in Å.

(iv) Schematic representation of energy profile for the Paal-Knorr furan synthetic paths obtained using B3LYP/6-311+G(2df,3pd) method.

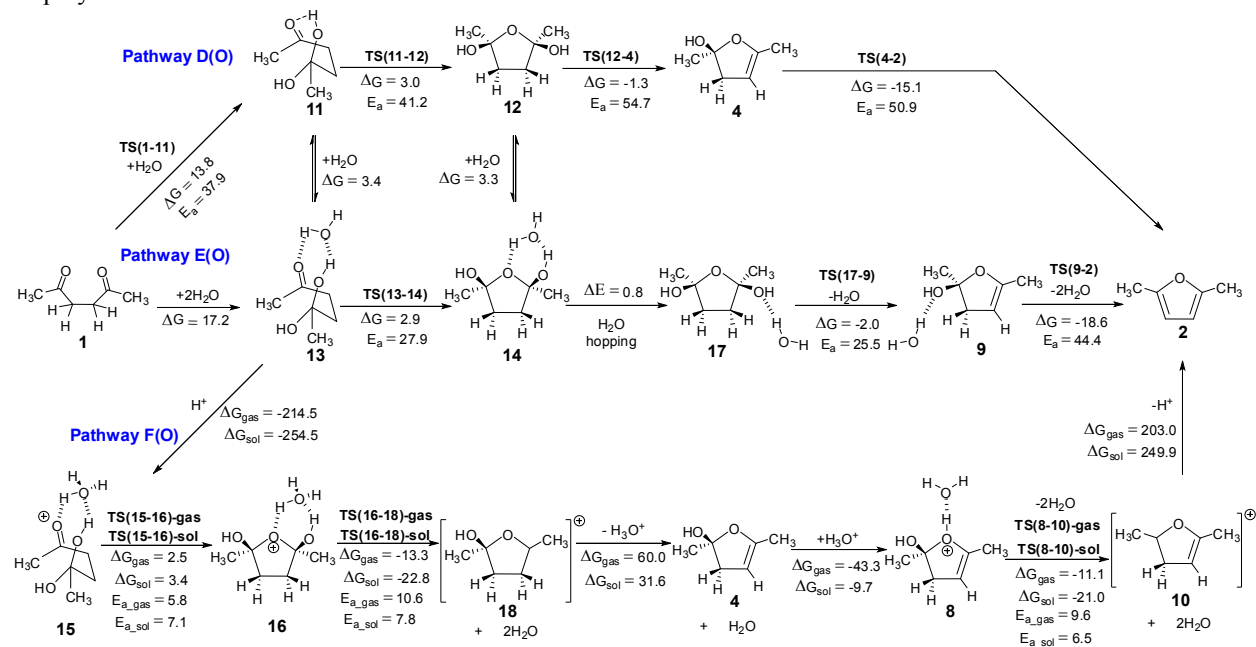
Monoenol Pathway

Scheme S2: Monoenol pathways for the Paal-Knorr synthesis of furan -- pathway A(O) without explicit water pathway B(O) with explicit water and pathway C(O) under protonated conditions. The energy values (kcal/mol) are obtained using B3LYP method.



Hemiketal Pathway

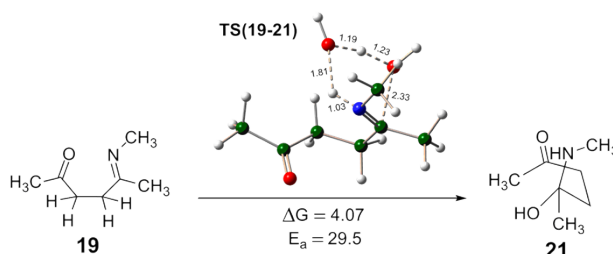
Scheme S3: Hemiketal pathways for the Paal-Knorr furan synthesis -- Pathway D(O) without explicit water, Pathway E(O) with explicit water and pathway F(O) under proton catalysis conditions. The energy values (kcal/mol) are obtained using B3LYP method. Structures **12**, **14** and **16** and **17** with cis arrangement of -OH groups are employed in this scheme.



(v) Formation of hemiaminal (21) from imine (19).

The hemiaminal (**21**) can be generated in a reaction between 1,4-diketone and methylamine directly, involving energy barrier of 26.4 kcal/mol via **TS(1-21)**. Alternatively, the hemiaminal **21** may be generated by the hydrolysis of an imine **19**, involving an energy barrier of 29.5 kcal/mol via **TS(19-21)** (Scheme S4).

Scheme S4: The formation of hemiaminal **21** from imine **19**. The energy values are given in kcal/mol.



(vi) Over-pyramidalization in transition state structure for water elimination step (under proton catalysis condition) in case of pyrrole as compared to in furan synthetic pathway.

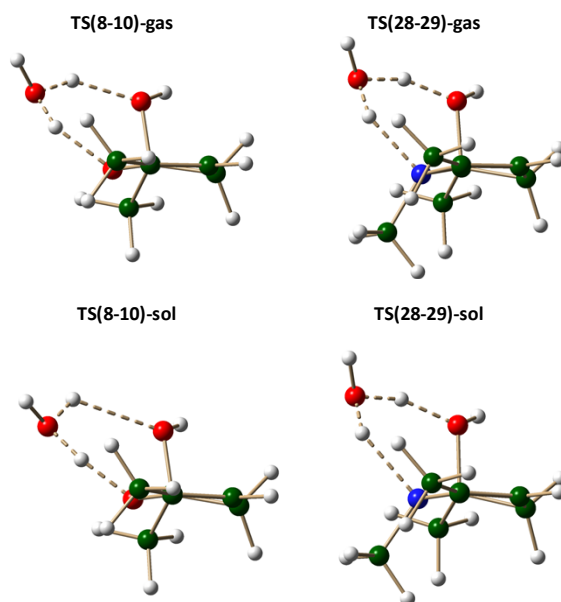
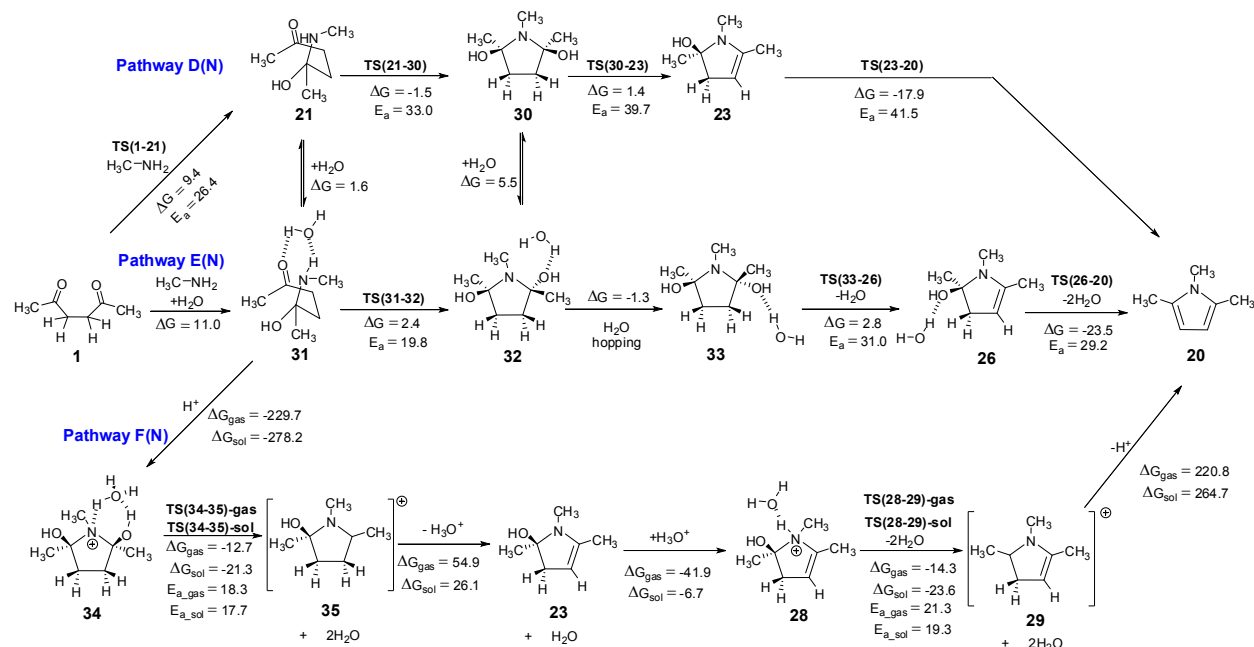


Figure S3: Over-pyramidalization of transition state structure for water elimination step (under proton catalysis conditions) in case of pyrrole as compared to furan.

(vii) Schematic representation of energy profile for the Paal-Knorr pyrrole synthesis hemiaminal pathway (trans w.r.t. -OH groups) obtained using M06/6-311+G(2df,3pd) method and 3D structures of the transition states.

Scheme S5: Hemiaminal pathways for the Paal-Knorr pyrrole synthesis – (i) Pathway D(N) without explicit water, (ii) Pathway E(N) with explicit water and (iii) Pathway F(N) under proton catalysis conditions. The energy values (kcal/mol) are obtained using M06 method. Structures **30**, **32**, **33** and **34** with trans arrangement of -OH groups are employed in the above scheme.



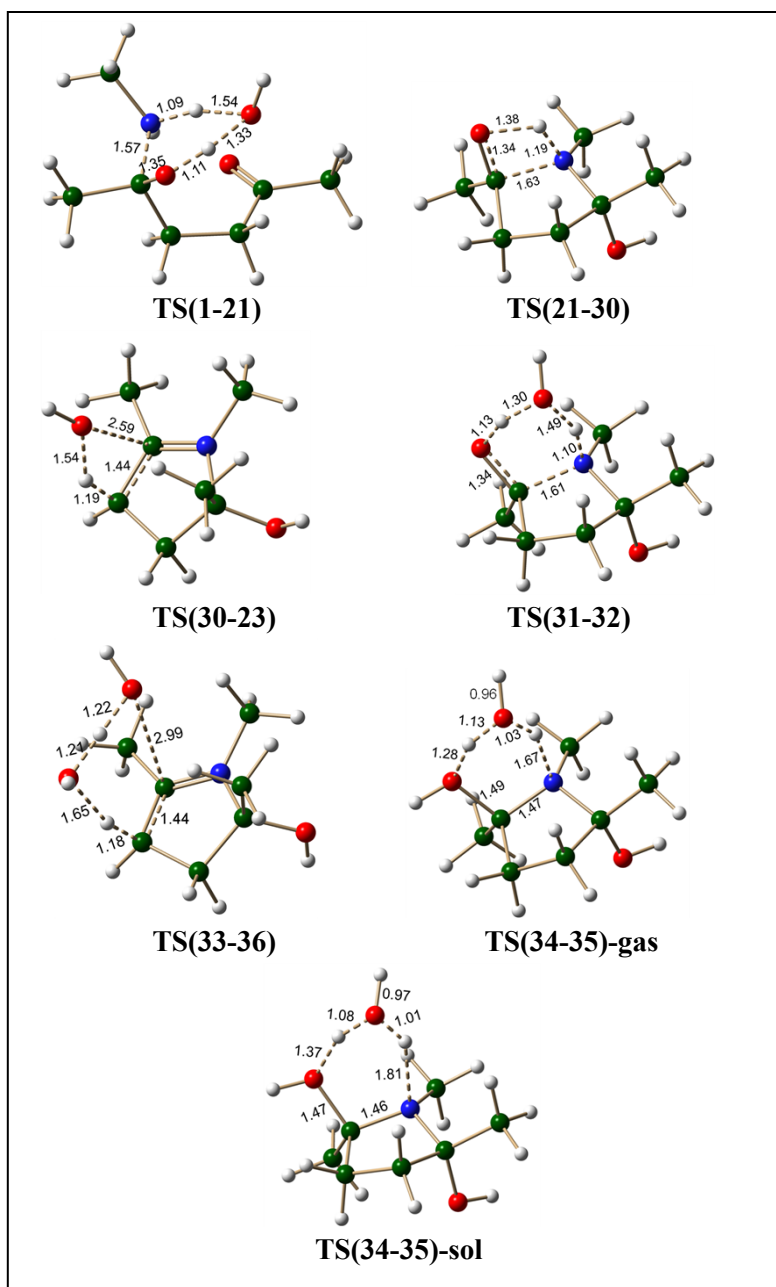
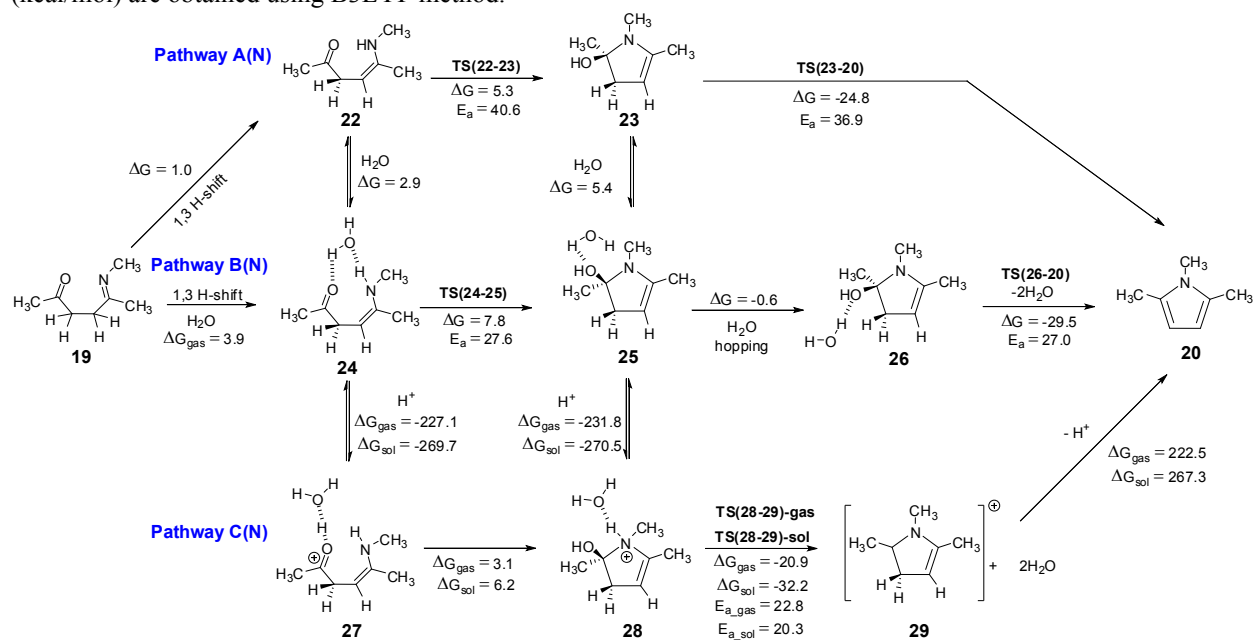


Figure S4: The 3D structures of the transition states on the potential energy surface of the hemiaminal pathways (referring to trans position of -OH group) for the Paal-Knorr synthesis of pyrrole. The distances are given in Å.

(viii) Schematic representation of energy profile for the Paal-Knorr pyrrole synthetic paths obtained using B3LYP/6-311+G(2df,3pd) method.

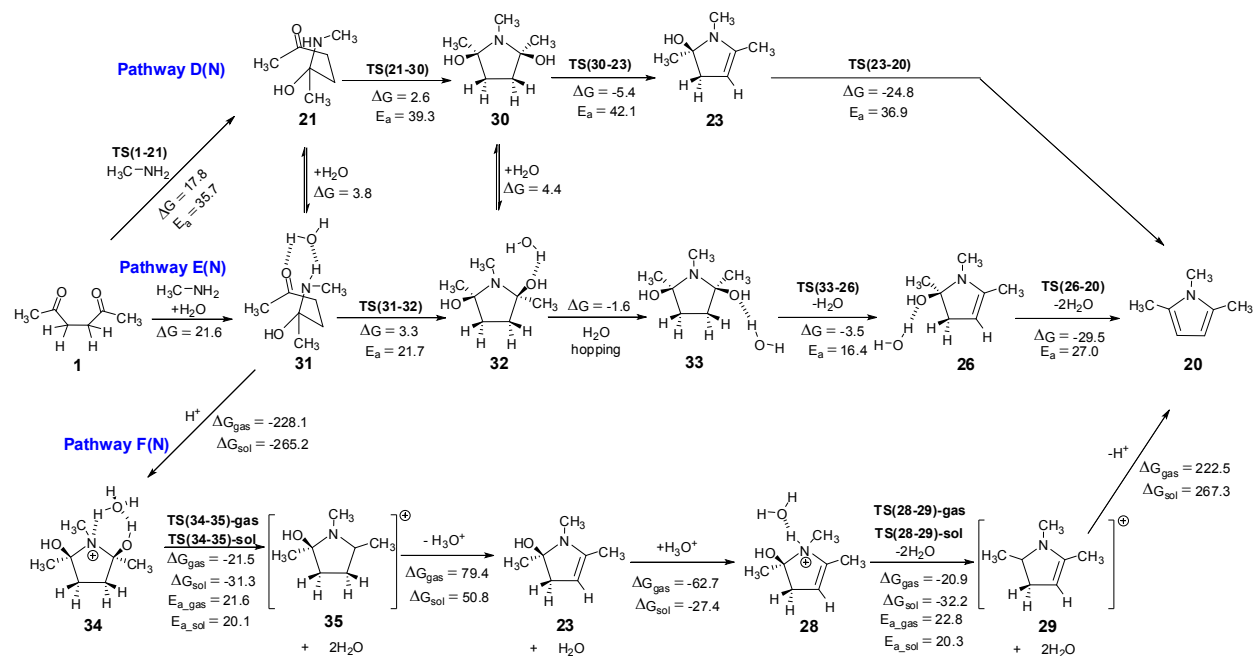
Enamine Pathway

Scheme S6: Enamine cyclization pathways for the Paal-Knorr pyrrole synthesis -- Pathway A(N) without explicit water, Pathway B(N) with explicit water and Pathway C(N) under proton catalysis conditions. The energy values (kcal/mol) are obtained using B3LYP method.



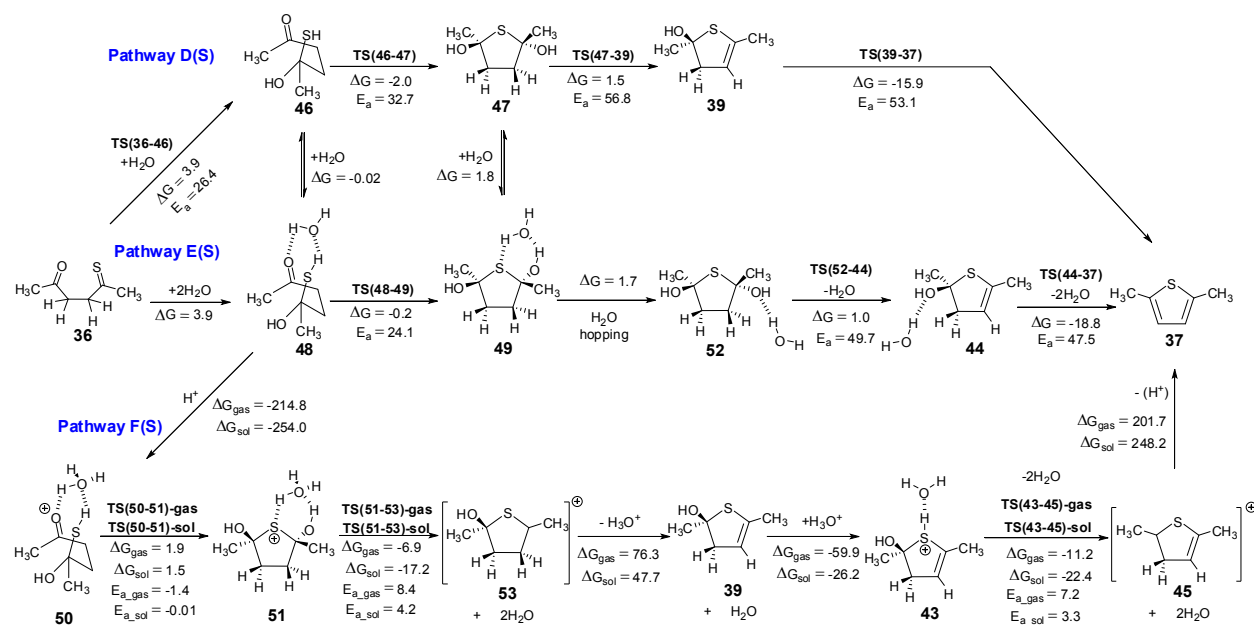
Hemiaminal Pathway

Scheme S7: Hemiaminal pathways for the Paal-Knorr pyrrole synthesis -- Pathway D(N) without explicit water, Pathway E(N) with explicit water and Pathway F(N) under proton catalysis conditions. The energy values (kcal/mol) are obtained using B3LYP method. Structures **29**, **31** and **32** with cis arrangement of -OH groups are employed in this scheme.



(ix) Schematic representation of energy profile for the Paal-Knorr thiophene synthesis hemithioketal pathway (trans w.r.t. -OH groups) obtained using M06/6-311+G(2df,3pd) method and 3D structures of the transition states.

Scheme S8: Hemithioketal pathways for the Paal-Knorr thiophene synthesis – (i) Pathway D(S) without explicit water, (ii) Pathway E(S) with explicit water and (iii) Pathway F(S) under proton catalysis condition. The energy values (kcal/mol) are obtained using M06 method. Structures **47**, **49**, **51** and **52** with trans arrangement of -OH groups are employed in this scheme.



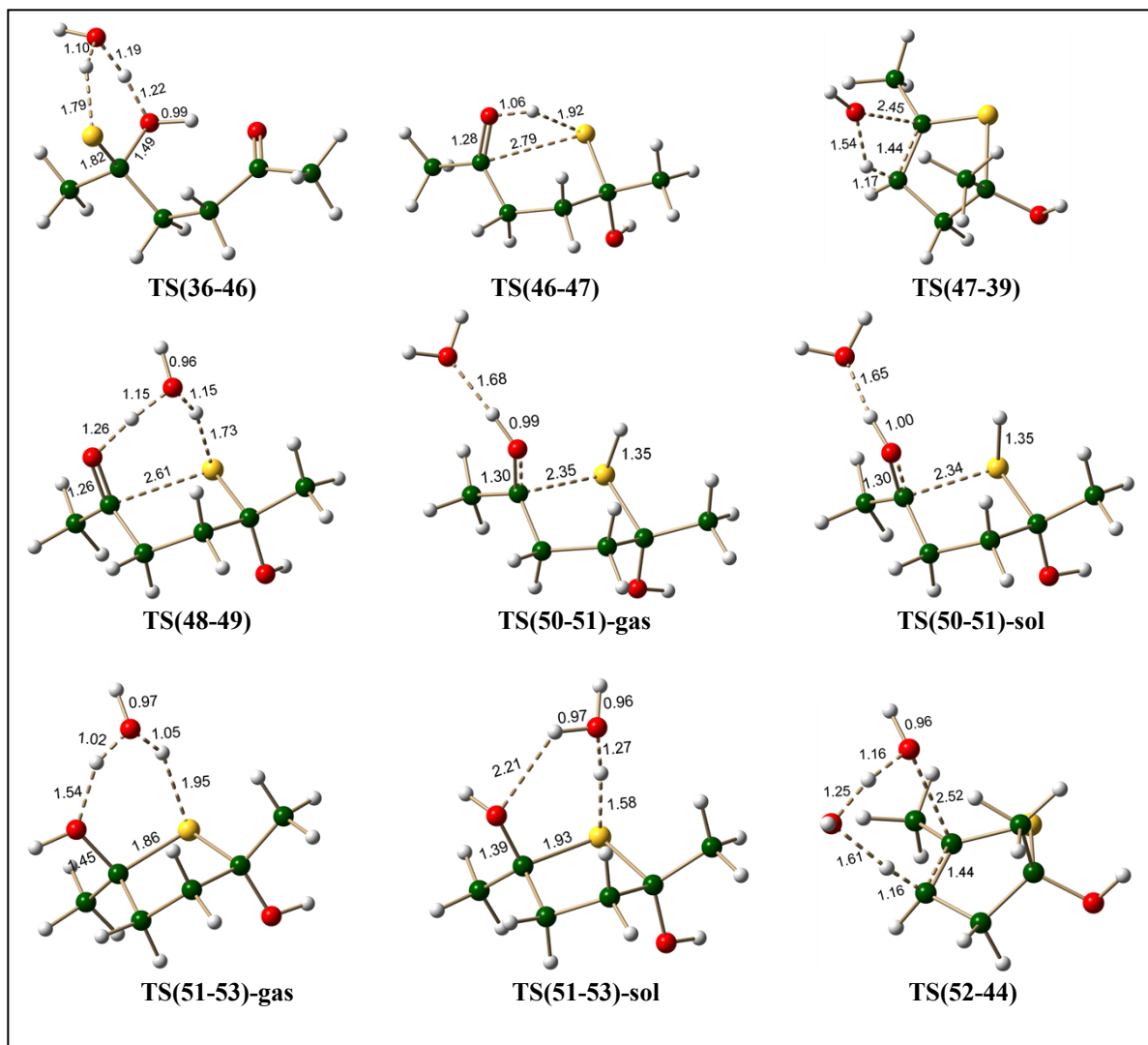
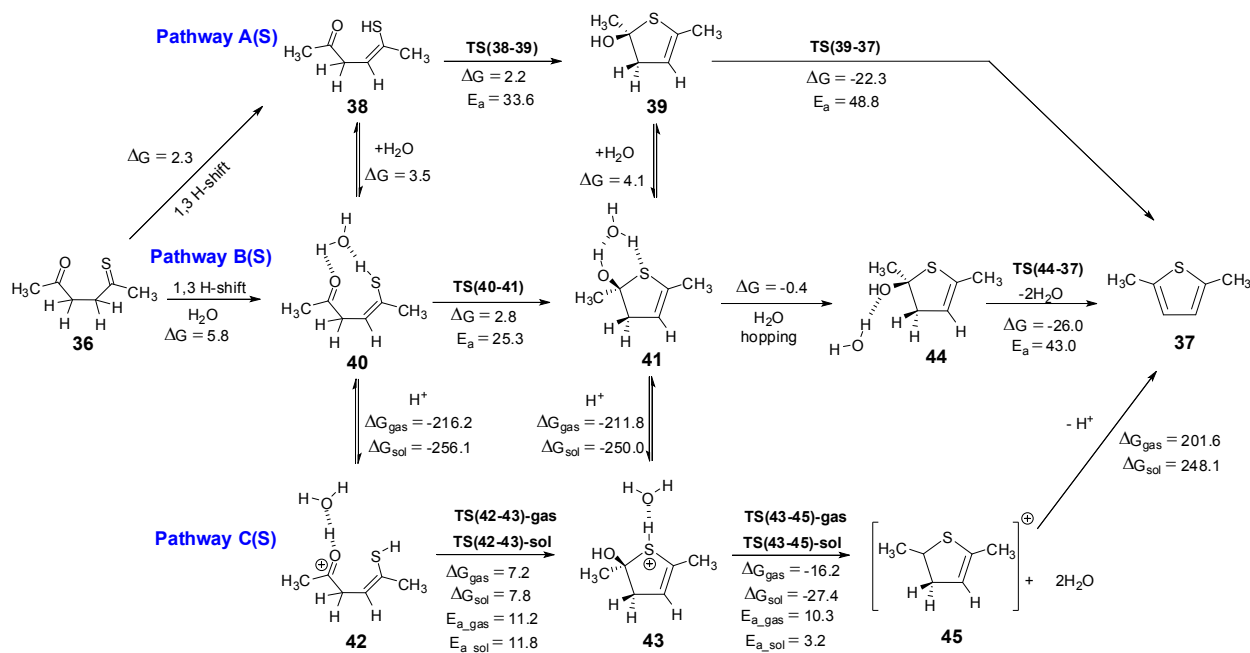


Figure S5: The 3D structures of the transition states on the potential energy surface of the hemithioketal pathways (referring to trans position of -OH group) for the Paal-Knorr synthesis of thiophene. The distances are given in Å.

(x) Schematic representation of energy profile for the Paal-Knorr thiophene synthetic paths obtained using B3LYP/6-311+G(2df,3pd) method.

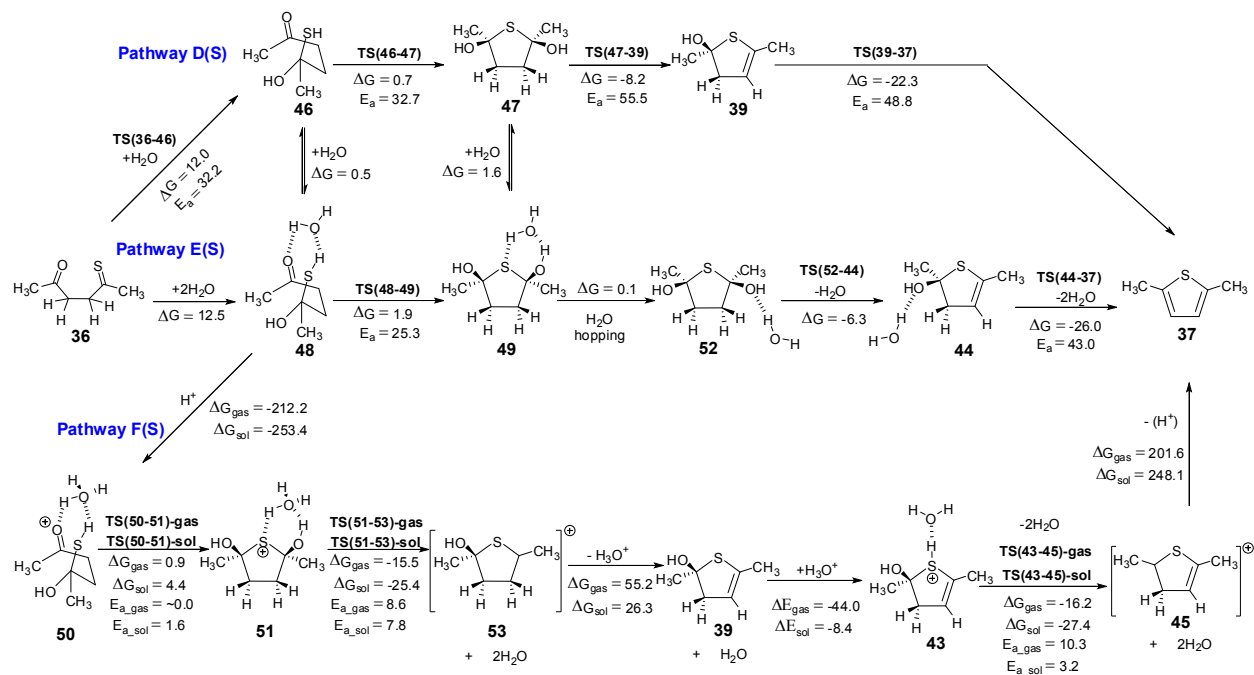
Thiol pathway

Scheme S9: Thiol pathways for the Paal-Knorr thiophene synthesis -- Pathway A(S) without explicit water, Pathway B(S) with explicit water and Pathway C(S) under proton catalysis conditions. The energy values (kcal/mol) are obtained using B3LYP method.



Hemithioketal Pathway

Scheme S10: Hemithioketal pathways for the Paal-Knorr thiophene synthesis -- Pathway D(S) without explicit water, Pathway E(S) with explicit water and pathway F(S) under proton catalysis conditions. The energy values (kcal/mol) are obtained using B3LYP method. Structures **47**, **49**, **51** and **52** with cis arrangement of -OH groups are employed in this scheme.



(xi) Table of free energies calculated using G2MP2 method

S. No.	Compound	Gibbs free energy (Hartrees)	S. No.	Compound	Gibbs free energy (Hartrees)
1	1_gas	-384.478406	9	30_gas	-707.064070
2	1_sol	-384.489012	10	30_sol	-707.072805
3	2_gas	-308.125190	11	31_gas	-630.740591
4	2_sol	-308.128591	12	31_sol	-630.743659
5	19_gas	-403.810943	13	NH₂Me_gas	-95.780594
6	19_sol	-403.821687	14	NH₂Me_sol	-95.784861
7	20_gas	-327.487491	15	Water_gas	-76.347604
8	20_sol	-327.493331	16	Water_sol	-76.354491

* 'gas' and 'sol' indicates the calculations carried out under gas phase and implicit solvent (water) phase conditions, respectively.

(xii) Table of free energies calculated using M06 method

S. No	Compound	Gibbs free energy (Hartrees)	S. No.	Compound	Gibbs free energy (Hartrees)
1	1 gas	-384.878231	97	47-cis gas	-784.249577
2	1 sol	-384.889038	98	47-trans gas	-784.249961
3	2 gas	-308.451895	99	48-cis gas	-860.664312
4	2 sol	-308.455114	100	48-cis sol	-860.678334
5	3 gas	-384.860292	101	48-trans gas	-860.666119
6	4 gas	-384.856225	102	48-trans sol	-860.677581
7	4 sol	-384.863074	103	49-cis gas	-860.667033
8	5 gas	-461.278218	104	49-trans gas	-860.666482
9	5 sol	-461.288565	105	50-cis-gas	-861.001591
10	6 gas	-461.273103	106	50-cis sol	-861.080845
11	6 sol	-461.281403	107	50-trans gas	-861.008489
12	7 gas	-461.620399	108	50-trans sol	-861.082332
13	7 sol	-461.694877	109	51-cis gas	-861.006932
14	8 gas	-461.603058	110	51-cis sol	-861.081571
15	8 sol	-461.679787	111	51-trans gas	-861.005464
16	9 gas	-461.269664	112	51-trans sol	-861.079897
17	10 gas	-308.774944	113	52-cis gas	-860.664148
18	10 sol	-308.852915	114	52-trans gas	-860.663706
19	11-cis gas	-461.285946	115	53 gas	-708.177824
20	11-trans gas	-461.287675	116	53 sol	-708.254235
21	12-cis gas	-461.284057	117	TS(1-11) gas	-537.664837
22	12-trans gas	-461.286261	118	TS(1-21) gas	-557.036037
23	13-cis gas	-537.701515	119	TS(3-4) gas	-384.796821
24	13-cis sol	-537.715654	120	TS(4-2) gas	-384.769118
25	13-trans gas	-537.702644	121	TS(5-6) gas	-461.232129
26	13-trans sol	-537.715616	122	TS(7-8) gas	-461.600249
27	14-cis gas	-537.702535	123	TS(7-8) sol	-461.676540
28	14-trans gas	-537.700905	124	TS(8-10) gas	-461.590196
29	15-cis gas	-538.042891	125	TS(8-10) sol	-461.674435
30	15-cis sol	-538.119877	126	TS(9-2) gas	-461.194388
31	15-trans gas	-538.046580	127	TS(11-12)-cis gas	-461.220725
32	15-trans sol	-538.122464	128	TS(11-12)-trans gas	-461.225001
33	16-cis gas	-538.040430	129	TS(12-4)-cis gas	-461.190041
34	16-cis sol	-538.117074	130	TS(12-4)-trans gas	-461.197305
35	16-trans gas	-538.039397	131	TS(13-14)-cis gas	-537.658399
36	16-trans sol	-538.117676	132	TS(13-14)-trans gas	-537.661394
37	17-cis gas	-537.699456	133	TS(15-16)-cis gas	-538.034383
38	17-trans gas	-537.700100	134	TS(15-16)-cis sol	-538.111119
39	18 gas	-385.211446	135	TS(15-16)-trans gas	-538.035235
40	18 sol	-385.289246	136	TS(15-16)-trans sol	-538.111426
41	19 gas	-404.229186	137	TS(16-18)-cis gas	-538.027000
42	19 sol	-480.673899	138	TS(16-18)-cis sol	-538.108087
43	20 gas	-327.833927	139	TS(16-18)-trans gas	-538.025522
44	20 sol	-327.839213	140	TS(16-18)-trans sol	-538.107933
45	21-cis gas	-480.642015	141	TS(17-9)-cis gas	-537.640052
46	21-trans gas	-480.643899	142	TS(17-9)-trans gas	-537.623643
47	22 gas	-404.226595	143	TS(21-30)-cis gas	-480.587486
48	23 gas	-404.224738	144	TS(21-30)-trans gas	-480.591378

49	24_gas	-480.644106	145	TS(22-23)_gas	-404.164134
50	24_sol	-480.653618	146	TS(23-20)_gas	-404.158564
51	25_gas	-480.637618	147	TS(24-25)_gas	-480.603861
52	25_sol	-480.649167	148	TS(26-20)_gas	-480.588517
53	26_gas	-480.635099	149	TS(28-29)_gas	-480.967634
54	26_sol	-480.646401	150	TS(28-29)_sol	-481.045806
55	27_gas	-480.986883	151	TS(30-23)-cis_gas	-480.570573
56	27_sol	-481.059767	152	TS(30-23)-trans_gas	-480.582938
57	28_gas	-481.001553	153	TS(31-32)-cis_gas	-557.031216
58	28_sol	-481.076578	154	TS(31-32)-trans_gas	-557.029064
59	29_gas	-328.185768	155	TS(33-26)-cis_gas	-557.024899
60	29_sol	-328.261038	156	TS(33-26)-trans_gas	-557.058876
61	30-cis_gas	-480.647507	157	TS(34-35)-cis_gas	-557.397400
62	30-trans_gas	-480.646270	158	TS(34-35)-cis_sol	-557.474535
63	31-cis_gas	-557.061773	159	TS(34-35)-trans_gas	-557.397512
64	31-cis_sol	-557.074591	160	TS(34-35)-trans_sol	-557.475258
65	31-trans_gas	-557.060610	161	TS(36-46)_gas	-860.630363
66	31-trans_sol	-557.060280	162	TS(38-39)_gas	-707.774931
67	32-cis_gas	-557.062627	163	TS(39-37)_gas	-707.743688
68	32-trans_gas	-557.056823	164	TS(40-41)_gas	-784.205063
69	33-cis_gas	-557.063447	165	TS(41-43)_gas	-784.570212
70	33-trans_gas	-557.058876	166	TS(41-43)_sol	-784.644083
71	34-cis_gas	-557.428332	167	TS(43-45)_gas	-784.564839
72	34-cis_sol	-557.503594	168	TS(43-45)_sol	-784.644571
73	34-trans_gas	-557.426709	169	TS(44-37)_gas	-784.167115
74	34-trans_sol	-557.503542	170	TS(46-47)-cis_gas	-784.191919
75	35_gas	-404.608361	171	TS(46-47)-trans_gas	-784.194599
76	35_sol	-404.684314	172	TS(47-39)-cis_gas	-784.153640
77	36_gas	-707.833742	173	TS(47-39)-trans_gas	-784.159459
78	36_sol	-707.842947	174	TS(48-49)-cis_gas	-860.624912
79	37_gas	-631.434181	175	TS(48-49)-trans_gas	-860.627789
80	37_sol	-631.437066	176	TS(50-51)-cis_gas	-861.003176
81	38_gas	-707.827529	177	TS(50-51)-cis_sol	-861.080075
82	38_sol	-707.828235	178	TS(50-51)-trans_gas	-861.010663
83	39_sol	-707.834738	179	TS(50-51)-trans_sol	-861.082344
84	40_gas	-784.242857	180	TS(51-53)-cis_gas	-860.994977
85	40_sol	-784.253392	181	TS(51-53)-cis_sol	-861.072027
86	41_gas	-784.243814	182	TS(51-53)-trans_gas	-860.992076
87	41_sol	-784.254049	183	TS(51-53)-trans_sol	-861.073212
88	42_gas	-784.586082	184	TS(52-44)-cis_gas	-860.603952
89	42_sol	-784.660632	185	TS(52-44)-trans_gas	-860.584575
90	43_gas	-784.576322	186	Water_gas	-76.419319
91	43_sol	-784.649888	187	Water_sol	-76.426560
92	44_gas	-784.242849	188	H ₃ O ⁺ _gas	-76.681373
93	45_gas	-631.755576	189	H ₃ O ⁺ _sol	-76.804402
94	45_sol	-631.832544	190	NH ₂ Me_gas	-95.780594
95	46-cis_gas	-784.240949	191	NH ₂ Me_sol	-95.784861
96	46-trans_gas	-784.246767			

**‘gas’ and ‘sol’ indicates the calculations carried out under gas phase and implicit solvent (water) phase conditions, respectively.

*‘-cis’ and ‘-trans’ refers to the arrangement of -OH groups on the same side of plane and on the opposite sides, respectively.

(xiii) Table of free energies calculated using B3LYP method

S. No	Compound	Gibbs free energy (Hartrees)	S. No.	Compound	Gibbs free energy (Hartrees)
1	1 gas	-385.141676	72	42 sol	-784.966304
2	1 sol	-385.153401	73	43 gas	-784.880734
3	2 gas	-308.680952	74	43 sol	-784.953852
4	2 sol	-308.684236	75	44 gas	-784.543884
5	3 gas	-385.124454	76	45 gas	-631.986317
6	4 gas	-385.116961	77	45 sol	-632.063356
7	4 sol	-385.123757	78	46-cis gas	-784.537766
8	5 gas	-461.57999	79	47-cis gas	-784.536582
9	5 sol	-461.590232	80	48-cis gas	-860.997129
10	6 gas	-461.570373	81	48-cis sol	-861.012144
11	6 sol	-461.579811	82	49-cis gas	-860.994179
12	7 gas	-461.923931	83	50-cis-gas	-861.335357
13	7 sol	-461.999241	84	50-cis sol	-861.415903
14	8 gas	-461.906976	85	51-cis gas	-861.333982
15	8 sol	-461.983296	86	51-cis sol	-861.408961
16	9 gas	-461.571590	87	52-cis gas	-860.994019
17	10 gas	-309.004428	88	53 gas	-708.438359
18	10 sol	-309.082540	89	53 sol	-708.515180
19	11-cis gas	-461.579804	90	TS(1-11) gas	-538.001578
20	12-cis gas	-461.575053	91	TS(1-21) gas	-557.404846
21	13-cis gas	-538.034498	92	TS(3-4) gas	-385.060723
22	13-cis sol	-538.048812	93	TS(4-2) gas	-385.035883
23	14-cis gas	-538.029859	94	TS(5-6) gas	-461.535474
24	15-cis gas	-538.376399	95	TS(7-8) gas	-461.904170
25	15-cis sol	-538.454365	96	TS(7-8) sol	-461.980720
26	16-cis gas	-538.372412	97	TS(8-10) gas	-461.891616
27	16-cis sol	-538.448985	98	TS(8-10) sol	-461.972944
28	17-cis gas	-538.028524	99	TS(9-2) gas	-461.500810
29	18 gas	-385.473379	100	TS(11-12)-cis gas	-461.514098
30	18 sol	-385.551071	101	TS(12-4)-cis gas	-461.487949
31	19 gas	-404.527466	102	TS(13-14)-cis gas	-537.990034
32	19 sol	-404.539167	103	TS(15-16)-cis gas	-538.367160
33	20 gas	-328.096844	104	TS(15-16)-cis sol	-538.443106
34	20 sol	-328.101987	105	TS(16-18)-cis gas	-538.355510
35	21-cis gas	-480.973190	106	TS(16-18)-cis sol	-538.436552
36	22 gas	-404.525900	107	TS(17-9)-cis gas	-537.987831
37	23 gas	-404.517473	108	TS(21-30)-cis gas	-480.910621
38	24 gas	-480.981429	109	TS(22-23) gas	-404.461169
39	24 sol	-480.990900	110	TS(23-20) gas	-404.458608
40	25 gas	-480.969004	111	TS(24-25) gas	-480.937476
41	25 sol	-480.979737	112	TS(26-20) gas	-480.927002
42	26 gas	-480.970029	113	TS(28-29) gas	-481.302010
43	26 sol	-480.981721	114	TS(28-29) sol	-481.378528
44	27 gas	-481.343322	115	TS(30-23)-cis gas	-480.901809
45	27 sol	-481.420744	116	TS(31-32)-cis gas	-557.392775
46	28 gas	-481.338340	117	TS(33-26)-cis gas	-557.398386
47	28 sol	-481.410864	118	TS(34-35)-cis gas	-557.756563
48	29 gas	-328.451437	119	TS(34-35)-cis sol	-557.833424

49	29_sol	-328.527908	120	TS(36-46)_gas	-860.965818
50	30-cis_gas	-480.968976	121	TS(38-39)_gas	-708.039618
51	31-cis_gas	-557.427359	122	TS(39-37)_gas	-708.011861
52	31-cis_sol	-557.442774	123	TS(40-41)_gas	-784.507352
53	32-cis_gas	-557.422037	124	TS(41-43)_gas	-784.874322
54	33-cis_gas	-557.424545	125	TS(41-43)_sol	-784.947449
55	33-cis_gas	-557.790931	126	TS(43-45)_gas	-784.864252
56	34-cis_gas	-557.790931	127	TS(43-45)_sol	-784.948828
57	34-cis_sol	-557.865390	128	TS(44-37)_gas	-784.475368
58	35_gas	-404.904884	129	TS(46-47)-cis_gas	-784.485672
59	35_sol	-404.981015	130	TS(47-39)-cis_gas	-784.448103
60	36_gas	-708.096815	131	TS(48-49)-cis_gas	-860.956805
61	36_sol	-708.107008	132	TS(50-51)-cis_gas	-861.336795
62	37_gas	-631.665038	133	TS(50-51)-cis_sol	-861.413393
63	37_sol	-631.667998	134	TS(51-53)-cis_gas	-861.320305
64	38_gas	-708.093112	135	TS(51-53)-cis_sol	-861.396567
65	39_gas	-708.089592	136	Water_gas	-76.460137
66	39_sol	-708.096247	137	Water_sol	-76.467116
67	40_gas	-784.547656	138	H₃O⁺_gas	-76.720996
68	40_sol	-784.558253	139	H₃O⁺_sol	-76.844148
69	41_gas	-784.543251	140	NH₂Me_gas	-95.859940
70	41_sol	-784.555409	141	NH₂Me_sol	-95.864308
71	42_gas	-784.892241			

* 'gas' and 'sol' indicates the calculations carried out under gas phase and implicit solvent (water) phase conditions, respectively.

* '-cis' and '-trans' refers to the arrangement of -OH groups on the same side of plane and on the opposite sides, respectively.

Cartesian coordinates of all the species involved in Paal-Knorr synthetic pathways for furan, pyrrole and thiophene

Coordinates of species optimized using G2MP2 method

1-gas

0 1			
C	1.46748100	-0.05965300	0.29698800
C	0.71798300	1.14269600	-0.24632500
C	-0.71854700	1.14462700	0.23508400
C	-1.46718500	-0.06364600	-0.29606900
O	-1.01877200	-0.73086000	-1.22376500
H	0.76027000	1.12368000	-1.33950700
H	-0.76076000	1.13633500	1.32841700
C	2.77326200	-0.40481500	-0.37150600
H	3.30983300	-1.14396900	0.22375600
H	2.55940600	-0.82269400	-1.36090200
H	3.39071600	0.48656300	-0.51606000
O	1.02132600	-0.71553700	1.23379300
H	1.24577700	2.04975500	0.07778000
H	-1.24700600	2.04808700	-0.09784300
C	-2.77497000	-0.40032700	0.37288300
H	-3.31016500	-1.14631400	-0.21505000
H	-2.56417800	-0.80649200	1.36780000
H	-3.39247400	0.49293100	0.50505400

1-sol

0 1			
C	-1.49447200	-0.07079200	-0.27694100
C	-0.71613200	1.11660400	0.24584800
C	0.71610200	1.11653100	-0.24631300
C	1.49448600	-0.07061100	0.27698900
O	1.05019900	-0.78171200	1.17703600
H	-0.75464100	1.10851800	1.33966600
H	0.75462700	1.10800900	-1.34012600
C	-2.83718100	-0.32960100	0.35347200
H	-3.37366900	-1.09503800	-0.20798200
H	-2.68951000	-0.67050100	1.38342100
H	-3.42774400	0.58981600	0.39579900
O	-1.05004500	-0.78241700	-1.17651000
H	-1.23851000	2.02740100	-0.07490400
H	1.23843000	2.02748300	0.07408400
C	2.83707700	-0.32980400	-0.35351400
H	3.37356800	-1.09507400	0.20816500
H	2.68923000	-0.67108700	-1.38330900
H	3.42771500	0.58954600	-0.39627000

2-gas

0 1			
C	-2.42492600	-0.68769800	0.00001900
C	-1.10724200	-0.00391500	0.00000400
C	-0.71322300	1.30448100	-0.00001900
C	0.71322300	1.30448100	-0.00002400
C	1.10724200	-0.00391500	-0.00000600
O	0.00000000	-0.81475600	0.00001300
H	-2.54508200	-1.32082700	0.88436500
H	-3.22204700	0.05902500	0.00001200
H	-1.36973900	2.16446900	-0.00003100
H	-2.54508900	-1.32085100	-0.88430900
H	1.36973900	2.16446900	-0.00004100
C	2.42492600	-0.68769800	0.00000500
H	2.54508700	-1.32082400	0.88435200
H	2.54508300	-1.32085400	-0.88432200

H	3.22204700	0.05902500	-0.00001000
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2-sol

O 1			
C	-2.42870500	-0.68680700	0.00001900
C	-1.10996500	-0.00431600	0.00000300
C	-0.71400100	1.30383000	-0.00001900
C	0.71400100	1.30383000	-0.00002300
C	1.10996500	-0.00431600	-0.00000400
O	0.00000000	-0.81575300	0.00001300
H	-2.55057100	-1.31938900	0.88450600
H	-3.22375500	0.06182700	0.00000800
H	-1.37109500	2.16375000	-0.00003100
H	-2.55057500	-1.31941900	-0.88444700
H	1.37109500	2.16375000	-0.00003900
C	2.42870500	-0.68680700	0.00000400
H	2.55057600	-1.31938900	0.88449100
H	2.55057000	-1.31941900	-0.88446200
H	3.22375500	0.06182700	-0.00001200

19-gas

O 1			
C	-1.22443900	-0.41148000	-0.06879600
C	-0.16629700	-1.47007800	-0.24680400
C	1.13217100	-0.94371300	-0.84432200
C	1.85963700	0.12073800	-0.04171700
H	1.83203000	-1.78378400	-0.96266300
C	-2.60445700	-0.87937200	0.32521900
H	-3.31463600	-0.71317200	-0.49278000
H	-2.60770800	-1.94423100	0.56654700
H	-2.97517200	-0.32426100	1.19258100
H	0.01276500	-1.95476400	0.72348700
H	0.95843600	-0.52312100	-1.83740600
O	2.52705300	0.97974000	-0.60656000
N	-0.87968800	0.81096100	-0.26119800
C	-1.89341400	1.84616000	-0.09032300
H	-1.47780800	2.79621300	-0.42767700
H	-2.80385300	1.63897200	-0.66535600
H	-2.17611000	1.95125200	0.96423100
H	-0.56970000	-2.26273800	-0.89183500
C	1.82968800	0.01229900	1.46653300
H	2.48920100	0.77257000	1.88607100
H	0.81383900	0.16538200	1.83795300
H	2.16276800	-0.98028700	1.78897500

19-sol

O 1			
C	-1.21187500	-0.41417000	-0.08424800
C	-0.14725000	-1.45979900	-0.28944700
C	1.15341100	-0.91730500	-0.86578400
C	1.85480400	0.13495700	-0.03457300
H	1.86168400	-1.75083000	-0.97783400
C	-2.56975200	-0.90474700	0.34803600
H	-3.31933400	-0.68657600	-0.42062600
H	-2.56207300	-1.98171500	0.52460700
H	-2.89131700	-0.40216500	1.26583700
H	0.02934200	-1.97093300	0.66662700
H	0.99112700	-0.49239500	-1.85922600
O	2.49314100	1.03886200	-0.57227600
N	-0.89636600	0.81739200	-0.28127900
C	-1.93677500	1.82252200	-0.06721900
H	-1.54262200	2.80064500	-0.34684800
H	-2.83058100	1.62347300	-0.66931500
H	-2.24127900	1.86253700	0.98502200
H	-0.54379200	-2.23531500	-0.95790700
C	1.83834300	-0.02657100	1.46500200
H	2.48455100	0.72722000	1.91638800

H	0.82079100	0.08997500	1.84546200
H	2.18750300	-1.02587200	1.74436500

20-gas

O 1			
C	2.50861400	0.27529700	-0.01379000
C	1.13133800	-0.29606700	-0.00816800
C	0.70672600	-1.61266500	0.01832700
C	-0.70674500	-1.61265700	0.01832700
C	-1.13134300	-0.29605500	-0.00816800
H	2.69766100	0.92677800	0.84724500
H	3.22956400	-0.54451500	0.02871400
H	1.35932800	-2.47704500	0.02670200
H	2.72189100	0.85385100	-0.92039100
H	-1.35935600	-2.47703000	0.02670100
N	0.00000200	0.49550000	-0.03663900
C	0.00001900	1.94235500	0.03443600
H	0.88427000	2.33209100	-0.47125400
H	-0.88435000	2.33209500	-0.47103900
H	0.00014500	2.29595000	1.07117900
C	-2.50861600	0.27531800	-0.01379000
H	-2.69766300	0.92679300	0.84724900
H	-2.72188900	0.85387700	-0.92038800
H	-3.22957000	-0.54449200	0.02870700

20-sol

O 1			
C	2.50909600	0.27666200	-0.00937500
C	1.13154100	-0.29642400	-0.00779300
C	0.70764600	-1.61566100	0.01459800
C	-0.70764500	-1.61566100	0.01459800
C	-1.13154100	-0.29642500	-0.00779300
H	2.69019300	0.92989900	0.85131700
H	3.23222900	-0.54132800	0.03512100
H	1.36254700	-2.47914500	0.02236000
H	2.72083400	0.85796300	-0.91388600
H	-1.36254400	-2.47914700	0.02236000
N	0.00000000	0.49368200	-0.03267100
C	-0.00000200	1.94558700	0.02784200
H	0.88441400	2.33010600	-0.47999100
H	-0.88440800	2.33010500	-0.48000800
H	-0.00001200	2.30080700	1.06266500
C	-2.50909600	0.27666100	-0.00937500
H	-2.69019300	0.92989800	0.85131700
H	-2.72083400	0.85796100	-0.91388700
H	-3.23222900	-0.54133000	0.03512200

30-gas

O 1			
C	1.67524300	-0.23898700	-0.15751700
C	0.95802000	-0.01357400	1.15883600
C	-0.39601900	-0.70050100	1.16923300
C	-1.35851700	-0.15987300	0.13347200
H	0.85030100	1.06359900	1.32541700
H	-0.26118600	-1.77363000	1.00284500
C	2.97469100	0.49890900	-0.36005500
H	3.46125500	0.14431000	-1.26894000
H	2.76903800	1.57061000	-0.45259400
H	3.63867100	0.36631500	0.49916600
O	1.20862700	-0.98141300	-1.01756300
H	1.59405700	-0.39265800	1.97025900
H	-0.86371400	-0.58344500	2.15636300
C	-2.21645800	-1.20025500	-0.51927800
H	-2.97106100	-0.75337000	-1.16666000
H	-1.56481200	-1.85394100	-1.11025200
H	-2.70377800	-1.82344500	0.23984000
S	-1.46497200	1.42329000	-0.22519300

30-sol

O 1			
C	-1.69244400	-0.26332100	0.22981300
C	-0.87881600	-0.75110300	-0.95021600
C	0.51549100	-1.19276800	-0.55719300
C	1.43881000	-0.10188900	-0.08082100
H	-0.85176200	0.02497700	-1.72085200
H	0.45496400	-1.94603700	0.23737400
C	-2.91045300	0.56118400	-0.08963300
H	-3.50210600	0.72284600	0.81194400
H	-2.59230600	1.52584800	-0.49776000
H	-3.51728100	0.06696700	-0.85398600
O	-1.38630200	-0.55613500	1.38414200
H	-1.42536400	-1.59916500	-1.38612900
H	1.00723700	-1.69005800	-1.40472700
C	2.75871900	-0.59957700	0.43155700
H	3.43026800	0.22159800	0.68214800
H	2.59363700	-1.21380000	1.32424800
H	3.23343600	-1.24447400	-0.31605100
S	1.05449100	1.47907600	-0.11564900

31-gas

O 1			
C	-2.70007900	-0.26573400	0.00003000
C	-1.25444400	0.11738700	-0.00000200
C	-0.70938700	1.37932300	-0.00002100
C	0.70938700	1.37932300	-0.00002400
C	1.25444400	0.11738700	-0.00001000
H	-2.96714500	-0.85293200	-0.88405600
H	-2.96713200	-0.85282900	0.88418900
H	-1.31992800	2.27775800	-0.00003000
H	-3.31276400	0.63957900	-0.00001700
H	1.31992800	2.27775800	-0.00003400
C	2.70007900	-0.26573400	0.00002600
H	2.96713800	-0.85280200	0.88420100
H	2.96713900	-0.85295900	-0.88404400
H	3.31276400	0.63957900	-0.00005400
S	0.00000000	-1.07467800	-0.00000900

31-sol

O 1			
C	-2.70311400	-0.26550300	0.00001200
C	-1.25711800	0.11778500	-0.00000300
C	-0.71025100	1.37942600	-0.00005100
C	0.71025100	1.37942600	-0.00005200
C	1.25711800	0.11778500	-0.00000500
H	-2.96907100	-0.85371900	-0.88347900
H	-2.96906800	-0.85365700	0.88354600
H	-1.32077000	2.27809800	-0.00008400
H	-3.31491100	0.64022200	-0.00001800
H	1.32077000	2.27809800	-0.00008700
C	2.70311400	-0.26550300	0.00000600
H	2.96907000	-0.85366100	0.88353700
H	2.96907000	-0.85371600	-0.88348700
H	3.31491100	0.64022200	-0.00002200
S	0.00000000	-1.07514900	0.00004100

Coordinates of all the species optimized using M06 method

1_gas

```
0 1
C      -1.46681500   -0.24614200   -0.18193200
C      -0.74035900    1.06400800   -0.36869600
C       0.69065300    0.85395700   -0.79532600
C       1.49876600    0.15082500    0.27337300
O       1.22436500    0.25967300    1.44157400
H      -0.79255800    1.62314300    0.57053700
H       0.74350500    0.28339600   -1.72560700
C      -2.82175500   -0.15785400    0.45010300
H      -3.35494300   -1.10034900    0.34809300
H      -2.69182000    0.06565400    1.51255600
H      -3.40607900    0.65997400    0.02377400
O      -0.97281400   -1.29510200   -0.51142600
H      -1.29766900    1.65551400   -1.10337900
H       1.18397000    1.81354300   -0.98789000
C       2.64799300   -0.67290300   -0.21406700
H       3.28371100   -0.98039700    0.61301500
H       2.23932900   -1.55822200   -0.70987000
H       3.22925700   -0.13016500   -0.96314300
```

1_sol

```
0 1
C       1.50938000   -0.05221900    0.30045900
C       0.71822700    1.08977200   -0.28457100
C      -0.71860000    1.10182900    0.17618500
C      -1.50739100   -0.09046200   -0.29166700
O      -1.10008400   -0.81752200   -1.14980200
H       0.75752400    0.97970600   -1.37244000
H      -0.78591900    1.14105500    1.26730700
C       2.79192800   -0.36951000   -0.39437000
H       3.37387400   -1.10453700    0.15672300
H       2.57479400   -0.73462600   -1.40111100
H       3.37934100    0.54247800   -0.52803700
O       1.12584100   -0.67041400    1.26350700
H       1.22535300    2.02460500   -0.03181600
H      -1.23372900    2.00315200   -0.17218900
C      -2.81178400   -0.32119000    0.39307000
H      -3.39120700   -1.09979600   -0.09601600
H      -2.61097600   -0.60490600    1.42996000
H      -3.38567400    0.60704000    0.44334000
```

2_gas

```
0 1
C      -2.40887400   -0.67738200    0.00001100
C      -1.09786300   -0.00559300    0.00000300
C      -0.71429100    1.29001700   -0.00001000
C       0.71429200    1.29001600   -0.00001500
C       1.09786300   -0.00559300   -0.00000500
O       0.00000000   -0.80652200    0.00000600
H      -2.53394100   -1.31253100    0.88027900
H      -3.20479800    0.06631600    0.00001000
H      -1.37450000    2.14259400   -0.00001600
H      -2.53394700   -1.31254000   -0.88024900
H       1.37450200    2.14259300   -0.00002600
C       2.40887300   -0.67738200    0.00000400
H       2.53396800   -1.31247900    0.88030500
H       2.53391800   -1.31259300   -0.88022300
H       3.20479800    0.06631500   -0.00006500
```

2_sol

0 1			
C	-2.41270400	-0.67692700	0.00001700
C	-1.10096500	-0.00567700	0.00000300
C	-0.71521900	1.28971900	-0.00001800
C	0.71521900	1.28971900	-0.00002200
C	1.10096500	-0.00567700	-0.00000300
O	0.00000000	-0.80744800	0.00001200
H	-2.53882900	-1.31153700	0.88043200
H	-3.20749100	0.06765800	0.00000700
H	-1.37563100	2.14254700	-0.00002900
H	-2.53883300	-1.31156600	-0.88037500
H	1.37563100	2.14254700	-0.00003700
C	2.41270400	-0.67692700	0.00000400
H	2.53883600	-1.31153200	0.88042100
H	2.53882500	-1.31157100	-0.88038700
H	3.20749100	0.06765800	-0.00001700

3_gas

0 1			
C	1.49276900	-0.07500800	0.00692400
C	0.55772800	-0.97151900	0.34464300
C	-0.73640100	-0.61176100	1.02282400
C	-1.57907800	0.17490300	0.05267100
O	-1.39467500	1.36447900	-0.09383600
H	-1.25357000	-1.51652600	1.34597800
C	2.81295500	-0.43576900	-0.56590700
H	3.61017400	-0.05353100	0.07585100
H	2.92526600	-1.51389900	-0.66383400
H	2.94236200	0.03085800	-1.54490000
O	1.37113600	1.25296300	0.17366600
H	0.76017600	-2.01526300	0.14254600
H	0.43869400	1.51211600	0.28738800
H	-0.55916900	0.01598000	1.90305400
C	-2.58013900	-0.58439900	-0.75418900
H	-3.02932500	0.04807700	-1.51612500
H	-2.09580200	-1.44828000	-1.21662400
H	-3.35749800	-0.97774700	-0.09377000

4_gas

0 1			
C	1.30752700	0.00240700	-0.06627800
C	0.96572900	1.28476800	-0.06603400
C	-0.52165200	1.38986700	-0.15610100
C	-0.95276900	-0.06623200	0.03499000
O	0.23932500	-0.84773600	-0.13937300
H	-0.85917300	1.78293700	-1.12141000
C	2.62474900	-0.65620900	-0.01844600
H	2.70202000	-1.29891000	0.86143100
H	2.76988800	-1.29131300	-0.89543800
H	3.42180400	0.08494400	0.01468500
H	1.65790600	2.11107300	-0.02484500
O	-1.37801700	-0.19657300	1.35915400
H	-1.53333500	-1.12847400	1.53812500
H	-0.97585000	2.00217000	0.62576000
C	-1.98226800	-0.58212700	-0.93384700
H	-2.18484600	-1.63839000	-0.74110200
H	-2.91026200	-0.02033500	-0.82139500
H	-1.62651500	-0.48406900	-1.95977000

4_sol

0 1			
C	1.31213600	0.00011900	-0.06409600
C	0.96913200	1.28302300	-0.05579500

C	-0.51751500	1.38779700	-0.16391600
C	-0.95455800	-0.06511600	0.03269800
O	0.24057400	-0.84848100	-0.14811000
H	-0.84125800	1.76993100	-1.13762000
C	2.62952200	-0.65893000	-0.01842400
H	2.70439800	-1.31633700	0.85084500
H	2.78242800	-1.27852600	-0.90524400
H	3.42552100	0.08226200	0.03123400
H	1.66152800	2.10943400	-0.01195400
O	-1.36777900	-0.19711800	1.36330100
H	-1.64229100	-1.10771100	1.51402600
H	-0.98208800	2.01417500	0.60036300
C	-1.99301800	-0.57815000	-0.92552700
H	-2.20804700	-1.63033700	-0.72506900
H	-2.91392200	-0.00481100	-0.81415200
H	-1.64281400	-0.48574500	-1.95359300

5_gas

0 1			
C	-1.67148500	-0.36773800	0.02142500
C	-0.60955000	-1.01456600	0.51938900
C	0.64600100	-0.38507000	1.04843600
C	1.68984000	-0.36000900	-0.04077600
O	1.96710500	0.64904900	-0.65405900
H	0.47518000	0.63136200	1.40819200
C	-2.89068600	-1.07840000	-0.44714700
H	-3.07949900	-0.84511500	-1.49744700
H	-2.79894000	-2.15663600	-0.33191300
H	-3.76065100	-0.73287000	0.11585300
O	-1.81715600	0.95580400	-0.10716000
H	-0.66978500	-2.09623800	0.54476600
H	-1.01628400	1.48665900	0.07946500
H	1.02353600	-0.97784400	1.88794100
H	1.04479300	2.13975100	-0.23869700
O	0.32891200	2.67921600	0.14962300
H	0.24210100	3.46557600	-0.38960100
C	2.35753400	-1.66241700	-0.34788700
H	1.61921100	-2.46122500	-0.43489000
H	2.94696200	-1.59054100	-1.25884900
H	3.01256800	-1.92623700	0.48731300

5_sol

0 1			
C	-1.66861800	-0.40055700	0.02293600
C	-0.58626600	-1.03154200	0.49201800
C	0.65569900	-0.39043100	1.03939100
C	1.70399900	-0.33829200	-0.04304200
O	1.93637100	0.68069000	-0.66637300
H	0.46728400	0.61873400	1.41000300
C	-2.87340600	-1.12341300	-0.46239300
H	-3.07417400	-0.86670600	-1.50531300
H	-2.75447200	-2.20179600	-0.38026400
H	-3.75056200	-0.82045200	0.11458400
O	-1.84646600	0.93155400	-0.05485900
H	-0.61344100	-2.11475100	0.47501000
H	-1.04301200	1.46755900	0.10892800
H	1.03597000	-0.98894900	1.87201500
H	0.97617200	2.14928800	-0.23937400
O	0.26480000	2.69851800	0.14440100
H	0.13954000	3.44118400	-0.45022100
C	2.42626200	-1.61019000	-0.32790800
H	1.72954100	-2.44870400	-0.37239800
H	2.99874200	-1.54207000	-1.24986600
H	3.10474700	-1.81288800	0.50552700

6_gas

O	1			
C		1.43952800	0.40389000	0.07775300
C		1.82986200	-0.79288800	-0.33779100
C		0.67422200	-1.73591000	-0.28008200
C		-0.50066800	-0.80178600	0.02124300
O		0.11811800	0.45133300	0.43661200
H		0.79176100	-2.49688400	0.49927500
C		2.17057200	1.67467700	0.22807200
H		1.73283300	2.44910800	-0.40700000
H		2.11918500	2.03224200	1.25940100
H		3.21671200	1.54846600	-0.04619900
H		2.83131200	-1.03855800	-0.65500900
O		-1.18424700	-0.58846600	-1.16283100
H		-1.83466000	0.11849700	-1.02889000
H		0.47822900	-2.25455000	-1.22083200
C		-1.40771100	-1.24410700	1.13898600
H		-2.19717700	-0.50808600	1.30257500
H		-1.87063500	-2.19529800	0.87307800
H		-0.84594700	-1.36850500	2.06537300
O		-2.14435300	1.94700600	-0.29780800
H		-2.68981600	2.40619800	0.34088100
H		-1.28276900	1.80513800	0.12048100

6_sol

O	1			
C		1.43936000	0.41260900	0.07708400
C		1.83130800	-0.77147100	-0.37587600
C		0.68794400	-1.73007100	-0.29974100
C		-0.48796400	-0.80925800	0.02873300
O		0.12293200	0.43401700	0.46486400
H		0.82956600	-2.48835500	0.47751200
C		2.16018100	1.68592700	0.25096600
H		1.69300300	2.47923500	-0.33767100
H		2.13734500	2.00370500	1.29604000
H		3.19832800	1.58252700	-0.06018400
H		2.82999400	-1.00289400	-0.71281600
O		-1.18149900	-0.56075700	-1.15441600
H		-1.81184700	0.16094500	-0.98842500
H		0.48344400	-2.25761000	-1.23375500
C		-1.39806800	-1.28130800	1.12949600
H		-2.18592200	-0.54865500	1.31541100
H		-1.86126100	-2.22475300	0.83819600
H		-0.83725100	-1.43553100	2.05161900
O		-2.15882900	1.95792100	-0.31335600
H		-2.80780200	2.20354700	0.34986000
H		-1.32500000	1.83982300	0.16349500

7_gas

1	1			
C		-1.67925000	-0.47680200	0.02490300
C		-0.52189500	-1.07975300	0.29561800
C		0.63520900	-0.44637500	1.02503300
C		1.71767700	-0.31822400	0.02210300
O		1.87361400	0.72173900	-0.66130400
H		0.36279900	0.52543100	1.43813300
C		-2.83782000	-1.14153100	-0.61479300
H		-3.11167100	-0.62814900	-1.54016900
H		-2.62280700	-2.18182900	-0.84647500
H		-3.70706100	-1.11590300	0.04922700
O		-1.86745600	0.83294800	0.35496900
H		-0.42277100	-2.11791700	0.00538000
H		-0.64235400	2.23876700	0.04178300
H		0.97038800	-1.09714500	1.83695400
H		1.23250600	1.50177000	-0.43779200

O	0.26918200	2.56005600	-0.04588400
H	0.26241100	3.45076900	-0.40380500
H	-2.80192500	1.05833400	0.29941100
C	2.62950800	-1.43549500	-0.23071100
H	3.17296300	-1.31711300	-1.16420800
H	3.34564500	-1.45815000	0.60016300
H	2.09857500	-2.38772800	-0.19375600

7_sol

1 1			
C	-1.66624800	-0.50646900	0.03086800
C	-0.49419300	-1.10091200	0.24882000
C	0.64936600	-0.48335200	1.00876100
C	1.74091500	-0.27492400	0.02835700
O	1.85802100	0.79211100	-0.61724000
H	0.35622000	0.45916600	1.47128000
C	-2.80786800	-1.14322400	-0.66560500
H	-3.09571300	-0.55640200	-1.54138800
H	-2.55858000	-2.15172500	-0.98678600
H	-3.67681700	-1.19522500	-0.00419900
O	-1.88295200	0.76156800	0.47792300
H	-0.36207900	-2.10773200	-0.12553800
H	-0.70768200	2.12788600	0.06958700
H	0.99994200	-1.16450300	1.78716100
H	1.15618000	1.53624800	-0.39237300
O	0.16149600	2.54685400	-0.06410400
H	0.04773000	3.24993100	-0.71005400
H	-2.80591900	1.01084600	0.36090600
C	2.69867100	-1.34693900	-0.23702900
H	3.29285600	-1.15488000	-1.12513700
H	3.35338400	-1.41587300	0.63868600
H	2.18409400	-2.30708000	-0.29980300

8_gas

1 1			
C	1.08726400	-0.95396200	0.08646800
C	0.28776000	-1.90006100	-0.35367800
C	-1.15110500	-1.51869400	-0.29683400
C	-1.17311500	-0.02534000	-0.02012400
O	0.31386800	0.17169600	0.52711200
H	-1.67899400	-2.06245300	0.49114200
C	2.53688500	-0.81136100	0.26941900
H	2.92863600	0.04047000	-0.29263400
H	2.78862600	-0.66353600	1.32194400
H	3.03806100	-1.71077000	-0.08283400
H	0.64148500	-2.86099400	-0.69457600
O	-1.23830100	0.66909800	-1.17404700
H	-1.56099300	1.56626900	-1.02934200
H	-1.67576900	-1.70644400	-1.23506900
O	1.11470800	2.53130700	-0.18747700
H	1.52991800	3.16666200	0.40246300
H	0.68753500	1.06429500	0.23822500
H	1.37482400	2.76603500	-1.08262200
C	-2.04786900	0.47809500	1.07942900
H	-1.89323100	1.54800600	1.24163500
H	-3.08936500	0.31405800	0.79838300
H	-1.85184700	-0.05046500	2.01050800

8_sol

1 1			
C	1.10225600	-0.91118500	0.09451900
C	0.32886900	-1.90552700	-0.28557700
C	-1.11811900	-1.55747700	-0.20120800

C	-1.15158100	-0.04884600	-0.02294300
O	0.30258100	0.19683400	0.50087600
H	-1.60263900	-2.05396800	0.64307900
C	2.55008200	-0.70977100	0.22831200
H	2.89413500	0.11762300	-0.39691700
H	2.81875500	-0.47952900	1.26138500
H	3.07137900	-1.61447800	-0.07717500
H	0.70587500	-2.86835100	-0.59263000
O	-1.23349000	0.55886300	-1.23124000
H	-1.50819200	1.47971900	-1.14229300
H	-1.67555100	-1.81780600	-1.10151300
O	1.00413300	2.51307300	-0.16545000
H	1.50752000	3.04394700	0.45942500
H	0.66007800	1.12934600	0.22379100
H	1.39500500	2.65632900	-1.03308700
C	-2.04717400	0.51513100	1.03033600
H	-1.89708700	1.59222600	1.12888900
H	-3.08190500	0.32976500	0.74142400
H	-1.85917000	0.04106300	1.99151000

9_gas

O 1			
C	1.82984100	-0.22826100	-0.02433400
C	1.22557500	-1.30775600	0.45405600
C	-0.19839300	-0.97165500	0.75721500
C	-0.33148200	0.41227200	0.12268200
O	1.00195800	0.86124400	-0.11705100
H	-0.40281100	-0.93208500	1.83232800
C	3.21966500	0.01311600	-0.44846600
H	3.25663400	0.31520300	-1.49762500
H	3.66500700	0.82189000	0.13563600
H	3.82042300	-0.88563100	-0.31895400
H	1.70020400	-2.26220500	0.61909800
O	-0.95610300	0.23450000	-1.13348900
H	-0.87815500	1.06027800	-1.62128800
H	-0.93126400	-1.65059100	0.31690200
O	-3.53700200	-0.62347900	-0.26137900
H	-2.74164800	-0.38855700	-0.76057600
H	-4.04975100	-1.19130600	-0.83619700
C	-1.04933900	1.44976300	0.93921500
H	-1.06256900	2.40522900	0.40941700
H	-2.07657200	1.12967300	1.11937300
H	-0.54553200	1.59510300	1.89503000

10_gas

1 1			
C	-2.37778500	-0.74803100	0.00002600
C	-1.06679100	-0.11818700	-0.00012100
C	-0.72802400	1.31121600	-0.00005900
C	0.75559800	1.27988600	0.00010900
C	1.15927700	0.02062400	0.00003100
O	-0.01510100	-0.82773600	-0.00014400
H	-2.94320400	-0.41151500	0.87428500
H	-2.94595200	-0.40714400	-0.87067000
H	-1.17909800	1.80857400	-0.86901200
H	-2.30281100	-1.83207800	-0.00252600
H	1.39909000	2.14451100	0.00020100
C	2.42485900	-0.71044600	0.00003500
H	2.50839000	-1.34783800	0.88214100
H	2.50847700	-1.34768400	-0.88217300
H	3.25252200	-0.00401300	0.00013700
H	-1.17941600	1.80870500	0.86864200

10_sol

1	1			
C		-2.37451700	-0.74618200	0.00001200
C		-1.06544900	-0.11858100	-0.00005800
C		-0.72880100	1.30713600	0.00012400
C		0.75264000	1.27790800	0.00017400
C		1.15312700	0.01901900	-0.00001600
O		-0.01220100	-0.83066300	-0.00017900
H		-2.93370900	-0.40310100	0.87414600
H		-2.93538900	-0.40040300	-0.87192800
H		-1.18116500	1.80090300	-0.86813300
H		-2.29858800	-1.82906700	-0.00158000
H		1.39555000	2.14170300	0.00030100
C		2.42414000	-0.70486500	-0.00012000
H		2.51031500	-1.34085200	0.88220800
H		2.51032500	-1.34057500	-0.88264600
H		3.24472000	0.00928700	-0.00000300
H		-1.18128700	1.80079700	0.86837100

11-cis_gas

0	1		
C	-1.46569000	-0.02515000	-0.02467100
C	-0.41427400	0.42144200	0.98469400
C	0.87712900	0.93022400	0.37789600
C	1.89151200	-0.13776500	0.05036300
O	1.62800200	-1.31623400	0.06184800
H	0.69980700	1.48616800	-0.55175300
H	-0.86550100	1.18903700	1.61746800
H	1.36840800	1.65067900	1.04102600
O	-0.92975300	-0.83268400	-1.03022200
H	-0.26931300	-1.42085700	-0.63660300
H	-0.20338700	-0.43347100	1.63297100
C	3.26803000	0.35643200	-0.27701100
H	3.22621900	1.20364500	-0.96438000
H	3.74449800	0.71655200	0.63876800
H	3.87046300	-0.44427100	-0.69943700
C	-2.14216700	1.13299900	-0.72538200
H	-2.85904900	0.74671400	-1.45315500
H	-2.67144400	1.75255700	-0.00123200
H	-1.42291500	1.74838500	-1.26840700
O	-2.40559400	-0.74371500	0.74269400
H	-3.04627800	-1.12316900	0.13484000

11-trans_gas

O	1			
C		-1.43527900	0.02248900	0.04040600
C		-0.45330700	-0.83153200	-0.76653100
C		0.91929100	-1.04862800	-0.15695500
C		1.84667600	0.12779200	-0.08493600
O		1.49005500	1.27051800	-0.26303600
H		0.81664800	-1.41533500	0.87147300
C		-2.86328400	-0.28018000	-0.35680800
H		-3.53718200	0.39446600	0.17505700
H		-3.00084500	-0.11908700	-1.42746400
H		-3.12024300	-1.31057600	-0.11003700
O		-1.22030600	-0.31419800	1.39987800
H		-0.90611000	-1.81741800	-0.90298200
H		1.44586600	-1.84845700	-0.69044200
H		-1.74093900	0.29957100	1.92514400
O		-1.26088300	1.38723700	-0.15610800
H		-0.30732900	1.57485100	-0.18372600
H		-0.37248900	-0.38244300	-1.76067100
C		3.27651300	-0.19752800	0.22513700
H		3.34616800	-0.94357200	1.01879100
H		3.73969000	-0.63708500	-0.66250900

H	3.82217000	0.70215900	0.49961500
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12-cis_gas

O	1		
C	1.13794500	-0.04977400	-0.09281700
C	0.74054600	-0.67624900	1.23478000
C	-0.70279900	-0.22006200	1.36448400
C	-1.15876900	0.02261000	-0.09229100
H	-1.34021800	-0.95181900	1.86116200
C	2.32741300	-0.65747000	-0.78030300
H	2.49496300	-0.15689800	-1.73381300
H	3.22107700	-0.54736100	-0.16125500
H	2.15986200	-1.71964300	-0.95977000
H	1.38535900	-0.36521500	2.05963300
H	-0.77998700	0.71474000	1.91995700
H	-0.87304900	1.91537000	-0.16242100
O	-1.62055300	1.32092100	-0.29739300
H	0.80950800	-1.76369800	1.14125100
O	1.31383100	1.36145700	0.06789700
H	2.09215000	1.52901400	0.60396400
C	-2.22996100	-0.91686500	-0.56819600
H	-3.15799600	-0.72741900	-0.02804200
H	-2.40278400	-0.76317300	-1.63322200
H	-1.92117700	-1.94997200	-0.40056200
O	0.00997700	-0.21076000	-0.88310800

12-trans_gas

O	1		
C	-1.16888900	0.04353700	-0.07186000
C	-0.70212900	-0.28716600	1.33404200
C	0.70207100	0.28507000	1.33444300
C	1.16888800	-0.04354600	-0.07194100
O	-0.00004300	0.00021800	-0.87322800
H	1.36779300	-0.15117600	2.07758300
C	-2.18747000	-0.89736500	-0.65839000
H	-2.42986000	-0.59938400	-1.68125600
H	-1.79275700	-1.91404300	-0.68075800
H	-3.10159000	-0.87741000	-0.06367000
H	-0.67634400	-1.37050500	1.46607400
H	0.67624500	1.36820500	1.46809200
H	-1.36782500	0.14799400	2.07784400
O	1.65677300	-1.36290700	-0.03973700
H	1.79030100	-1.65209100	-0.94650800
O	-1.65611300	1.36312000	-0.03782600
H	-1.78948800	1.65361900	-0.94419800
C	2.18693300	0.89870700	-0.65723000
H	3.10109000	0.87845200	-0.06257400
H	2.42943800	0.60228100	-1.68051900
H	1.79163200	1.91519300	-0.67816000

13-cis_gas

O	1		
C	1.40992000	-0.20645000	-0.05630500
C	0.56691000	-0.28577900	1.21018700
C	-0.70050800	-1.10861200	1.05127800
C	-1.75603900	-0.45547900	0.19069500
O	-2.13846000	0.67185400	0.41278000
H	-0.47734300	-2.11200800	0.68001300
H	1.18590800	-0.70486800	2.00727600
H	-1.16536200	-1.23644800	2.03514500
O	0.67924900	0.31650700	-1.12913600
H	0.40051000	1.22247200	-0.89680900
H	0.31689800	0.73563200	1.50950800

O	-0.39456500	2.73759900	-0.15528800
H	-1.17768100	2.26554500	0.16773700
H	-0.71528400	3.50958300	-0.62174100
C	-2.33017200	-1.28097500	-0.91283000
H	-3.15255500	-0.76386000	-1.40190100
H	-1.53357900	-1.47741900	-1.63656900
H	-2.66270800	-2.25010400	-0.53300000
C	1.93810100	-1.54936500	-0.51314100
H	2.59679800	-1.40198000	-1.37147000
H	2.50450900	-2.02516100	0.28825700
H	1.13350300	-2.21494500	-0.82901300
O	2.47552100	0.64742900	0.28310100
H	3.00314200	0.78640900	-0.50839100

13-cis_sol

O 1			
C	1.40852600	-0.24504500	-0.05867900
C	0.55207700	-0.31640900	1.19851600
C	-0.73512200	-1.10243800	1.02560700
C	-1.77988800	-0.41510400	0.18466100
O	-2.10058200	0.73881800	0.39202100
H	-0.54142200	-2.10524400	0.63937900
H	1.15145800	-0.76679800	1.99297900
H	-1.20105700	-1.23983900	2.00765000
O	0.70287700	0.31700700	-1.13336700
H	0.44457600	1.22370300	-0.88358800
H	0.32650500	0.70627600	1.51369600
O	-0.28784000	2.78187100	-0.13307700
H	-1.07271000	2.29723900	0.16793100
H	-0.61452200	3.49803500	-0.68198300
C	-2.42723000	-1.23621600	-0.87518300
H	-3.21887400	-0.68739200	-1.37986800
H	-1.65872900	-1.53350700	-1.59460100
H	-2.82060100	-2.15995200	-0.44427100
C	1.90411700	-1.59347100	-0.52689200
H	2.58987400	-1.45631000	-1.36566900
H	2.43051300	-2.10586100	0.27891000
H	1.08182100	-2.22250200	-0.86991100
O	2.49413700	0.58497400	0.29710500
H	3.09954600	0.62288700	-0.45029200

13-trans_gas

O 1			
C	1.35654600	-0.38886500	-0.07784300
C	0.52221700	-0.40412300	1.19556500
C	-0.82339900	-1.07279400	0.99143700
C	-1.80262100	-0.24959000	0.19435700
O	-1.98202900	0.92861600	0.41974400
H	-0.69081000	-2.05389200	0.53090300
C	2.65060800	0.37308800	0.12020000
H	3.24431000	0.33010100	-0.79554200
H	2.44723800	1.42021300	0.35395200
H	3.22895200	-0.06747200	0.93369600
O	1.60650900	-1.72613900	-0.40860900
H	1.08937500	-0.93271600	1.96582900
H	-1.30402200	-1.23777400	1.96295900
H	1.96886700	-1.73774200	-1.29889900
O	0.63121300	0.15274800	-1.15793200
H	0.53281400	1.11003900	-1.01742700
H	0.38660800	0.62450900	1.54044500
O	0.04456500	2.71020800	-0.10516900
H	-0.77780500	2.30389000	0.21844600
H	-0.20053400	3.55625300	-0.47988500
C	-2.58108400	-0.97677000	-0.85067100
H	-3.32947800	-0.33081400	-1.30388100
H	-1.87768400	-1.32896900	-1.60999000

H	-3.05351000	-1.86476600	-0.42315200
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13-trans_sol

O 1			
C	1.40569600	-0.40105900	-0.07939100
C	0.48797700	-0.56890900	1.12454300
C	-0.84090400	-1.19328300	0.76017100
C	-1.86241000	-0.24547700	0.19830700
O	-1.91473200	0.92597900	0.51855500
H	-0.70482200	-2.03004000	0.07108500
C	2.65124000	0.38088500	0.27983300
H	3.32082200	0.42579700	-0.58196100
H	2.39492100	1.40069000	0.57247200
H	3.17503000	-0.10056500	1.10702200
O	1.73734600	-1.69285700	-0.51197300
H	1.01016500	-1.18641800	1.85895900
H	-1.31900000	-1.61967200	1.65117400
H	2.27822100	-1.61026600	-1.30376300
O	0.73143400	0.21611000	-1.15563300
H	0.59828300	1.15728300	-0.94193800
H	0.32845500	0.40864900	1.58800600
O	0.08604000	2.74762000	-0.08960800
H	-0.71184000	2.31281400	0.25445500
H	-0.22184400	3.50089400	-0.59800200
C	-2.84924100	-0.84130300	-0.74677400
H	-3.66534300	-0.15345700	-0.95499900
H	-2.32423000	-1.07972600	-1.67654300
H	-3.23366100	-1.78593200	-0.35682600

14-cis_gas

O 1			
C	-1.25090900	0.31589300	0.04246200
C	-1.47542700	-1.05071200	-0.63633700
C	-0.25967800	-1.87809600	-0.24879300
C	0.77338900	-0.81082700	0.04396900
O	0.01172400	0.19301500	0.70218300
H	0.07807100	-2.56437000	-1.02493100
H	-1.53450800	-0.91015700	-1.71610100
H	-0.44094700	-2.44620300	0.66661700
H	-2.41603900	-1.49812100	-0.31419400
O	1.23828900	-0.33205800	-1.19407200
H	1.80760400	0.43487500	-1.01780000
C	1.90729200	-1.21342600	0.94522400
H	2.47596600	-2.01633200	0.47503700
H	2.57470700	-0.36658100	1.11504000
H	1.52801200	-1.55825800	1.90746800
O	2.01753000	2.07962600	0.09287200
H	1.17692700	1.79874900	0.48703600
H	1.89058200	2.98659500	-0.18731100
C	-2.27643400	0.67595200	1.07940000
H	-2.34612000	-0.11693700	1.82505500
H	-1.99071600	1.60475900	1.57401400
H	-3.25016700	0.81375900	0.60868300
O	-1.20585600	1.36844200	-0.87656500
H	-0.55626100	1.13331200	-1.54950100

14-trans_gas

O 1			
C	0.76639700	-0.82290700	-0.02029600
C	-0.33555500	-1.76892900	-0.45223800
C	-1.40071700	-0.80027600	-0.93081900
C	-1.28889100	0.32608100	0.08308800
O	0.05782100	0.29206800	0.54245800

H	-2.41043400	-1.20770800	-0.93805300
C	1.71506900	-1.34607600	1.02436300
H	2.44010000	-0.57583800	1.29552700
H	1.17108100	-1.64710600	1.92034300
H	2.25643200	-2.20491600	0.62613500
H	-0.68912000	-2.33673400	0.41115100
H	-1.15801900	-0.42870400	-1.92767800
H	0.01880000	-2.45904800	-1.21647500
O	-2.14128700	0.00651800	1.14965900
H	-1.94724200	0.59961400	1.88058600
O	1.43845200	-0.41708900	-1.17442900
H	2.01263400	0.33055800	-0.94794900
C	-1.57232100	1.70578000	-0.45469400
H	-2.59660500	1.76417300	-0.82478700
H	-1.44704600	2.45286900	0.33433200
H	-0.88255200	1.93725600	-1.26932800
O	2.20650700	2.03568200	0.10966800
H	2.11185800	2.91036600	-0.26803100
H	1.32427600	1.76575300	0.40895600

15-cis_gas

1 1			
C	-1.54561300	-0.32463600	-0.09367100
C	-0.45566800	-0.68894000	0.90172700
C	0.46575300	0.47875800	1.24033300
C	1.20389600	1.03252400	0.07719500
O	2.02121300	0.33937000	-0.58303200
H	-0.08323200	1.28894500	1.72282100
H	-0.91131300	-1.06315600	1.81904500
H	1.22530600	0.13462300	1.95326100
O	-0.85692200	0.38719400	-1.11264700
H	-1.43058400	0.53174000	-1.87078500
H	0.11195300	-1.51704200	0.47431100
O	2.47440100	-2.14864100	0.02799900
H	2.12605100	-0.63271400	-0.32798600
H	2.12862800	-2.86954600	-0.50638100
C	1.14383000	2.45925000	-0.24284700
H	1.62590000	2.68255800	-1.19080700
H	0.11089600	2.80550000	-0.22700600
H	1.66615500	2.99250600	0.56145200
H	3.36364200	-2.40422600	0.28904000
C	-2.64971100	0.52652700	0.48937200
H	-3.38027100	0.77709800	-0.28504400
H	-3.16426400	-0.00438800	1.29132600
H	-2.26035200	1.46598400	0.88443300
O	-2.03167500	-1.53136200	-0.58208700
H	-2.95958100	-1.46127100	-0.82219100

15-cis_sol

1 1			
C	-1.54105800	-0.35911500	-0.09422400
C	-0.41476200	-0.79189300	0.82512800
C	0.50506000	0.35756400	1.22588800
C	1.16515600	1.02171700	0.07484100
O	2.00047300	0.41420100	-0.64354000
H	-0.02929100	1.10893000	1.80768600
H	-0.83428400	-1.24012900	1.72596800
H	1.30382900	-0.03805000	1.86208100
O	-0.89664800	0.30851700	-1.16465600
H	-1.52581600	0.84602500	-1.65648300
H	0.15073700	-1.57224300	0.31203100
O	2.58733500	-1.99589000	0.01987300
H	2.19956900	-0.55444000	-0.39032300
H	2.54435800	-2.66376100	-0.67116600
C	0.99463000	2.45249400	-0.17254400
H	1.37406800	2.74148300	-1.14856800

H	-0.04322500	2.75039800	-0.03657400
H	1.57222700	2.96999600	0.60318000
H	3.44740700	-2.09699100	0.43861000
C	-2.56186700	0.54282500	0.55994600
H	-3.35013400	0.79419100	-0.15484100
H	-3.01903100	0.03906400	1.41166500
H	-2.11367200	1.47581700	0.90223400
O	-2.13710100	-1.54563600	-0.53521300
H	-2.99217100	-1.35137300	-0.93142200

15-trans_gas

1 1			
C	-1.53393400	-0.34067700	-0.06063500
C	-0.43285800	-0.81142900	0.86769600
C	0.50713400	0.33839100	1.24451500
C	1.09805100	1.03327000	0.07536300
O	1.99780500	0.49365600	-0.62619000
H	-0.03213300	1.06613000	1.85036600
C	-2.49936000	-1.44194900	-0.41926800
H	-3.25336900	-1.07070600	-1.11931800
H	-1.97733500	-2.26994400	-0.89780100
H	-3.00714400	-1.81236900	0.47210400
O	-2.17924100	0.73646300	0.55687200
H	-0.87069000	-1.20976900	1.78326300
H	1.33351700	-0.06460900	1.83901600
H	-3.11737700	0.74111900	0.35074900
O	-0.83065300	0.11466600	-1.20388200
H	-1.44402100	0.48803400	-1.84462100
H	0.11867800	-1.61890500	0.38185100
O	2.74971400	-1.94142700	-0.03413400
H	2.25200200	-0.44887100	-0.37983300
H	2.68539200	-2.61898900	-0.71323700
C	0.79658600	2.43671400	-0.20408800
H	1.12154700	2.72929500	-1.19925500
H	-0.26021500	2.64077200	-0.03892700
H	1.35162400	3.02910700	0.53533300
H	3.58479800	-2.09308500	0.41748700

15-trans_sol

1 1			
C	-1.54249800	-0.28673400	-0.05372600
C	-0.42550800	-0.79551700	0.83136900
C	0.53560200	0.32751300	1.22665900
C	1.17206700	0.99441600	0.06623400
O	2.01364000	0.39423900	-0.65414600
H	0.01447400	1.07593100	1.82183800
C	-2.48237400	-1.38543200	-0.48635400
H	-3.25522500	-0.98021300	-1.14500900
H	-1.93887100	-2.15691900	-1.03125800
H	-2.96544300	-1.83542800	0.38147000
O	-2.21949000	0.71178300	0.66031900
H	-0.84966700	-1.22492600	1.73905500
H	1.33964800	-0.09455200	1.83738400
H	-3.09778300	0.84227500	0.29092300
O	-0.87525700	0.27047600	-1.17119300
H	-1.50906000	0.69296200	-1.76001300
H	0.10795500	-1.59043700	0.30749900
O	2.55892100	-2.03886400	-0.01566100
H	2.21519600	-0.57034500	-0.39522700
H	2.54489600	-2.67752600	-0.73482200
C	0.97090100	2.41917100	-0.19343200
H	1.31232100	2.69935200	-1.18613700
H	-0.06776300	2.69679600	-0.02695200
H	1.56768100	2.95688200	0.55325200
H	3.38999000	-2.17542200	0.44894700

16-cis_gas

1	1			
C		-1.23313300	-0.39102700	-0.01897800
C		-0.72590800	-1.80839000	-0.08136400
C		0.70785500	-1.72001100	0.42657800
C		1.24733800	-0.35199000	0.01656600
O		-0.03038600	0.29178900	-0.61079600
H		1.33859900	-2.50858200	0.01889100
C		-2.41425000	-0.03378600	-0.86429400
H		-2.62702000	1.03705000	-0.80250700
H		-2.24295400	-0.29671600	-1.90674900
H		-3.28636200	-0.57952400	-0.50305100
H		-0.75666000	-2.14672000	-1.11888700
H		0.74221400	-1.80920700	1.51361100
H		-1.35217400	-2.46755800	0.51693500
O		-1.33882100	-0.00057600	1.29243100
H		-1.92102900	0.76071600	1.38818900
O		-0.02901100	2.82133400	-0.05143900
H		0.70999600	3.08306300	0.50645300
H		-0.23347600	3.57124900	-0.61681000
H		-0.02382100	1.29029900	-0.45590500
C		2.25744500	-0.32732200	-1.08263600
H		2.47147900	0.69924900	-1.38243600
H		3.18036200	-0.78000500	-0.72010100
H		1.89839900	-0.89050900	-1.94357600
O		1.64123200	0.45644200	1.03272500
H		1.12225600	0.28043300	1.82734900

16-cis_sol

1	1			
C		1.00463800	-0.75157500	0.00325800
C		0.03572400	-1.90335500	-0.06609100
C		-1.23047200	-1.28194300	-0.62931800
C		-1.33903500	0.10537500	-0.01062300
O		0.08146200	0.29486700	0.56508200
H		-2.12205400	-1.86280000	-0.39954200
C		2.15710700	-0.86881100	0.94981400
H		2.72642600	0.06279000	0.98110200
H		1.80869200	-1.10417100	1.95381700
H		2.81349300	-1.66713200	0.60406200
H		-0.12504500	-2.29274800	0.94085600
H		-1.16339300	-1.19315800	-1.71485900
H		0.43535400	-2.70230100	-0.68710400
O		1.35504300	-0.37649800	-1.26799100
H		2.09878600	0.23725600	-1.25167400
O		1.25740900	2.49526200	0.04980200
H		0.83228600	3.11409000	-0.55195500
H		1.60741800	3.01959400	0.77661300
H		0.44963300	1.23486500	0.40762000
C		-2.24634200	0.22116500	1.17252200
H		-2.14530300	1.20331300	1.63369000
H		-3.27516100	0.09034400	0.83805200
H		-2.01089400	-0.54871800	1.90650800
O		-1.57434900	1.12787800	-0.87428500
H		-1.17648600	0.95156900	-1.73542000

16-trans_gas

1	1			
C		1.00550500	-0.79066500	-0.04217500
C		-0.02139400	-1.86392500	-0.30060600
C		-1.21662900	-1.11011200	-0.85207900
C		-1.38548100	0.07754600	0.06888400
O		0.09285400	0.30300000	0.52692500
H		-2.13249900	-1.69803500	-0.85114800
C		2.04420000	-1.06272100	0.99949400

H	2.67668700	-0.18552900	1.15859800
H	1.58201700	-1.33701600	1.94611500
H	2.67329900	-1.88830100	0.66401800
H	-0.27409300	-2.36294300	0.63676400
H	-1.01991900	-0.76739300	-1.86872500
H	0.38293300	-2.59990600	-0.99314900
O	-2.05975200	-0.29998700	1.17534800
H	-2.34729300	0.45363500	1.70130700
O	1.49839500	-0.32033600	-1.22476100
H	2.36413300	0.08333500	-1.10395500
C	-1.84197800	1.36264300	-0.55081500
H	-2.85744700	1.22324100	-0.92318100
H	-1.85272500	2.17696100	0.17795000
H	-1.20552000	1.63913700	-1.39251200
O	1.34782500	2.58184700	0.08797200
H	1.37957100	3.08408800	-0.73045000
H	1.62058100	3.17983500	0.78910800
H	0.47036000	1.20609900	0.32916300

16-trans_sol

1 1			
C	1.00596200	-0.76166400	-0.04383800
C	0.00736900	-1.87842000	-0.21138600
C	-1.22919300	-1.18630000	-0.75459200
C	-1.36900100	0.07562700	0.07241400
O	0.08288700	0.31491300	0.50281100
H	-2.13364300	-1.78283600	-0.65817100
C	2.09021600	-0.94350200	0.97087300
H	2.67828700	-0.02856900	1.07205700
H	1.66985900	-1.20346200	1.94047800
H	2.74796800	-1.74720900	0.64013900
H	-0.19333500	-2.33085700	0.76118900
H	-1.09550300	-0.92557500	-1.80460800
H	0.40753700	-2.64017900	-0.87716300
O	-2.06082700	-0.20182200	1.21005700
H	-2.29092800	0.60746200	1.68016500
O	1.44728100	-0.35113300	-1.27064400
H	2.23273500	0.20157800	-1.18553900
C	-1.82767900	1.30505800	-0.65072600
H	-2.84126800	1.13215900	-1.01222000
H	-1.83991300	2.17262900	0.01204400
H	-1.18611500	1.51399000	-1.50719900
O	1.35667300	2.48794100	0.08058300
H	1.20316800	3.03997100	-0.69209700
H	1.50154400	3.08660100	0.81940600
H	0.46544400	1.24031100	0.33259400

17-cis_gas

0 1			
C	-1.61142300	-0.22768000	-0.04751100
C	-0.75815100	-1.05758800	0.92961500
C	0.44960800	-0.18326500	1.21024500
C	0.54744200	0.61629100	-0.07197500
O	-0.77781500	0.87552400	-0.42286600
H	1.36814300	-0.72521200	1.43546400
H	-0.46251900	-1.99157500	0.44848900
H	0.24998600	0.51557200	2.02690400
H	-1.32430400	-1.31783500	1.82408500
O	1.13797000	-0.24729600	-1.05243300
H	1.13200900	0.22528200	-1.89059700
C	1.30331100	1.91218000	0.00695500
H	2.34199500	1.72350700	0.28095400
H	1.27766900	2.42302700	-0.95849300
H	0.84810200	2.56809200	0.74892400
O	3.62243900	-0.86615100	0.21979100
H	4.13935100	-1.60737600	-0.09532300

H	2.86210500	-0.79811100	-0.37543200
C	-2.86804100	0.33756300	0.55390600
H	-3.34377600	1.00988800	-0.15997300
H	-3.56107100	-0.46746400	0.79925200
H	-2.62853100	0.89487100	1.46108000
O	-1.99199600	-0.95104200	-1.17687200
H	-1.20042500	-1.32595800	-1.57369300

17-trans_gas

O 1			
C	1.66422400	-0.15409800	-0.02033200
C	0.83103900	-1.13600200	-0.82631400
C	-0.40699900	-0.31742100	-1.14118800
C	-0.58005600	0.47201000	0.14014700
O	0.72366000	0.70701500	0.61489500
H	-1.29778200	-0.89882300	-1.37609800
C	2.54099500	-0.76549100	1.04031900
H	3.07331200	0.01645900	1.58714800
H	1.93373600	-1.32967500	1.74982100
H	3.27331000	-1.43155800	0.58239000
H	0.57739100	-2.00046600	-0.20964700
H	-0.21216300	0.37586500	-1.96197800
H	1.37968200	-1.47582700	-1.70321000
O	-1.24580900	-0.38739300	1.06255400
H	-1.18611300	0.02005800	1.93163400
O	2.41753400	0.59457800	-0.93694300
H	2.82163400	1.32793200	-0.46515500
C	-1.30924800	1.78133500	0.01903400
H	-2.32965200	1.61180700	-0.32749500
H	-1.34476800	2.28247300	0.98936200
H	-0.79050500	2.43337000	-0.68432600
O	-3.77324800	-0.67315800	-0.21172800
H	-4.32248600	-1.41916200	0.02788000
H	-2.99242000	-0.72278500	0.35945300

18_gas

1 1			
C	1.06740800	-0.01924800	0.04238800
C	0.52369400	1.29878100	-0.46071700
C	-0.94126100	1.28649800	-0.05385300
C	-1.27636800	-0.15311300	-0.04027900
O	-0.28004200	-0.90583900	-0.06220000
H	-1.61550400	1.85644200	-0.69414900
C	2.06342600	-0.75387500	-0.78483600
H	2.28298600	-1.73145300	-0.35221400
H	1.70458000	-0.89426600	-1.80322700
H	2.98506800	-0.17058000	-0.81845600
H	0.62227800	1.35084600	-1.54535700
H	-1.09974400	1.65853800	0.96719400
H	1.08662700	2.11946100	-0.02123900
O	1.31864200	0.05482200	1.35776300
H	1.83824000	-0.69378800	1.67408000
C	-2.62864300	-0.70174900	0.00259200
H	-3.13268200	-0.45136700	-0.93687700
H	-2.62984700	-1.77856200	0.14594600
H	-3.20033900	-0.20089500	0.78801700

18_sol

1 1			
C	1.05281300	-0.02343500	0.04062600
C	0.51782300	1.30976400	-0.43225800
C	-0.95201400	1.28771300	-0.05072600
C	-1.27493600	-0.14911700	-0.03061200

O	-0.26939500	-0.89584400	-0.03574300
H	-1.62004600	1.83973700	-0.71072000
C	2.03238200	-0.74082900	-0.82374900
H	2.26821200	-1.72088300	-0.40715800
H	1.64232700	-0.86618600	-1.83227200
H	2.94669500	-0.14879700	-0.87238500
H	0.63089300	1.38980700	-1.51253100
H	-1.13974600	1.66573700	0.96179600
H	1.07426500	2.11662000	0.03768300
O	1.35893500	0.03215400	1.35326100
H	1.84889800	-0.75042400	1.63281200
C	-2.61838600	-0.71020200	-0.00265400
H	-3.09570900	-0.47949800	-0.96010000
H	-2.61008900	-1.78338200	0.16014000
H	-3.20811500	-0.19657600	0.75881800

19_gas

O 1			
C	-1.22661800	-0.40470400	-0.08041700
C	-0.14853500	-1.42777300	-0.28355500
C	1.14371600	-0.88585400	-0.85807700
C	1.89622700	0.14005700	-0.03985000
H	1.84269900	-1.72042400	-0.99660000
C	-2.56620800	-0.92981100	0.34401900
H	-3.32264000	-0.71066500	-0.41447800
H	-2.54812000	-2.00756100	0.50482200
H	-2.90051900	-0.44738600	1.26579300
H	0.01940800	-1.93892000	0.67416200
H	0.97982700	-0.44512000	-1.84271700
O	2.56464900	0.98416100	-0.57742500
N	-0.95340000	0.81625700	-0.26478900
C	-1.98191400	1.80858000	-0.07235000
H	-1.58464900	2.79878900	-0.29037500
H	-2.84411500	1.63814200	-0.72762400
H	-2.35682600	1.81556600	0.95817600
H	-0.54280600	-2.21082800	-0.94240400
C	1.86280200	-0.00498600	1.45617700
H	2.58296700	0.67443800	1.90651700
H	0.86463400	0.22755100	1.83260000
H	2.08992600	-1.03372300	1.74936700

19_sol

O 1			
C	-1.21129400	-0.40767300	-0.09962400
C	-0.12793400	-1.41434200	-0.33894400
C	1.16550900	-0.85105400	-0.88906900
C	1.88483900	0.15581800	-0.03177000
H	1.87358300	-1.67831200	-1.02376800
C	-2.52341500	-0.95739500	0.36629300
H	-3.32476600	-0.67834000	-0.32240000
H	-2.50061000	-2.04296200	0.45005800
H	-2.78887100	-0.53994800	1.34099100
H	0.03965800	-1.95975400	0.59824600
H	1.01343500	-0.40100500	-1.87159800
O	2.50477200	1.06993600	-0.53161800
N	-0.96851500	0.82375000	-0.28210800
C	-2.02387500	1.78087200	-0.03375600
H	-1.65632100	2.79240200	-0.20282300
H	-2.88206700	1.62022600	-0.69572800
H	-2.39636600	1.72416200	0.99515700
H	-0.51596900	-2.17396900	-1.02644500
C	1.88213500	-0.07068900	1.44808300
H	2.58169900	0.60447200	1.93583000
H	0.87969000	0.10093900	1.84633100
H	2.14253900	-1.10687300	1.67657300

20_gas

O 1			
C	2.49363800	0.26593900	-0.01068100
C	1.12435700	-0.29778500	-0.00885400
C	0.70810600	-1.60034000	0.01528400
C	-0.70800300	-1.60038400	0.01528500
C	-1.12432600	-0.29785300	-0.00885600
H	2.67095200	0.93761700	0.83517900
H	3.21856800	-0.54498600	0.05521000
H	1.36274300	-2.45848000	0.02755700
H	2.71559200	0.82977800	-0.92276300
H	-1.36258800	-2.45856200	0.02755800
N	-0.00000900	0.49778400	-0.03285700
C	-0.00010500	1.93476300	0.02930500
H	0.88035200	2.33395900	-0.47293300
H	-0.88007400	2.33389300	-0.47385100
H	-0.00065700	2.29924600	1.06160100
C	-2.49362400	0.26582600	-0.01068200
H	-2.67094400	0.93753100	0.83515600
H	-2.71560500	0.82963300	-0.92277800
H	-3.21853500	-0.54511400	0.05524600

20_sol

O 1			
C	2.49364400	0.26793700	-0.00711400
C	1.12448600	-0.29786200	-0.00873300
C	0.70938500	-1.60360600	0.01247800
C	-0.70931800	-1.60363600	0.01248000
C	-1.12446800	-0.29790800	-0.00873200
H	2.66298900	0.94162600	0.83794000
H	3.22126600	-0.54056300	0.06034800
H	1.36645400	-2.46083600	0.02427400
H	2.71322900	0.83476600	-0.91710100
H	-1.36635200	-2.46089200	0.02427800
N	-0.00000800	0.49527000	-0.03045000
C	-0.00006700	1.93705500	0.02451200
H	0.88027700	2.33174700	-0.47963000
H	-0.88006900	2.33171400	-0.48026100
H	-0.00043900	2.30086600	1.05546700
C	-2.49363600	0.26786600	-0.00711500
H	-2.66295400	0.94162500	0.83788800
H	-2.71325400	0.83462300	-0.91714000
H	-3.22124800	-0.54063500	0.06043400

21-cis_gas

O 1			
C	-1.17728800	-0.45656000	-0.00697200
C	-0.05730400	-1.18121100	-0.77182400
C	1.35200100	-1.11908900	-0.21191100
C	2.04746200	0.21607700	-0.19445600
O	1.65237900	1.17430800	-0.81330800
H	1.40460900	-1.54690100	0.79538300
H	-0.35137700	-2.23301500	-0.80001200
H	2.00308600	-1.77049800	-0.81092100
H	-0.39743000	1.26265100	-0.78956300
H	-0.06917200	-0.82195100	-1.80589100
C	3.28688600	0.27893600	0.64818000
H	2.98991200	0.29589600	1.70118700
H	3.90585000	-0.60986100	0.51152800
H	3.85682600	1.17829100	0.42634800
N	-1.29888800	0.88800700	-0.52145500
C	-2.09109600	1.82498200	0.24136100
H	-2.24413200	2.73043800	-0.34671900
H	-3.07418400	1.39618600	0.44581800
H	-1.64733500	2.12220000	1.20234200

C	-0.98644200	-0.55787100	1.49678300
H	-0.85856300	-1.60134100	1.79339800
H	-0.11407800	0.01342800	1.82559200
H	-1.86492600	-0.17301300	2.01370600
O	-2.40276600	-1.13112200	-0.26027400
H	-2.68907900	-0.83563700	-1.13033100

21-trans_gas

O 1			
C	-1.10616800	-0.43559800	0.00992400
C	-0.06202300	-1.18929500	-0.82926200
C	1.35758300	-1.14966500	-0.29695700
C	1.99950200	0.20833900	-0.20289300
O	1.63542600	1.15292800	-0.86161100
H	1.41767600	-1.62949600	0.68291800
C	-2.40768700	-1.21457100	0.05400700
H	-3.16753500	-0.69442000	0.64198400
H	-2.79729300	-1.35135300	-0.95618600
H	-2.23949900	-2.19166300	0.50911700
O	-0.56480500	-0.37035800	1.34086600
H	-0.35699200	-2.23993700	-0.89206300
H	2.00864800	-1.74072400	-0.95497700
H	-1.23951000	-0.02561800	1.92996000
H	-0.43461000	1.27495700	-0.82840600
H	-0.10348000	-0.79336200	-1.84611000
C	3.13727800	0.31134100	0.76521200
H	2.71980800	0.27840700	1.77583200
H	3.81208400	-0.54268400	0.67512900
H	3.68053000	1.24352900	0.62789900
N	-1.32577600	0.86044500	-0.57977000
C	-2.15430200	1.79214000	0.14593600
H	-2.15613300	2.74719100	-0.37903800
H	-3.19155000	1.45169200	0.18572800
H	-1.82177600	1.99365600	1.17676500

22_gas

O 1			
C	1.10436700	-0.62544400	0.06952000
C	-0.05122800	-1.24961000	0.37279800
C	-1.20693900	-0.56862200	1.04929400
C	-1.85517500	0.35522900	0.05071000
O	-1.51128900	1.51250800	-0.04904500
H	-1.92350300	-1.31330600	1.40301700
C	2.24553000	-1.38238800	-0.52135100
H	3.12015200	-1.35011100	0.13368000
H	1.97273100	-2.42569400	-0.66794600
H	2.55188500	-0.96763700	-1.48507700
H	-0.14086400	-2.30279900	0.14021500
H	0.47837000	1.26310400	0.45114300
H	-0.87351300	0.02805100	1.90604200
C	-2.89139800	-0.24802400	-0.84757100
H	-2.54449700	-1.20718600	-1.23708400
H	-3.79385600	-0.44992900	-0.26344300
H	-3.13593700	0.42683600	-1.66480800
N	1.31553900	0.70671200	0.33009100
C	2.46208900	1.43611700	-0.14758700
H	3.39500900	0.98432200	0.19427300
H	2.50624800	1.51769300	-1.24112700
H	2.42584000	2.44605700	0.25795700

23_gas

O 1			
C	-1.27249500	-0.34622600	-0.10357700

C	-0.81689500	-1.59828200	0.01524500
C	0.66221400	-1.58830400	-0.20997200
C	1.01856800	-0.11390000	0.00598600
H	1.25297500	-2.21526400	0.46225300
C	-2.67801700	0.11844400	-0.06472900
H	-2.94715200	0.62756400	-0.99458900
H	-3.34968300	-0.72846300	0.06919100
H	-2.85380200	0.82585500	0.75005100
H	-1.43758000	-2.47576500	0.11516700
H	0.90987300	-1.88714300	-1.23687400
N	-0.23637600	0.56193000	-0.34941100
C	-0.38098500	1.95055500	0.01214200
H	0.49470500	2.50704900	-0.32190700
H	-1.24963100	2.37926200	-0.48862800
H	-0.48566800	2.11143000	1.09348200
C	2.19678800	0.36734900	-0.79634800
H	3.06927700	-0.24525200	-0.56447000
H	1.98299600	0.29682200	-1.86253700
H	2.44251700	1.40073200	-0.54736600
O	1.34711300	0.12763200	1.36361000
H	0.67383600	-0.28921400	1.91074100

24_gas

O 1			
C	1.16617300	-0.93009000	0.15095900
C	-0.01675000	-1.35592400	0.64395300
C	-1.12630100	-0.44938200	1.09274900
C	-1.97314200	-0.08548300	-0.09897700
H	-1.74853700	-0.96523600	1.83094800
C	2.20236700	-1.91708200	-0.27358500
H	3.13144300	-1.78478000	0.28660400
H	1.84943700	-2.93416300	-0.11568100
H	2.44897000	-1.79849700	-1.33193400
H	-0.18553400	-2.42391000	0.70025800
H	-0.75100800	0.47027900	1.55236900
O	-1.91470200	1.00119800	-0.63611200
N	1.49665500	0.38289700	0.00062800
C	2.79026200	0.87396400	-0.38945400
H	3.57247500	0.67168300	0.35237800
H	3.11953900	0.45890300	-1.34589300
H	2.71382500	1.95379600	-0.50814800
H	0.84672800	1.09821400	0.29603100
O	-0.05526700	2.87218600	0.22323500
H	-0.81872600	2.37329600	-0.12148100
H	-0.41308500	3.56381000	0.77878700
C	-2.89110100	-1.15154100	-0.61222600
H	-3.27846900	-0.88675200	-1.59340300
H	-2.38586900	-2.11724600	-0.64901300
H	-3.72707300	-1.25352200	0.08629000

24_sol

O 1			
C	1.17122200	-0.92263700	0.12614100
C	-0.00425300	-1.33876200	0.64428600
C	-1.11593600	-0.43138100	1.09134100
C	-1.96717300	-0.10566700	-0.10439100
H	-1.72767200	-0.93888200	1.84200100
C	2.21078400	-1.91520400	-0.27710400
H	3.13336700	-1.77917600	0.29259100
H	1.85483400	-2.93022600	-0.11241200
H	2.47089700	-1.80597900	-1.33314000
H	-0.17528000	-2.40605900	0.71198100
H	-0.74306700	0.49899800	1.53007200
O	-1.87939700	0.95731600	-0.69368700
N	1.48620200	0.39153900	-0.08571900
C	2.82553000	0.87426900	-0.31826800

H	3.50490500	0.69095700	0.52243800
H	3.26796000	0.42990900	-1.21215300
H	2.77276400	1.95053300	-0.47714900
H	0.84221800	1.09995900	0.24033000
O	-0.12431500	2.92611500	0.19552100
H	-0.84830600	2.34577000	-0.10551400
H	-0.45651300	3.36870600	0.97882600
C	-2.91499400	-1.16673400	-0.55589300
H	-3.27016900	-0.97491800	-1.56596800
H	-2.46103600	-2.15579000	-0.49039100
H	-3.76969000	-1.16534000	0.12718900

25_gas

O 1			
C	0.95774700	-0.85854100	-0.24082200
C	0.56016900	-0.79485400	-1.51462600
C	-0.89846100	-0.46862900	-1.54711300
C	-1.18468900	-0.01503400	-0.10734800
H	-1.50637200	-1.34784400	-1.79515000
C	2.29495200	-1.21191900	0.28515700
H	2.73710600	-0.37613100	0.83443300
H	2.23842400	-2.06257600	0.96978600
H	2.96234200	-1.47530800	-0.53458900
H	1.16467000	-1.06057000	-2.36845800
O	-1.06249300	1.41376700	0.00095400
H	-1.78940300	1.82947800	-0.46908500
H	-1.17880400	0.32127900	-2.25096700
O	1.70712200	2.26063700	-0.26626900
H	1.91049900	1.58488200	-0.91809800
H	0.75517000	2.15014600	-0.13688200
N	-0.08717100	-0.58035700	0.64601000
C	0.16971100	-0.10558000	1.98608900
H	0.76884900	-0.83549400	2.53160700
H	0.68814700	0.85975100	2.00805500
H	-0.77505500	0.00353600	2.51809200
C	-2.54180500	-0.43197200	0.40810300
H	-3.32868400	-0.02365400	-0.23249900
H	-2.63182400	-1.51815600	0.40631800
H	-2.70764600	-0.06289000	1.42124600

25_sol

O 1			
C	-1.01881200	-0.60679300	0.57260200
C	-0.69735900	0.17134500	1.61124000
C	0.76844200	0.46494200	1.55926100
C	1.16189400	0.02346800	0.14126700
H	1.32575800	-0.11716800	2.30306000
C	-2.33308700	-1.20619400	0.24895400
H	-2.71597700	-0.84308400	-0.70905300
H	-2.26288700	-2.29452600	0.17353000
H	-3.05879500	-0.95933800	1.02276300
H	-1.36424800	0.43246900	2.41946000
O	1.09928800	1.14259400	-0.76386800
H	1.82679400	1.74105000	-0.56876500
H	1.03680400	1.51421800	1.71226800
O	-1.52059500	2.25076600	-0.87159600
H	-1.81746600	1.81735800	-0.06397800
H	-0.60033800	1.94601000	-0.94047600
N	0.08888900	-0.87449900	-0.23856100
C	-0.07038200	-1.23441500	-1.62857400
H	-0.69290700	-2.12487800	-1.71542000
H	-0.52106700	-0.43566600	-2.23031200
H	0.90258600	-1.47243400	-2.05716900
C	2.53070000	-0.60488200	0.04830100
H	3.29013400	0.10152300	0.39250000
H	2.58296200	-1.49397200	0.67671300

H	2.76850500	-0.88178200	-0.97979500
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26_gas

O	1		
C		1.67127600	-0.61823900
C		0.90814000	-1.69109700
C		-0.44853200	-1.25145200
C		-0.44949200	0.24260700
H		-0.58918900	-1.39398200
C		3.10097200	-0.56908600
H		3.25225300	-0.06799200
H		3.69123400	-0.02719200
H		3.49906600	-1.57966100
H		1.24794500	-2.71385300
O		-1.04560200	0.36292900
H		-1.13510500	1.29484800
H		-1.28748200	-1.74218800
O		-3.73332300	-0.48256200
H		-2.84321800	-0.27504500
H		-4.14456100	-1.00755300
N		0.97053800	0.57209600
C		1.36036600	1.80266800
H		2.40606000	2.02386400
H		1.23519200	1.79025000
H		0.77422600	2.63010100
C		-1.21499800	1.09789900
H		-2.25410600	0.76665900
H		-0.77226200	1.02321400
H		-1.20881900	2.15112400

26_sol

O	1		
C		1.64659600	-0.64702100
C		0.86127500	-1.68730800
C		-0.45987900	-1.17954000
C		-0.43363400	0.29181100
H		-0.55170500	-1.25495600
C		3.05959400	-0.65805400
H		3.18067500	-0.20233600
H		3.69420000	-0.09701600
H		3.42822900	-1.68173900
H		1.17145600	-2.72138200
O		-1.07783000	0.35010200
H		-1.12119200	1.26593000
H		-1.33455200	-1.67445400
O		-3.77308100	-0.53074800
H		-2.85580300	-0.25806700
H		-3.90823500	-1.31045500
N		0.99083300	0.57320800
C		1.39996800	1.76898600
H		2.45507200	1.96926000
H		1.25157900	1.71209200
H		0.84126500	2.62612600
C		-1.14072000	1.22528400
H		-2.18304000	0.91791800
H		-0.66676600	1.20092500
H		-1.12891600	2.25591400

27_gas

1	1		
C		-1.31170100	-0.84565200
C		-0.07897200	-1.12808800
C		0.85231900	-0.24359500

C	2.01197800	-0.01905100	0.13086000
O	1.99619900	0.86862300	-0.75414000
H	0.40561300	0.71675500	1.28471000
C	-2.03538100	-1.79357000	-1.10296100
H	-2.34054700	-1.28644700	-2.02285800
H	-1.41959300	-2.64615800	-1.37869100
H	-2.94456300	-2.16070800	-0.62001800
H	0.32465700	-2.09773900	-0.03251000
H	-0.96881400	1.63977900	-0.76409500
H	1.19055400	-0.73146700	1.94715700
H	1.12266400	1.42648200	-0.81673200
O	-0.15087900	2.16891300	-0.88180100
H	-0.31406400	2.87599300	-1.50956900
H	-2.95843100	0.26661200	-0.32637200
C	3.19803500	-0.87069200	0.22282100
H	3.88674000	-0.71165100	-0.60189600
H	3.69610100	-0.64994400	1.17401300
H	2.89464900	-1.91874300	0.28946500
C	-2.09072500	0.85726700	1.44279500
H	-1.36255400	1.65459700	1.60204800
H	-3.07563800	1.28835400	1.60891400
H	-1.92867000	0.07375500	2.18582200
N	-2.03485400	0.31721800	0.08013800

27_sol

1 1			
C	-1.30989600	-0.84119700	-0.21200200
C	-0.08374800	-1.14602100	0.23425700
C	0.85196500	-0.27284200	1.03027200
C	2.00553800	-0.01995900	0.13107000
O	1.97397900	0.88499400	-0.73389600
H	0.40690500	0.68050400	1.31069100
C	-2.04001100	-1.75866300	-1.13223300
H	-2.31400900	-1.22749500	-2.04802800
H	-1.43551500	-2.62005500	-1.40707800
H	-2.96860400	-2.10687000	-0.67305800
H	0.31798900	-2.11055200	-0.05583500
H	-0.94578900	1.62943000	-0.72488600
H	1.20169700	-0.77488400	1.93492600
H	1.08117100	1.44324500	-0.78371300
O	-0.14811600	2.18799800	-0.86701400
H	-0.27734700	2.68122400	-1.68182600
H	-2.92990600	0.31710100	-0.33329600
C	3.19505100	-0.86565600	0.20455200
H	3.88287300	-0.68246600	-0.61503800
H	3.68562000	-0.66525900	1.16294700
H	2.89275900	-1.91478200	0.24270100
C	-2.07966600	0.83193300	1.46705100
H	-1.35099100	1.62272300	1.65483300
H	-3.06624200	1.25746400	1.63623600
H	-1.91822900	0.02994200	2.19038500
N	-2.01495600	0.32731800	0.09421600

28_gas

1 1			
C	1.52124700	0.30005200	-0.18934200
C	1.77336600	-0.95407500	-0.51298800
C	0.62082300	-1.86217700	-0.26460000
C	-0.55936400	-0.91569600	-0.10700900
H	0.76949400	-2.47579100	0.62958300
C	2.32597200	1.53236300	-0.29476300
H	1.81571600	2.28935300	-0.89701400
H	2.54390700	1.97833100	0.67870000
H	3.27707900	1.30892400	-0.77476900
H	2.71939000	-1.27995600	-0.92188000
O	-1.03374300	-0.61729200	-1.35978900
H	-1.84031800	-0.08801600	-1.29192600

H	0.41966300	-2.54036700	-1.09506600
O	-2.17732200	1.91425500	-0.56127500
H	-2.88591000	2.24832600	-0.00410200
H	-0.37829100	1.17370700	-0.03403600
H	-2.19652300	2.46734500	-1.34809000
C	-1.64265000	-1.36068600	0.83385700
H	-2.43055500	-0.60925500	0.92516300
H	-2.08768000	-2.26096900	0.40829600
H	-1.27073800	-1.61231000	1.82596000
C	0.20386700	0.62099900	1.85477100
H	-0.80514100	0.75032200	2.23941700
H	0.68429200	-0.23674100	2.32228700
H	0.78386600	1.51718400	2.06325300
N	0.15867200	0.40421800	0.38902500

28_sol

1 1			
C	1.52012600	0.25114300	-0.19097200
C	1.72763900	-1.01078300	-0.51714500
C	0.54056500	-1.87269600	-0.26480300
C	-0.59630400	-0.87521900	-0.10912200
H	0.66360000	-2.48534200	0.63301900
C	2.37149400	1.45089100	-0.28969200
H	1.89517500	2.22141200	-0.90109300
H	2.58163300	1.89244800	0.68685800
H	3.32146200	1.18615400	-0.75042300
H	2.66136400	-1.37112200	-0.92436800
O	-1.05707600	-0.55928800	-1.37029000
H	-1.75437600	0.11285800	-1.29997700
H	0.31045000	-2.54795400	-1.08970200
O	-2.07110600	1.93488900	-0.57199700
H	-2.75124600	2.20518500	0.05127400
H	-0.34338200	1.20412200	-0.00448800
H	-2.04453200	2.62489000	-1.24087100
C	-1.70409200	-1.28451400	0.81952400
H	-2.46307200	-0.50553000	0.91137800
H	-2.17516700	-2.16509700	0.38186200
H	-1.34501500	-1.55610500	1.81062700
C	0.23132800	0.58587500	1.86488700
H	-0.76768500	0.76036200	2.25525900
H	0.67152000	-0.30264000	2.31249600
H	0.85458600	1.44976500	2.07895000
N	0.16651500	0.40051600	0.39306200

29_gas

1 1			
C	2.47887800	0.36397100	0.00005200
C	1.11218400	-0.17893000	-0.00007700
C	0.75163300	-1.60831800	-0.00001900
C	-0.72802200	-1.59323300	0.00001700
C	-1.15044900	-0.33142400	-0.00005300
H	2.65484000	0.98698700	0.88057100
H	3.20847700	-0.44285000	-0.00113200
H	1.19671800	-2.10902100	-0.86969500
H	2.65438500	0.98938300	-0.87880900
H	-1.35958900	-2.46712400	0.00008000
C	-2.50281700	0.25524400	0.00006400
H	-2.68055400	0.87367900	0.88266200
H	-2.68058800	0.87413600	-0.88219800
H	-3.24095100	-0.54429700	-0.00011400
H	1.19679300	-2.10900700	0.86962600
N	0.01659200	0.52206400	-0.00013600
C	-0.08238300	1.97262000	-0.00001500
H	0.90916200	2.41474500	0.00013300
H	-0.62444000	2.29980300	-0.88633400
H	-0.62454300	2.29953400	0.88633900

29_sol

1	1			
C	2.47285900	0.36566900	0.00005700	
C	1.10977100	-0.17924900	-0.00001900	
C	0.75252200	-1.60732600	-0.00016100	
C	-0.72644500	-1.59330000	-0.00016400	
C	-1.14652800	-0.33118900	-0.00004200	
H	2.64013400	0.98984300	0.88023800	
H	3.20087900	-0.44151500	-0.00006300	
H	1.19908300	-2.10351100	-0.87002600	
H	2.64013200	0.99010300	-0.87993800	
H	-1.35858200	-2.46610000	-0.00025200	
C	-2.49874100	0.25471500	0.00000100	
H	-2.67112200	0.87529700	0.88167000	
H	-2.67104800	0.87557400	-0.88148800	
H	-3.23499700	-0.54645100	-0.00015400	
H	1.19908000	-2.10367900	0.86960900	
N	0.01545800	0.52177600	0.00004300	
C	-0.08276400	1.97036500	0.00021700	
H	0.90946000	2.40897900	-0.00006500	
H	-0.62291500	2.29554200	-0.88702300	
H	-0.62235000	2.29537800	0.88786500	

30-cis_gas

0	1			
C	1.15962200	-0.15106400	-0.06577900	
C	0.75772500	-1.55292900	-0.48706800	
C	-0.72939500	-1.60838500	-0.15646600	
C	-1.18227300	-0.14053900	-0.00645400	
H	-1.30373400	-2.12001200	-0.92990000	
C	2.43350200	0.34578900	-0.70280000	
H	2.72031600	1.31756100	-0.29912400	
H	3.24786000	-0.35700100	-0.50563400	
H	2.31064000	0.43034200	-1.78347100	
H	1.35296600	-2.31257800	0.02515500	
H	-0.92186500	-2.12622900	0.78370400	
H	-0.77896000	0.02188000	1.87928600	
O	-1.55965100	0.15317400	1.32762300	
N	0.00182700	0.60736100	-0.42249600	
C	0.02142300	2.02605200	-0.14811500	
H	-0.94517000	2.45875600	-0.40307300	
H	0.22897000	2.26198200	0.90178700	
H	0.77213600	2.51739800	-0.76978300	
H	0.93114300	-1.65962900	-1.56076800	
O	1.29985500	-0.10285200	1.37794900	
H	2.10372200	-0.55821500	1.63815600	
C	-2.38828400	0.19138500	-0.84976500	
H	-3.23050700	-0.42878700	-0.53913500	
H	-2.68137700	1.23426500	-0.72294100	
H	-2.17447500	0.00431500	-1.90268600	

30-trans_gas

0	1			
C	1.18410000	-0.14647600	0.00980300	
C	0.74801300	-1.56989600	-0.30607800	
C	-0.68757300	-1.58133200	0.18010500	
C	-1.20147700	-0.15376600	-0.07266200	
H	-1.32924000	-2.30517200	-0.32146800	
C	2.42294900	0.28721000	-0.74058700	
H	2.73353500	1.29026800	-0.44459000	
H	3.24811800	-0.39704700	-0.52346700	
H	2.24479600	0.27350100	-1.81680300	

H	1.38783100	-2.30591400	0.18511500
H	-0.71302800	-1.79154900	1.25100500
N	0.01661000	0.60080000	-0.34153800
C	0.00730200	2.02557800	-0.12811400
H	-0.90561800	2.44561600	-0.55245400
H	0.06679800	2.30714200	0.93057100
H	0.84645500	2.48942200	-0.64934000
H	0.81319500	-1.73149900	-1.38673700
O	1.40670900	-0.00028100	1.42228100
H	2.25869500	-0.37807600	1.65184700
C	-2.03183500	0.35007700	1.08714600
H	-2.45272600	1.33271300	0.87247300
H	-2.86117800	-0.33826300	1.25912800
H	-1.42514900	0.40590600	1.99229600
O	-2.05453900	-0.07691200	-1.20388100
H	-1.49497800	-0.15348200	-1.98168700

31-cis_gas

0 1			
C	-1.31537000	-0.25745100	-0.32852700
C	-0.28492200	-0.62069600	-1.39030800
C	0.87791200	-1.44650400	-0.86986400
C	1.84991600	-0.65399600	-0.02697300
O	2.35686400	0.35927900	-0.45347700
H	0.52686100	-2.32670500	-0.32529900
H	-0.80181200	-1.15505700	-2.19097400
H	1.46065500	-1.81453000	-1.72143200
H	-0.24565300	1.34056800	0.28875700
H	0.09296600	0.30964500	-1.82545500
O	1.04793800	2.83621700	-0.31950800
H	1.70586400	2.14064300	-0.46634800
H	0.93512000	3.26950800	-1.16574900
C	2.21271100	-1.22347700	1.30577200
H	2.61004200	-2.23465200	1.17971500
H	2.94497000	-0.59686800	1.80995500
H	1.30761300	-1.30696500	1.91259400
N	-0.65575600	0.50403400	0.70148200
C	-1.42970800	0.85806900	1.86961500
H	-2.40847800	1.31427400	1.64941300
H	-1.60474000	-0.01142900	2.50808400
H	-0.86689500	1.58357900	2.45627100
C	-1.99347700	-1.48500100	0.25378500
H	-2.86658500	-1.20184200	0.84599800
H	-2.33619800	-2.13207100	-0.55486800
H	-1.32386300	-2.05056100	0.90468600
O	-2.28398200	0.50270300	-1.05545700
H	-3.00849700	0.73296900	-0.46918000

31-cis_sol

0 1			
C	-1.28517800	-0.21129900	-0.37066300
C	-0.21690100	-0.24190200	-1.45728900
C	0.97455700	-1.12242100	-1.13126400
C	1.88240500	-0.56676200	-0.06445000
O	2.33189500	0.56091300	-0.14203500
H	0.65844300	-2.13445400	-0.86956700
H	-0.68642100	-0.58380700	-2.38234000
H	1.60128100	-1.21735300	-2.02489800
H	-0.33353800	1.21909300	0.67065200
H	0.11888600	0.78448300	-1.63585800
O	0.88443200	2.95231700	-0.01097000
H	1.47318900	2.21339700	-0.23435300
H	0.65145000	3.35701100	-0.84892400
C	2.27106900	-1.49517100	1.03372600
H	2.72511400	-2.39428500	0.60861300
H	2.96111700	-1.02250700	1.72909600

H	1.36823200	-1.81868900	1.55820800
N	-0.68805900	0.28251400	0.84596400
C	-1.50488500	0.27031500	2.04261300
H	-2.49208900	0.74095900	1.92393900
H	-1.66047500	-0.75073000	2.39617800
H	-0.98269200	0.80969600	2.83238500
C	-1.91740200	-1.57219200	-0.15113100
H	-2.81620600	-1.48749700	0.46320900
H	-2.20402900	-2.00479600	-1.11047200
H	-1.23521200	-2.25562500	0.35678000
O	-2.27671100	0.68372400	-0.89781700
H	-3.06956300	0.62845300	-0.35708100

31-trans_gas

O 1			
C	-1.25478600	-0.20279300	-0.38058000
C	-0.23856100	0.05219600	-1.48343700
C	1.00855100	-0.80153900	-1.33161900
C	1.87262200	-0.40724500	-0.15916200
O	2.30280800	0.72172900	-0.04023000
H	0.73142000	-1.85519800	-1.26449000
H	-0.72028700	-0.16588200	-2.44026000
H	1.63651000	-0.68056500	-2.22087100
H	-0.37296400	1.04965700	0.95859500
H	0.02524900	1.11292000	-1.48723000
O	0.51232200	2.82568200	0.22388900
H	1.29411900	2.27022700	0.06133700
H	0.84015300	3.64654200	0.59062200
C	2.26589500	-1.50387900	0.77685200
H	2.84488700	-2.25530000	0.23138700
H	2.85694700	-1.11653800	1.60400700
H	1.36522200	-1.99942800	1.14594600
N	-0.60663100	0.06128000	0.90083600
C	-1.30129400	-0.38509100	2.08431300
H	-2.33713100	-0.02260200	2.18222000
H	-1.32249300	-1.47707400	2.12194600
H	-0.75593400	-0.04520100	2.96503600
C	-2.49070600	0.65387600	-0.60294100
H	-2.94444800	0.43109500	-1.57075300
H	-3.23968100	0.47701400	0.17408900
H	-2.21809500	1.71104500	-0.57631600
O	-1.58883600	-1.57455900	-0.45886600
H	-2.41773100	-1.72563700	-0.00002100

31-trans_sol

O 1			
C	-1.26672600	-0.30510600	-0.35596900
C	-0.19838600	-0.17012700	-1.43887000
C	1.04001300	-0.98606800	-1.12574900
C	1.96933000	-0.36341200	-0.11678000
O	2.25641300	0.81459300	-0.14426300
H	0.75384600	-1.98971900	-0.80302300
H	-0.63904100	-0.51367800	-2.37886000
H	1.64423900	-1.10637800	-2.03373200
H	-0.33997300	1.02357200	0.84919700
H	0.05800700	0.88451000	-1.57278900
O	0.40067100	2.86728100	-0.02985100
H	1.19599600	2.32628300	-0.16802200
H	0.70614400	3.69991400	0.32967400
C	2.58944600	-1.29644600	0.87125300
H	3.03415400	-2.15187900	0.35632900
H	3.33899500	-0.78697700	1.47269400
H	1.79632400	-1.68978500	1.51177900
N	-0.66723100	0.06303600	0.91557200
C	-1.49853500	-0.10882700	2.08805500
H	-2.40389400	0.51566200	2.10447600

H	-1.80575900	-1.15138300	2.16779500
H	-0.91635000	0.13703000	2.97688300
C	-2.47932300	0.53464300	-0.72213700
H	-2.86642600	0.25185900	-1.70533000
H	-3.27872900	0.41202100	0.01221100
H	-2.20202700	1.59006700	-0.75648000
O	-1.63271900	-1.67373400	-0.25298000
H	-2.53471800	-1.78542500	-0.55387300

32-cis_gas

0 1			
C	-1.31116900	-0.01345000	-0.15448100
C	-0.88591600	-0.28577400	-1.59502000
C	0.62585500	-0.17040200	-1.55499100
C	1.01211900	-0.67130800	-0.16383000
H	1.13175800	-0.73424700	-2.33990500
C	-2.65760600	-0.61731100	0.17284900
H	-2.95886800	-0.36568100	1.19071600
H	-3.41100600	-0.20717600	-0.50175500
H	-2.62882500	-1.70187000	0.06299200
H	-1.36499200	0.41392600	-2.28005800
H	0.93819700	0.87128000	-1.65133100
H	2.42362200	-0.15253800	1.12050900
O	1.99248900	0.24627100	0.36070500
N	-0.23193300	-0.66093700	0.57502300
C	-0.18125300	-0.51997600	2.00266300
H	0.55830100	-1.20614800	2.42578300
H	0.06354000	0.49859100	2.33507400
H	-1.14472600	-0.78636800	2.43940000
H	-1.19051000	-1.30023500	-1.87042400
O	-1.44856000	1.36123900	0.12472200
H	-0.62339900	1.84875500	-0.03624800
C	1.62382800	-2.05714900	-0.17339300
H	2.58465300	-2.05215100	-0.69191000
H	1.77483600	-2.42856000	0.84456900
H	0.94949900	-2.74936000	-0.68010800
O	1.02006500	2.79197200	-0.04430700
H	1.54857500	2.02897100	0.24557800
H	1.10578000	3.46574900	0.63021200

32-trans_gas

0 1			
C	1.27852900	-0.52040600	-0.17710500
C	0.94013200	-0.18779600	-1.61933200
C	-0.47610000	0.34568900	-1.54473300
C	-0.57077600	1.02125200	-0.17529100
H	-0.72755600	1.03545000	-2.35144800
H	1.05010700	-1.05048000	-2.27758300
H	-1.19912200	-0.47261400	-1.57368600
H	-1.99456400	1.09757700	1.19805300
O	-1.79847300	0.56216800	0.42522000
N	0.60420000	0.56670300	0.52098800
C	0.62405200	0.59044200	1.95270500
H	0.34413700	1.58083500	2.32277800
H	-0.04317300	-0.14767600	2.42314300
H	1.64128200	0.40542000	2.30426800
H	1.64247000	0.58385700	-1.94466500
C	-0.61593900	2.53380500	-0.24911400
H	-1.52615400	2.86698600	-0.75135400
H	-0.58558300	2.98194900	0.74849800
H	0.25170100	2.89769200	-0.80178800
O	-2.64252400	-2.12622000	0.16205900
H	-2.46569200	-1.18110500	0.28880400
H	-3.52175500	-2.17969700	-0.21174300
C	0.81442400	-1.90382000	0.24297400
H	1.34695900	-2.66635600	-0.32972600

H	1.01414500	-2.07231600	1.30564700
H	-0.25737400	-2.03953700	0.08458000
O	2.67507700	-0.41566800	-0.00270200
H	2.96219000	-1.04413600	0.66207200

33-cis_gas

O 1			
C	-1.52578800	-0.42129400	-0.02646400
C	-0.89381700	-1.46147200	0.88179500
C	0.58302900	-1.07974700	0.89894200
C	0.64939800	0.35269100	0.33543600
H	1.00407000	-1.11827200	1.90391500
C	-3.00794100	-0.23650100	0.18240600
H	-3.42830700	0.44400300	-0.55883500
H	-3.51847400	-1.19859900	0.08571500
H	-3.20590800	0.15508500	1.18120500
H	-1.08307700	-2.47486900	0.52013500
H	1.19191600	-1.73586900	0.27679700
H	0.68897000	-0.15000800	-1.54385800
O	1.26033300	0.36838200	-0.96150800
N	-0.74871700	0.74346400	0.26798400
C	-1.07044300	1.96422300	-0.43591000
H	-0.37927600	2.74995000	-0.13398800
H	-1.01400800	1.86506700	-1.52573700
H	-2.07470800	2.29662900	-0.16840400
H	-1.33873700	-1.37563100	1.87602200
O	-1.28367200	-0.77657800	-1.41341400
H	-1.79550500	-1.55651600	-1.63956700
C	1.48079400	1.28288900	1.18236400
H	2.49243400	0.88359500	1.27457300
H	1.55066400	2.27328500	0.73076000
H	1.04072200	1.37198100	2.17608500
O	3.80809300	-0.76096300	-0.46374800
H	4.53381300	-0.37138400	-0.95061400
H	3.00700300	-0.31416600	-0.78214500

33-trans_gas

O 1			
C	1.59949800	-0.42779200	-0.00111300
C	0.82841500	-1.51474200	-0.73980800
C	-0.62227200	-1.20906900	-0.42751200
C	-0.68069000	0.31777900	-0.26466200
H	-1.32481200	-1.56073800	-1.18352500
H	1.14440800	-2.51726600	-0.44773200
H	-0.92484200	-1.67539000	0.51443400
H	-1.02039900	0.29162000	1.67617100
O	-1.43548000	0.68343300	0.90237100
N	0.70773100	0.70974200	-0.16821200
C	1.04268500	1.95964500	0.46072700
H	0.46027300	2.76988800	0.01935700
H	0.86126800	1.97954400	1.54444400
H	2.09894400	2.17298500	0.29081700
H	1.02686200	-1.39989000	-1.81034700
C	-1.38415300	1.01431300	-1.40647700
H	-2.43684000	0.72838200	-1.43793600
H	-1.31900600	2.09801200	-1.29738700
H	-0.91138300	0.72890800	-2.34779000
O	-3.86226900	-0.74184000	0.41800800
H	-4.66624700	-0.31703300	0.71651000
H	-3.13944100	-0.15232300	0.68182800
C	1.90112800	-0.79389900	1.44003600
H	2.60804600	-1.62381500	1.47357100
H	2.34802800	0.05107700	1.96534500
H	0.99336100	-1.09745400	1.96734300
O	2.85346400	-0.15471000	-0.57677200
H	2.69427800	0.18282800	-1.46362300

34-cis_gas

1	1			
C		0.83804500	-0.84823900	-0.20481300
C		-0.21132400	-1.85441200	-0.61679200
C		-1.48871800	-1.04740600	-0.84799000
C		-1.31257000	0.32982900	-0.19181000
H		-2.36108000	-1.55386900	-0.43495500
C		2.03293000	-1.39110900	0.52905300
H		2.69000600	-0.58489300	0.86629800
H		1.76486700	-2.01391400	1.38069500
H		2.59304200	-2.00906600	-0.17313000
H		-0.34123800	-2.59908000	0.17025500
H		-1.69211500	-0.89273900	-1.90799900
H		0.13307400	-2.38246600	-1.50492900
O		1.21699300	-0.15008000	-1.34343700
H		1.89425500	0.50623300	-1.11976600
O		1.94929500	2.22909700	0.05746900
H		1.55613400	2.97008600	-0.41441100
H		2.71797200	2.58946200	0.50863500
H		0.50021600	1.03731000	0.65561000
C		-2.47037700	0.77446200	0.65528000
H		-2.26493700	1.73201300	1.13625800
H		-3.31632300	0.91807800	-0.01714900
H		-2.75732400	0.03488500	1.40056500
O		-1.04909200	1.35113500	-1.07776800
H		-0.43509400	1.03453100	-1.75369400
C		-0.20153100	-0.29434000	2.05791600
H		-0.71842200	-1.25232400	2.08339200
H		0.76125400	-0.38496500	2.55362900
H		-0.79516500	0.44997600	2.58102300
N		0.00208200	0.13526100	0.65921400

34-cis_sol

1	1			
C		0.82328500	-0.83579200	-0.20105800
C		-0.22717000	-1.85255200	-0.58139700
C		-1.50781300	-1.05434400	-0.81292200
C		-1.32014900	0.33506800	-0.18675500
H		-2.37126900	-1.55246500	-0.37306700
C		2.01878200	-1.37228400	0.53612500
H		2.68678400	-0.56980500	0.85501100
H		1.74412700	-1.97355900	1.40048900
H		2.56321800	-2.01159300	-0.15895300
H		-0.34650400	-2.57810700	0.22377900
H		-1.72380800	-0.91903900	-1.87265700
H		0.10867400	-2.39813400	-1.46190900
O		1.19970500	-0.16226900	-1.36016900
H		1.84534900	0.52901200	-1.13445000
O		2.01853800	2.12969600	0.02065900
H		1.79493700	2.96412200	-0.40170800
H		2.77357700	2.31866800	0.58483800
H		0.49829900	1.06924200	0.61777100
C		-2.47156400	0.79472100	0.66106300
H		-2.26051300	1.75993000	1.12296900
H		-3.32609600	0.91502100	-0.00510500
H		-2.74301700	0.06885600	1.42449700
O		-1.07976000	1.33727900	-1.11035200
H		-0.40730600	1.03091700	-1.73542000
C		-0.18751200	-0.23126900	2.05414100
H		-0.69661200	-1.19145400	2.10815500
H		0.78432500	-0.29791900	2.53381500
H		-0.77576600	0.52496100	2.56393000
N		-0.00334500	0.16748700	0.64167400

34-trans_gas

1	1			
C		0.99298700	-0.85605300	-0.13561300
C		-0.00832200	-1.85149300	-0.68761000
C		-1.13593700	-0.98826100	-1.21429200
C		-1.38409800	0.01358600	-0.10474100
H		-2.05337000	-1.53002000	-1.44647100
C		1.92387200	-1.41276100	0.90353000
H		2.63670900	-0.66422800	1.25846700
H		1.39138000	-1.82199900	1.76146100
H		2.48594000	-2.22460400	0.44032500
H		-0.34278000	-2.51878900	0.11320500
H		-0.81960100	-0.46717900	-2.12042600
H		0.47006200	-2.46667600	-1.44792900
O		1.67164300	-0.30223800	-1.20994200
H		2.50500600	0.08576400	-0.92425300
O		1.31465300	2.71661900	-0.39485900
H		1.55238500	2.96237600	-1.29268500
H		1.34984600	3.53095800	0.11327400
H		0.41293400	1.12854500	-0.08177100
C		0.13582600	0.61717400	1.84593000
H		-0.13571400	-0.24211800	2.45077300
H		1.14240500	0.95223100	2.08768100
H		-0.56873600	1.42259500	2.04642700
N		0.07274900	0.28665700	0.40930500
C		-1.99368900	1.31943500	-0.52957200
H		-2.98868000	1.12377000	-0.92883200
H		-2.10430800	1.99514400	0.32009900
H		-1.39564500	1.80360000	-1.30260700
O		-2.11894600	-0.49793200	0.94302400
H		-2.16971100	-1.45732300	0.91654600

34-trans_sol

1	1			
C		0.79944100	-0.89575100	-0.17471700
C		-0.33176000	-1.84683800	-0.47593400
C		-1.41193600	-0.94095100	-1.02688900
C		-1.40869700	0.29210300	-0.13019500
H		-2.40449900	-1.38611500	-1.00822200
C		1.91548100	-1.44668900	0.66864300
H		2.66761500	-0.68423000	0.88206300
H		1.56386200	-1.87596900	1.60529000
H		2.39195400	-2.23884800	0.09075200
H		-0.65408100	-2.33529700	0.44748500
H		-1.18395500	-0.65522200	-2.05328700
H		-0.00240500	-2.61692300	-1.17201000
O		1.26271900	-0.39326800	-1.38061400
H		1.95702000	0.26351200	-1.21270000
O		2.20003700	2.00683300	-0.26901100
H		2.12772300	2.78686200	-0.82648000
H		2.86874500	2.21961900	0.38818700
H		0.54880800	1.12047700	0.22799000
C		0.04269700	0.26524700	1.99204400
H		-0.41103500	-0.64769500	2.36650000
H		1.06973300	0.34924200	2.33758900
H		-0.51622800	1.12458600	2.35342900
N		0.04155200	0.27269300	0.51461900
O		-2.34058800	0.10125600	0.86539000
H		-2.61216500	0.94014900	1.25238800
C		-1.57329000	1.60670000	-0.84178500
H		-1.53168300	2.44329200	-0.13912700
H		-0.79624200	1.74314700	-1.59525900
H		-2.54298600	1.61905600	-1.34004300

35_gas

1	1			
C		-1.05145100	-0.18468700	0.03231300
C		-0.57799300	-1.56937600	-0.38220200
C		0.89396000	-1.59352900	-0.01215600
C		1.28679800	-0.16352400	-0.04837300
H		1.52413800	-2.20036900	-0.66362900
C		-2.12500600	0.39878400	-0.84224900
H		-2.45411100	1.37855000	-0.48855100
H		-1.78849200	0.49532000	-1.87506600
H		-2.98494700	-0.27245900	-0.82928700
H		-0.69852000	-1.68925300	-1.46016600
H		1.06884800	-1.95148500	1.00985100
H		-1.17269200	-2.33006100	0.11799400
O		-1.37637700	-0.18373800	1.37712900
H		-2.13231700	0.37981200	1.56416900
C		2.69384300	0.25376400	-0.02770500
H		3.16440900	-0.07149500	-0.96017600
H		2.85154900	1.32154900	0.09020800
H		3.21140600	-0.28196200	0.77133100
N		0.25469700	0.60626700	-0.08100100
C		0.21932400	2.05475100	-0.01263300
H		1.20435100	2.46093400	0.19330200
H		-0.14724200	2.46283800	-0.95402900
H		-0.45510200	2.34702300	0.79205300

35_sol

1	1			
C		-1.04780600	-0.18446200	0.03092200
C		-0.57563800	-1.57241700	-0.36945500
C		0.89961000	-1.59518200	-0.01400600
C		1.28694800	-0.16545000	-0.03572400
H		1.52352000	-2.18326500	-0.68696500
C		-2.09739200	0.40477700	-0.86871800
H		-2.42636200	1.38576900	-0.52013900
H		-1.72883200	0.50016800	-1.89015700
H		-2.95951800	-0.26255300	-0.87255500
H		-0.70437000	-1.70011800	-1.44446400
H		1.09382300	-1.96948700	0.99728200
H		-1.16685900	-2.32860100	0.14098200
O		-1.42941100	-0.19910100	1.36650400
H		-2.03728000	0.52166100	1.55954700
C		2.68956700	0.25834400	-0.02622900
H		3.12437300	0.00340800	-0.99651900
H		2.83970900	1.31708500	0.15847400
H		3.23234500	-0.32859500	0.71601000
N		0.25296400	0.60133700	-0.05477700
C		0.22117000	2.04995600	-0.00645700
H		1.20368400	2.45019900	0.21798800
H		-0.11669600	2.44306200	-0.96409800
H		-0.47175300	2.36132300	0.77401900

36_gas

0	1			
C		-1.71743400	-0.29197700	0.20801500
C		-0.87208800	-0.68019400	-0.98552200
C		0.50606400	-1.15084100	-0.59864900
C		1.43993900	-0.10159300	-0.07906100
H		-0.82712200	0.15215000	-1.69196900
H		0.42931200	-1.92973000	0.17021200
C		-2.82262000	0.67909100	-0.06799000
H		-3.48791400	0.76102800	0.78841300
H		-2.37759500	1.65485600	-0.28177300
H		-3.38367700	0.38564200	-0.95867800
O		-1.52101800	-0.76194700	1.29955300

H	-1.41344400	-1.48887800	-1.49220100
H	1.00392700	-1.63393700	-1.44899300
C	2.73604600	-0.64547700	0.41274300
H	3.45344600	0.14285600	0.62659700
H	2.55415300	-1.21384200	1.33107900
H	3.16213500	-1.35157000	-0.30644600
S	1.08971800	1.48518400	-0.02936800

36_sol

O 1			
C	-1.73026700	-0.26165900	0.22129500
C	-0.85604600	-0.79714500	-0.88284700
C	0.52450500	-1.20528500	-0.43981400
C	1.46301800	-0.10517000	-0.06289800
H	-0.82000600	-0.07229900	-1.69977800
H	0.46042500	-1.87987700	0.42305500
C	-2.87855700	0.58625100	-0.21992500
H	-3.56574600	0.77657000	0.60135500
H	-2.48663700	1.53543600	-0.59561900
H	-3.40418300	0.11433800	-1.05273600
O	-1.53324800	-0.53295800	1.38463600
H	-1.38675400	-1.66975400	-1.28331600
H	1.01684000	-1.79930700	-1.21854800
C	2.81893700	-0.57769000	0.32129100
H	3.47166900	0.23798800	0.62106600
H	2.74234300	-1.30295200	1.13695700
H	3.27232700	-1.11390600	-0.51816200
S	1.05726000	1.47510100	-0.06962300

37_gas

O 1			
C	-2.68640700	-0.26028700	0.00001100
C	-1.25211500	0.12381600	-0.00000100
C	-0.70926500	1.36813000	-0.00004000
C	0.70926400	1.36813000	-0.00004400
C	1.25211400	0.12381600	-0.00000800
H	-2.95325000	-0.85108700	-0.87950100
H	-2.95323800	-0.85107800	0.87953200
H	-1.31716400	2.26493200	-0.00006200
H	-3.30811900	0.63614600	0.00001100
H	1.31716300	2.26493200	-0.00007300
C	2.68640700	-0.26028600	0.00001000
H	2.95325600	-0.85099400	0.87958200
H	2.95323200	-0.85116900	-0.87945200
H	3.30811900	0.63614700	-0.00008700
S	0.00000100	-1.07360900	0.00003000

37_sol

O 1			
C	-2.68965900	-0.26028100	0.00001300
C	-1.25479200	0.12408000	-0.00000300
C	-0.71023300	1.36860400	-0.00005400
C	0.71023300	1.36860400	-0.00005600
C	1.25479200	0.12408000	-0.00000600
H	-2.95534200	-0.85226200	-0.87873000
H	-2.95533500	-0.85221400	0.87878900
H	-1.31802100	2.26576400	-0.00009000
H	-3.31070800	0.63639800	-0.00000900
H	1.31802100	2.26576500	-0.00009300
C	2.68965900	-0.26028100	0.00000700
H	2.95533800	-0.85220900	0.87878500
H	2.95533900	-0.85226600	-0.87873300
H	3.31070800	0.63639800	-0.00002200

S	0.00000000	-1.07401300	0.00004400
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38_gas

O 1			
C	1.31380100	-0.49110600	0.02804200
C	0.20342000	-1.06486900	0.49457600
C	-0.96526600	-0.35562000	1.10723800
C	-1.84520500	0.21300500	0.01470600
O	-1.75292000	1.36634700	-0.32863300
H	-1.53941200	-1.05668800	1.71856200
C	2.46161200	-1.28303200	-0.50242300
H	3.38663100	-1.02328400	0.01995900
H	2.28911800	-2.35246400	-0.37845600
H	2.62697000	-1.07235600	-1.56158000
H	0.14318300	-2.14804300	0.42480700
H	-0.63160000	0.46922900	1.74253200
C	-2.79644200	-0.74522300	-0.63389000
H	-3.25367100	-0.29925200	-1.51416100
H	-2.28103200	-1.67007100	-0.90305300
H	-3.57636200	-1.01577800	0.08318100
S	1.64122600	1.24468800	-0.00768000
H	0.36840300	1.68399100	0.07066500

38_gas

O 1			
C	1.45227200	0.13945500	-0.06345900
C	0.92044700	1.35145800	-0.17313900
C	-0.55036900	1.38816000	-0.41121100
C	-1.12854000	0.06343600	0.06522700
H	-0.76276600	1.52137600	-1.47959000
C	2.87675500	-0.22427700	0.12141300
H	3.02619100	-0.76811200	1.05744000
H	3.22807300	-0.87378300	-0.68471600
H	3.50145400	0.66983700	0.13627600
H	1.52381900	2.25122200	-0.13269000
O	-1.39178800	0.21824300	1.43548400
H	-1.54240200	-0.64660700	1.82646400
H	-1.05933000	2.19458500	0.12470200
C	-2.36503100	-0.38920300	-0.67357900
H	-2.72039800	-1.34748000	-0.28646400
H	-3.15832600	0.34770800	-0.52669200
H	-2.17403000	-0.50117600	-1.74094800
S	0.25242600	-1.16048000	-0.18557300

39_sol

O 1			
C	1.45929400	0.13889100	-0.05718100
C	0.92474600	1.35107000	-0.16511600
C	-0.54479400	1.38533700	-0.41270100
C	-1.13260700	0.06487400	0.06397600
H	-0.74793500	1.50876800	-1.48360100
C	2.88496100	-0.22410800	0.12426700
H	3.03767500	-0.77757100	1.05408800
H	3.23680900	-0.86543700	-0.68796000
H	3.50731400	0.67131200	0.14686700
H	1.52703400	2.25188800	-0.12804500
O	-1.40001000	0.21388400	1.43448500
H	-1.75962200	-0.61030400	1.77778600
H	-1.05811800	2.20074400	0.10458800
C	-2.36314800	-0.38581100	-0.68249200
H	-2.72637600	-1.34143800	-0.29714800
H	-3.15347100	0.35692500	-0.54962700
H	-2.16178300	-0.49882000	-1.74743500

S	0.25799000	-1.16179100	-0.18062000
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39_gas

O 1			
C	1.65300300	-0.07812600	0.22966000
C	0.85297200	-0.85415500	0.96074600
C	-0.61955300	-0.67048700	1.13424100
C	-1.45385200	-1.01981400	-0.08139400
O	-2.42928000	-0.37267300	-0.38880000
H	-0.97731300	-1.33940600	1.92609400
C	3.11286200	-0.34635000	0.07623500
H	3.70503600	0.47604100	0.48474900
H	3.39491000	-1.26796400	0.58601200
H	3.38624800	-0.43940400	-0.97846900
H	1.31844500	-1.69674000	1.46529300
H	-0.88384700	0.34260600	1.45069500
C	-1.03677200	-2.21448100	-0.87754500
H	-1.85828900	-2.55114900	-1.50588200
H	-0.19636900	-1.92506300	-1.51449600
H	-0.68033900	-3.02146900	-0.23465100
S	1.15633000	1.34930000	-0.68434600
H	-0.06384800	1.55862700	-0.14209500
O	-2.03648600	2.24738800	0.45858500
H	-2.53348600	2.95884600	0.05486000
H	-2.43825400	1.41903700	0.14749000

40_sol

O 1			
C	1.66458700	-0.09225000	0.21549800
C	0.85610200	-0.88584400	0.91626900
C	-0.61088400	-0.68589000	1.12194500
C	-1.45818900	-1.03536600	-0.07984700
O	-2.39466900	-0.33972100	-0.41894000
H	-0.95686200	-1.35021600	1.92175800
C	3.11516500	-0.38160000	0.02114100
H	3.73440900	0.41270800	0.44502400
H	3.38666000	-1.32564800	0.49333000
H	3.36348500	-0.44466400	-1.04169800
H	1.30586200	-1.77075700	1.35807900
H	-0.85777600	0.33172800	1.43637800
C	-1.10205400	-2.27572700	-0.82639200
H	-1.93548300	-2.60311600	-1.44361600
H	-0.24866300	-2.05243800	-1.47296500
H	-0.78409600	-3.06967400	-0.14905300
S	1.18696000	1.39708100	-0.61664300
H	-0.04744400	1.57143800	-0.09774800
O	-2.09664200	2.30367000	0.45211100
H	-2.42258800	2.94167800	-0.18573900
H	-2.38674300	1.43413000	0.12547700

41_gas

O 1			
C	1.70476000	0.25924700	-0.02459700
C	1.71498200	-0.96491900	-0.53916100
C	0.49733200	-1.78422400	-0.28076400
C	-0.65717300	-0.83167700	-0.00142700
H	0.65532700	-2.43782000	0.58652700
C	2.77698700	1.28132800	-0.06244200
H	2.44335000	2.18546100	-0.57803800
H	3.07480100	1.58092900	0.94589200
H	3.65738400	0.89422500	-0.57740600
H	2.57209300	-1.35409600	-1.07728400
O	-1.17827500	-0.45856100	-1.23147700

H	-1.84295400	0.23754000	-1.10610500
H	0.21447000	-2.42019000	-1.12415700
C	-1.72419900	-1.37617300	0.91733100
H	-2.50903000	-0.63419400	1.08055000
H	-2.18022600	-2.25156300	0.44785300
H	-1.31154000	-1.66422300	1.88438200
S	0.19739700	0.63126100	0.83471200
O	-2.50061400	1.89797700	-0.38473300
H	-1.60398900	2.08282300	-0.06983300
H	-2.77305200	2.66411500	-0.89173000

41_sol

0 1			
C	1.72264000	0.29114600	-0.03674900
C	1.74323300	-0.92571500	-0.57108400
C	0.53893900	-1.76503400	-0.31085200
C	-0.62361000	-0.83582500	0.00915300
H	0.71944500	-2.43429600	0.53959200
C	2.78251900	1.32702400	-0.06009400
H	2.43442500	2.23936400	-0.55068900
H	3.08362000	1.60746400	0.95261200
H	3.66316000	0.96166000	-0.58985900
H	2.60338800	-1.29922300	-1.11569800
O	-1.19066900	-0.44731400	-1.20508700
H	-1.84671700	0.25301600	-1.03776300
H	0.25358500	-2.39474100	-1.15828800
C	-1.65976700	-1.41828200	0.93904700
H	-2.45613800	-0.69694400	1.13399000
H	-2.10638200	-2.29654400	0.46593900
H	-1.21997500	-1.71700200	1.89056600
S	0.21243000	0.63534000	0.83216000
O	-2.64561100	1.81020600	-0.37564000
H	-1.82946100	2.20719400	-0.04864700
H	-3.03130700	2.46159700	-0.96701500

42_gas

1 1			
C	-1.41241000	-0.80250300	-0.12551300
C	-0.15073300	-1.16484500	0.10884700
C	0.84818700	-0.42458800	0.96237900
C	2.03501600	-0.18954100	0.10385400
O	2.13191700	0.82328700	-0.62584200
H	0.44927600	0.52676900	1.32232100
C	-2.33470000	-1.61959000	-0.95998500
H	-2.71048400	-1.03742100	-1.80511700
H	-1.83072200	-2.50302800	-1.35041300
H	-3.20034100	-1.94199000	-0.37755700
H	0.18938300	-2.10096300	-0.32499700
H	-0.64119700	2.21209700	-0.31094400
H	1.14016200	-1.02701700	1.82781300
H	1.35917900	1.51078400	-0.56702200
O	0.27412600	2.50728000	-0.45315300
H	0.26728500	3.36427800	-0.88633400
H	-3.23139300	0.66099000	-0.11338400
C	3.11646900	-1.17279600	0.05174900
H	3.80505800	-0.98506500	-0.76713200
H	3.65507300	-1.11864500	1.00566700
H	2.70599800	-2.18421600	0.00602800
S	-2.11353700	0.63888000	0.63281500

42_sol

1 1			
C	1.41213100	-0.79804200	0.13951800

C	0.14838800	-1.16405400	-0.06398200
C	-0.85028200	-0.46100400	-0.94256600
C	-2.04773800	-0.17669200	-0.11175800
O	-2.12946200	0.86026500	0.58233800
H	-0.45073000	0.47187300	-1.34533500
C	2.33705100	-1.56236300	1.01960900
H	2.71656100	-0.92675800	1.82351700
H	1.82842900	-2.41631900	1.46642200
H	3.20160700	-1.92112300	0.45732000
H	-0.19862700	-2.06658100	0.43117100
H	0.63113700	2.14077700	0.24512300
H	-1.14218500	-1.09763700	-1.78164800
H	-1.32227600	1.52619900	0.52726800
O	-0.24384100	2.50346000	0.47246600
H	-0.13206600	3.03154400	1.26905200
H	3.17232800	0.73921100	0.10976200
C	-3.14701100	-1.13513600	-0.05532600
H	-3.85600200	-0.90176200	0.73269200
H	-3.64763800	-1.11405000	-1.02935200
H	-2.74999000	-2.14737300	0.04797200
S	2.11379000	0.59724600	-0.70658500

43_gas

1 1			
C	-1.55388000	-0.24040100	0.17043500
C	-0.96336200	-0.45478200	1.33735000
C	0.51395600	-0.35661200	1.42556800
C	1.12729600	-0.59755600	0.05534600
H	0.94159000	-1.07548700	2.13059400
C	-2.98637500	-0.23330100	-0.19909200
H	-3.29789200	0.73969300	-0.58532200
H	-3.20652400	-0.97403700	-0.97042400
H	-3.59200000	-0.45982500	0.67841100
H	-1.55881700	-0.66053800	2.22075200
O	2.22794500	0.17242600	-0.13521200
H	2.82918500	-0.22161400	-0.77736300
H	0.80076200	0.64314200	1.77059100
O	0.53268900	2.80327700	0.17054100
H	0.14835900	3.68094800	0.24119500
H	-0.06705200	1.37736500	-0.82007900
H	1.48587000	2.92660900	0.16208500
C	1.30671800	-2.04203800	-0.31370200
H	1.64632300	-2.15357000	-1.34537400
H	2.05788500	-2.47371500	0.35231900
H	0.38115700	-2.60504300	-0.19027900
S	-0.33250300	0.06241100	-1.12532300

43_sol

1 1			
C	-1.52780600	-0.31729800	0.16505100
C	-0.93787500	-0.53712000	1.33056800
C	0.53484200	-0.39489100	1.42745800
C	1.15975400	-0.54288700	0.04945600
H	0.98038800	-1.13742900	2.09491700
C	-2.95846900	-0.35253300	-0.20804700
H	-3.29629300	0.61659700	-0.58097800
H	-3.14539300	-1.08645000	-0.99427800
H	-3.55784200	-0.61474400	0.66358800
H	-1.52872300	-0.78434300	2.20572400
O	2.21190700	0.30253300	-0.09863800
H	2.79152700	0.01612300	-0.81442800
H	0.79371400	0.59121600	1.82650400
O	0.32228700	2.82920900	0.22957800
H	-0.05176700	3.68643200	0.00739200
H	-0.13465300	1.38263300	-0.79352300
H	1.27632200	2.94120100	0.17809800

C	1.43259000	-1.96023200	-0.36296300
H	1.78429300	-2.01542500	-1.39370000
H	2.20516100	-2.36088600	0.29662200
H	0.53991300	-2.57789000	-0.26220000
S	-0.32177600	0.05742500	-1.11815000

44_gas

0 1			
C	1.84090400	-0.46935100	0.03483300
C	1.00181500	-1.33087500	0.59772800
C	-0.33395500	-0.78142600	0.96470200
C	-0.56312800	0.46488300	0.12338400
H	-0.35773500	-0.51205300	2.02797100
C	3.24457900	-0.68840700	-0.38535300
H	3.36688300	-0.52118300	-1.45829800
H	3.92327600	0.00058500	0.12428800
H	3.55769400	-1.70771400	-0.15549900
H	1.28696400	-2.35411600	0.81433200
O	-1.11351700	0.02081300	-1.10816100
H	-0.97291000	0.69985700	-1.77410900
H	-1.16250200	-1.47500300	0.79477700
O	-3.65773500	-0.96787200	-0.28784500
H	-2.85972200	-0.70861600	-0.77100000
H	-4.06494100	-1.66233100	-0.80526300
C	-1.45509100	1.50503100	0.75426700
H	-1.56978200	2.36843000	0.09448600
H	-2.44458100	1.07487300	0.92658100
H	-1.04467400	1.85103100	1.70295600
S	1.13133100	1.14522400	-0.18065800

45_gas

1 1			
C	-2.65283900	-0.33304400	0.00003800
C	-1.22986900	0.02368900	-0.00001900
C	-0.71623600	1.40267400	-0.00002900
C	0.75852400	1.35993900	0.00001400
C	1.29259400	0.14041900	0.00001300
H	-3.14222300	0.10662000	0.87470700
H	-3.14254500	0.10737500	-0.87406000
H	-1.13084400	1.94281400	-0.86425700
H	-2.82351600	-1.40702000	-0.00035800
H	1.36019600	2.26010000	0.00002500
C	2.70137000	-0.30987000	0.00002900
H	2.93025400	-0.91283800	0.88077000
H	2.93027900	-0.91282700	-0.88071200
H	3.36229600	0.55600200	0.00004400
H	-1.13093900	1.94291800	0.86408300
S	-0.00838900	-1.08662400	-0.00003300

45_sol

1 1			
C	-2.64794400	-0.33082400	0.00002800
C	-1.22711900	0.02505600	-0.00001300
C	-0.71551600	1.40120000	-0.00000800
C	0.75729500	1.35758900	0.00001700
C	1.28767400	0.13747700	0.00000700
H	-3.13127200	0.11213000	0.87490200
H	-3.13150800	0.11267900	-0.87443000
H	-1.13027900	1.93900900	-0.86395700
H	-2.81492600	-1.40452500	-0.00026100
H	1.35907100	2.25671800	0.00003100
C	2.69865900	-0.30585900	0.00001500
H	2.92714400	-0.90897800	0.88026100

H	2.92716000	-0.90896600	-0.88023500
H	3.35269700	0.56516500	0.00002700
H	-1.13033000	1.93904800	0.86389000
S	-0.00912800	-1.08813200	-0.00003200

46-cis_gas

O 1			
C	-1.21222700	-0.41156400	0.06083200
C	-0.20514600	-0.76831900	-1.04247200
C	1.23761400	-0.98337700	-0.63132100
C	2.00364300	0.22100100	-0.15101100
O	1.59192600	1.34868600	-0.26609200
H	1.33696000	-1.77460900	0.12036600
H	-0.56805400	-1.70329200	-1.47756700
H	1.79862400	-1.36300800	-1.49540400
H	-0.52097200	1.89437100	0.11187700
H	-0.25639600	-0.01726200	-1.83181500
C	3.32489700	-0.07708900	0.49508100
H	3.13834700	-0.50580900	1.48454900
H	3.88548800	-0.82464900	-0.06962500
H	3.91009900	0.83253000	0.60793600
S	-1.75151900	1.36910700	-0.02993500
C	-0.73937400	-0.73728700	1.46225500
H	-0.49296700	-1.80086500	1.53798300
H	0.13090800	-0.14471500	1.75159100
H	-1.53288600	-0.51534800	2.17812200
O	-2.36822500	-1.16032100	-0.23496900
H	-3.05089800	-0.95017500	0.40925400

46-trans_gas

O 1			
C	-1.15044300	-0.37905400	0.09236300
C	-0.23471000	-0.78050700	-1.07965900
C	1.21095700	-1.02540500	-0.69791100
C	1.94998100	0.18216700	-0.18280200
O	1.63339200	1.30880700	-0.47827800
H	1.29737900	-1.83360300	0.03199600
C	-2.43572300	-1.18360200	0.07765500
H	-3.10975400	-0.86017700	0.87459200
H	-2.95296800	-1.07370800	-0.87705200
H	-2.19736500	-2.23818400	0.23263400
O	-0.44256500	-0.61564300	1.29118000
H	-0.62645400	-1.70274800	-1.51918000
H	1.76524700	-1.36261500	-1.58356700
H	-0.90796500	-0.16445000	2.00105400
H	-0.44991900	1.88113300	-0.19061500
H	-0.28932300	-0.02078700	-1.85980200
C	3.11942100	-0.11018800	0.70513000
H	2.73646300	-0.48512200	1.65860200
H	3.74205800	-0.90262000	0.28334600
H	3.71019900	0.78650100	0.87739200
S	-1.68757000	1.38816200	0.00492100

47-cis_gas

O 1			
C	1.35238700	0.06062700	-0.01514900
C	0.67925100	1.06993000	-0.92430900
C	-0.67462900	1.36101700	-0.32120300
C	-1.36817200	0.04286300	0.03229500
H	-1.31705200	1.94662100	-0.98432200
C	2.56012000	-0.60913800	-0.62553200
H	2.97949400	-1.35444300	0.05500300
H	2.30577500	-1.10845100	-1.56081600

H	3.32794600	0.14452600	-0.81742300
H	0.58182900	0.63485400	-1.92328100
H	-0.54363300	1.93912100	0.59679700
H	1.30335900	1.96486900	-1.00430100
O	1.70855200	0.75448000	1.16040400
H	1.97831100	0.11662600	1.82608000
S	0.02818800	-1.18181100	0.30263900
C	-2.26128000	-0.46672300	-1.07114600
H	-2.63583900	-1.46306200	-0.83458400
H	-3.11461600	0.20703000	-1.18206800
H	-1.71821300	-0.51494100	-2.01561800
O	-2.17216700	0.15187300	1.16926000
H	-1.61551900	0.39395100	1.91526800

47-trans_gas

O 1			
C	-1.36160000	-0.05433800	0.04282800
C	-0.67648200	-1.35110300	-0.33860200
C	0.67648200	-1.35110400	0.33859900
C	1.36160000	-0.05433800	-0.04282800
H	1.30794600	-2.18819700	0.02978900
C	-2.48125600	0.35250400	-0.88431000
H	-2.91529400	1.30769600	-0.57825400
H	-2.12398100	0.45241200	-1.90941900
H	-3.26883500	-0.40436000	-0.84822700
H	-0.55227900	-1.39170200	-1.42313400
H	0.55227800	-1.39170500	1.42313000
H	-1.30794600	-2.18819700	-0.02979400
O	1.83895300	-0.22481800	-1.35652900
H	2.07696600	0.63177200	-1.71978000
O	-1.83895200	-0.22482200	1.35652900
H	-2.07696500	0.63176800	1.71978200
C	2.48125600	0.35250100	0.88431200
H	3.26883400	-0.40436200	0.84822700
H	2.91529400	1.30769400	0.57825800
H	2.12398000	0.45240900	1.90942000
S	0.00000000	1.21357300	0.00000100

48-cis_gas

O 1			
C	-1.48118100	-0.26703000	-0.18181600
C	-0.41802500	-0.33826600	-1.26847600
C	0.77755000	-1.21109700	-0.94701900
C	1.90772000	-0.52549900	-0.21773600
O	2.20085800	0.62995900	-0.41930700
H	0.49216300	-2.11900900	-0.40841200
H	-0.92300000	-0.70512000	-2.16840500
H	1.23630700	-1.56228600	-1.88085700
H	-0.34784400	1.46139300	1.01004100
H	-0.08753100	0.67849600	-1.49444800
O	0.61248700	2.92641100	-0.20571400
H	1.28931600	2.26256500	-0.40728400
H	1.08656800	3.72470300	0.02716600
C	2.70206200	-1.38606100	0.71110200
H	3.60383100	-0.87431100	1.03892800
H	2.07710100	-1.62032200	1.57748300
H	2.95434400	-2.33659700	0.23488200
S	-0.78323500	0.25968000	1.45391600
C	-2.16010700	-1.60149900	0.06499700
H	-2.96703400	-1.48355600	0.79125700
H	-2.58982200	-1.96248200	-0.87212400
H	-1.47357400	-2.35514300	0.45333100
O	-2.40899300	0.67275800	-0.64903400
H	-3.02199400	0.88048500	0.06191500

48-cis_sol

O	1			
C		-1.48505500	-0.29229200	-0.18748900
C		-0.39521800	-0.34586700	-1.24766700
C		0.80932000	-1.19750000	-0.90969200
C		1.93837600	-0.49839600	-0.20145600
O		2.15801400	0.68877400	-0.32991900
H		0.53916100	-2.09825700	-0.35225900
H		-0.87425600	-0.72360500	-2.15657500
H		1.26809600	-1.57079800	-1.83459800
H		-0.37053300	1.42146400	1.05222500
H		-0.07579600	0.67534000	-1.46905800
O		0.56130100	3.00007500	-0.26024800
H		1.19545600	2.27245300	-0.36706800
H		1.04899200	3.70349600	0.17266700
C		2.81854200	-1.37254400	0.62516100
H		3.71965400	-0.84800800	0.93378800
H		2.25437200	-1.68358700	1.50923800
H		3.07354700	-2.28466800	0.08185200
S		-0.83008700	0.22451100	1.47597400
C		-2.16034800	-1.63053500	0.03004900
H		-2.98638100	-1.52869300	0.73713000
H		-2.55974900	-1.98878200	-0.92114500
H		-1.47394900	-2.37965700	0.42539200
O		-2.40512000	0.65546600	-0.66375100
H		-3.14447000	0.70940500	-0.04926400

48-trans_gas

O	1			
C		-1.41268000	-0.43706500	-0.17647100
C		-0.35981300	-0.35703200	-1.26792200
C		0.92843500	-1.08460300	-0.95212200
C		1.97607800	-0.26315900	-0.24629500
O		2.06643300	0.93720200	-0.37687500
H		0.73586700	-2.00234800	-0.38970900
C		-2.58462100	0.46050600	-0.49661900
H		-3.36593400	0.35795600	0.25936400
H		-2.27504400	1.50609300	-0.53376300
H		-2.99762200	0.17895100	-1.46973200
O		-1.80228400	-1.78555100	-0.09861900
H		-0.82284500	-0.78601900	-2.16279800
H		1.41592900	-1.40913100	-1.88132200
H		-2.49656600	-1.86971000	0.56125900
H		-0.56807300	1.30285900	1.27154800
H		-0.15589400	0.69239100	-1.48878500
O		0.04031300	2.87717300	-0.15110100
H		0.82912600	2.33418200	-0.31212900
H		0.36010700	3.76689400	-0.00146900
C		2.95455400	-1.03586800	0.57856300
H		3.79647600	-0.41249000	0.87056000
H		2.43479000	-1.39131700	1.47261900
H		3.30102800	-1.92135000	0.04100600
S		-0.72742200	-0.01713900	1.50883100

48-trans_sol

O	1			
C		-1.42351800	-0.44686400	-0.17818200
C		-0.35093500	-0.37817000	-1.25068200
C		0.93429300	-1.10282400	-0.91795900
C		1.98939700	-0.27912300	-0.23286500
O		2.06110600	0.92800400	-0.35045700
H		0.74667900	-2.00863400	-0.33541300
C		-2.59334400	0.44079700	-0.53005600
H		-3.39252000	0.33797900	0.20648100
H		-2.28760800	1.48752500	-0.56503200

H	-2.98156200	0.15504500	-1.51186700
O	-1.81034100	-1.79288400	-0.07524800
H	-0.80011800	-0.80793500	-2.15185100
H	1.42044800	-1.45200200	-1.83822800
H	-2.57224000	-1.85919300	0.50961200
H	-0.56831700	1.32286000	1.24014000
H	-0.14328300	0.66943900	-1.47663700
O	0.06616100	2.92853400	-0.20096800
H	0.81590900	2.32355300	-0.32592800
H	0.45000100	3.75252000	0.10551100
C	2.99459300	-1.04916500	0.55562000
H	3.83927800	-0.42503500	0.83761000
H	2.50391300	-1.42812300	1.45680600
H	3.33422800	-1.92238700	-0.00471300
S	-0.76269600	0.01482900	1.51197700

49-cis_gas

O 1			
C	-0.89102300	-0.85367800	0.02387200
C	0.16812600	-1.87889000	0.37624300
C	1.50609200	-1.16873200	0.58490000
C	1.45544700	0.28166800	0.06705500
H	2.30307700	-1.70554600	0.06622700
C	-2.11156500	-1.42505900	-0.65085500
H	-2.83607900	-0.63724100	-0.86806700
H	-1.84943200	-1.92396600	-1.58459200
H	-2.58475500	-2.14747100	0.01893000
H	0.23785500	-2.58876400	-0.45039100
H	1.78773900	-1.12444200	1.63938100
H	-0.15619200	-2.43240000	1.26215600
O	-1.23387700	-0.19351500	1.21707300
H	-1.86394800	0.52067800	1.02065300
S	0.02624300	0.27311400	-1.13906600
O	-2.21412400	2.17012500	0.19790900
H	-2.82103800	2.78808000	-0.20976800
H	-1.46036800	2.06813200	-0.40366200
C	2.71194100	0.71201000	-0.64210400
H	2.61641500	1.73973400	-0.99412400
H	3.54820300	0.67126700	0.06015800
H	2.92639700	0.06064700	-1.48928200
O	1.23340900	1.19782900	1.09266300
H	0.41486400	0.94202700	1.54160500

49-trans_gas

O 1			
C	-0.88087400	-0.85701100	0.04873700
C	0.29575700	-1.68884600	0.51815600
C	1.31664800	-0.72777300	1.08601100
C	1.60988800	0.29863500	0.00939900
H	2.25309500	-1.21595500	1.36776700
C	-1.78526700	-1.54674300	-0.94391100
H	-2.58681200	-0.87611100	-1.26371600
H	-1.23326600	-1.87454800	-1.82499600
H	-2.24399300	-2.41390800	-0.46154300
H	0.72262900	-2.23005700	-0.32928900
H	0.90748000	-0.22605000	1.96568500
H	-0.05973100	-2.41407500	1.25450100
O	2.48487200	-0.31761500	-0.90405800
H	2.53260200	0.21037900	-1.70479000
O	-1.58169700	-0.46030200	1.18196600
H	-2.27307900	0.17281300	0.93490800
C	2.19397000	1.59233100	0.52262300
H	3.16294600	1.38925000	0.98591500
H	2.35148100	2.30188900	-0.29370700
H	1.53488600	2.05586400	1.25690100
S	-0.04414100	0.60821500	-0.79192700

O	-2.84124600	1.87128200	0.21145600
H	-3.42102000	2.19515800	-0.47897100
H	-1.93713400	2.02343600	-0.09884300

50-cis-gas

1 1			
C	1.55722000	-0.40236400	-0.15411600
C	0.32421700	-0.82229700	-0.95237400
C	-0.60234200	0.32485900	-1.34882900
C	-1.31123200	1.00551900	-0.23320700
O	-2.17962200	0.39616600	0.45861800
H	-0.06156200	1.07104700	-1.93147700
H	0.68082800	-1.31021700	-1.86329400
H	-1.39038600	-0.07557500	-2.00006400
H	-0.23165400	-1.58438100	-0.39511900
O	-2.64286200	-2.15505700	0.10427800
H	-2.31510500	-0.58387900	0.27239300
H	-2.72401300	-2.68604900	0.90215000
C	-1.25534000	2.45985700	-0.06267000
H	-1.63154200	2.76252600	0.91151800
H	-0.25470600	2.84590100	-0.24375100
H	-1.91195300	2.88749400	-0.83337500
H	-3.30898700	-2.48446600	-0.50565900
S	0.88473600	0.28734400	1.44620900
H	1.91179900	1.11429700	1.71212900
O	2.37578900	-1.50009200	0.06780500
H	1.94012600	-2.15692400	0.61915600
C	2.41545200	0.61683400	-0.86435900
H	3.31730500	0.80249000	-0.28126900
H	2.72360100	0.21076200	-1.83102100
H	1.90618300	1.56688400	-1.02394600

50-cis_sol

1 1			
C	1.55588900	-0.40071000	-0.16206800
C	0.27587300	-0.89057400	-0.83238600
C	-0.68560500	0.19657700	-1.30741000
C	-1.37692500	0.95887900	-0.23822600
O	-2.18368400	0.39547700	0.54814300
H	-0.18601700	0.89506300	-1.97780200
H	0.57876300	-1.47174100	-1.70707800
H	-1.47889300	-0.28825800	-1.88853100
H	-0.24095800	-1.58722400	-0.16529100
O	-2.64682400	-2.08948200	0.15278500
H	-2.34068300	-0.60625000	0.40370400
H	-2.69987200	-2.64621600	0.93564400
C	-1.29577400	2.41769700	-0.17084300
H	-1.68635200	2.79944500	0.76838000
H	-0.28232400	2.76616200	-0.35823200
H	-1.91565500	2.79486800	-0.99462400
H	-3.43657000	-2.27507400	-0.36438700
S	1.03290600	0.40786900	1.43740100
H	2.03856500	1.29779600	1.50080200
O	2.39783900	-1.49133700	0.07880100
H	1.93613000	-2.15627200	0.60022500
C	2.35211700	0.56096300	-1.00860300
H	3.30409000	0.77437100	-0.52186800
H	2.55742400	0.09893900	-1.97762400
H	1.83377500	1.50422800	-1.17235800

50-trans_gas

1 1			
C	1.54736700	-0.35078500	-0.19468600

C	0.33392300	-0.88780700	-0.93264500
C	-0.64580300	0.21136900	-1.34173500
C	-1.26146900	0.98525500	-0.23088300
O	-2.20080400	0.49508100	0.46645600
H	-0.13873500	0.90930800	-2.00797600
C	2.61021100	-1.40504800	-0.01541800
H	3.44833500	-1.01425300	0.56561900
H	2.21812600	-2.27183600	0.51686300
H	2.97766800	-1.72727900	-0.99315100
O	2.01331200	0.75497200	-0.89856900
H	0.67536800	-1.38548800	-1.84438100
H	-1.46982600	-0.25129700	-1.89581900
H	2.94805500	0.89576800	-0.72121000
H	1.75830500	1.17257900	1.66850600
H	-0.16038100	-1.64889600	-0.32148000
O	-2.79877600	-2.03898300	0.13172800
H	-2.41673400	-0.47165800	0.30030900
H	-2.81822600	-2.58504300	0.92304400
C	-1.02767600	2.42517500	-0.09369800
H	-1.35428600	2.79596300	0.87468800
H	0.01310000	2.67104400	-0.29543800
H	-1.63186200	2.91102000	-0.87272400
H	-3.54399500	-2.32199900	-0.40565200
S	0.87787000	0.17278400	1.48539300

50-trans_sol

1 1			
C	1.54263200	-0.32708000	-0.20696700
C	0.29385800	-0.90901100	-0.84231300
C	-0.70770300	0.14495100	-1.31171300
C	-1.36751100	0.92992300	-0.24021000
O	-2.20452100	0.39925000	0.54094200
H	-0.21869400	0.83389600	-1.99869600
C	2.59568400	-1.38653300	0.00771300
H	3.47056800	-0.96469800	0.50622500
H	2.21006200	-2.19609700	0.62772200
H	2.90252100	-1.79573200	-0.95823500
O	1.99797300	0.69903100	-1.03071200
H	0.60073900	-1.48172500	-1.72154300
H	-1.50831800	-0.36414200	-1.85886500
H	2.90543900	0.92390100	-0.80185400
H	1.91498600	1.33762700	1.50114400
H	-0.17197100	-1.61886500	-0.15405500
O	-2.62731300	-2.11164600	0.19732700
H	-2.36265100	-0.60036700	0.41100000
H	-2.67413700	-2.64737000	0.99502700
C	-1.23211300	2.38560800	-0.18067800
H	-1.58087400	2.78521900	0.76766300
H	-0.21029100	2.68849300	-0.39916400
H	-1.86220100	2.78282200	-0.98712900
H	-3.40433100	-2.33649900	-0.32323500
S	0.99443500	0.35833100	1.46115900

51-cis_gas

1 1			
C	1.26204900	-0.75856800	0.12071800
C	0.48149200	-0.54145000	1.40060800
C	-0.98245100	-0.83918100	1.19662800
C	-1.54120500	0.06493500	0.11455800
O	-1.55694300	1.36017300	0.56959400
H	-1.13559600	-1.88174900	0.90410400
H	0.92288600	-1.19104300	2.16243800
H	-1.56419200	-0.67066800	2.10582400
H	0.25485200	1.18876700	-1.13132100
H	0.61173500	0.48879200	1.74193200
O	1.46588400	2.59296200	0.00625000

H	0.98453200	3.08460500	0.67751900
H	2.05280000	3.22813700	-0.41478100
C	-2.84994800	-0.39120600	-0.46471500
H	-3.20247800	0.28598500	-1.24544500
H	-2.76975500	-1.38987600	-0.89403600
H	-3.59305400	-0.41918100	0.33611800
S	-0.17324600	-0.08943900	-1.26515400
H	-2.22280300	1.87765700	0.10472300
C	1.50975800	-2.17819800	-0.28053500
H	0.59998400	-2.77728300	-0.27237400
H	1.96440700	-2.22556300	-1.26860000
H	2.21324700	-2.60621300	0.43794700
O	2.35957300	-0.02711900	-0.04807300
H	2.22909600	0.89254400	0.25268100

51-cis_sol

1 1			
C	1.23757600	-0.72933200	0.10059900
C	0.48978800	-0.50264200	1.40121100
C	-0.97381500	-0.81610600	1.21756100
C	-1.54356800	0.05502300	0.11692000
O	-1.60460700	1.34827700	0.55404500
H	-1.12292000	-1.86602500	0.95493500
H	0.94853200	-1.13677300	2.16415800
H	-1.55225200	-0.62427600	2.12366400
H	0.26860300	1.20815700	-1.09937700
H	0.62091600	0.53521900	1.71756100
O	1.40828500	2.55483000	0.01059800
H	0.93699900	3.01678500	0.70976400
H	1.92299900	3.22603600	-0.44648500
C	-2.81499700	-0.44714900	-0.50146600
H	-3.16123800	0.21510400	-1.29616800
H	-2.68463000	-1.44709900	-0.91373500
H	-3.57871500	-0.48737200	0.27843800
S	-0.12617200	-0.08218300	-1.24112000
H	-2.17318700	1.87963200	-0.01497400
C	1.48412700	-2.16405100	-0.26057500
H	0.56914400	-2.75460600	-0.24689900
H	1.93900300	-2.23726400	-1.24725400
H	2.17568400	-2.57955300	0.47541700
O	2.37200200	-0.01841500	-0.05752500
H	2.22970800	0.91496300	0.19642900

51-trans_gas

1 1			
C	1.33512000	-0.66915100	0.07880300
C	0.60078900	-0.51820200	1.39164200
C	-0.81626500	-1.00281200	1.19793600
C	-1.49039900	-0.20237800	0.10109900
O	-1.85214200	1.02807400	0.57309500
H	-0.81424500	-2.05907500	0.92182800
C	2.61229600	0.10423500	-0.06184700
H	3.04108300	-0.00194700	-1.06055800
H	2.46320600	1.16252600	0.15034900
H	3.32754000	-0.29677500	0.66103200
O	1.43384000	-1.99378900	-0.23046200
H	1.13557200	-1.10363300	2.14361200
H	-1.42193200	-0.89266300	2.09956200
H	2.10926800	-2.15382000	-0.89820100
H	0.19168000	1.37993900	-0.80245600
H	0.62372600	0.52964500	1.70064300
O	0.59097800	3.00015300	0.08333100
H	-0.04206600	3.25281200	0.76039200
H	0.97953400	3.81770700	-0.23790900
C	-2.57833100	-0.91997600	-0.64153200
H	-3.00572500	-0.30048200	-1.43274500

H	-2.20977400	-1.84323300	-1.08814300
H	-3.36901400	-1.17332800	0.06923800
S	0.01242000	0.07838600	-1.17746700
H	-2.56825100	1.40234300	0.04850400

51-trans_sol

1 1			
C	1.32044400	-0.66980900	0.07077900
C	0.57909800	-0.57919900	1.38544500
C	-0.83703000	-1.05275800	1.16085700
C	-1.49193600	-0.19289800	0.09974600
O	-1.82257800	1.02073000	0.63215800
H	-0.84005200	-2.09304200	0.83065600
C	2.58755200	0.12857000	-0.02301000
H	3.02545500	0.06979800	-1.02071300
H	2.41497800	1.17395200	0.22920300
H	3.29898100	-0.29258400	0.69120900
O	1.46153300	-1.98850700	-0.27508400
H	1.11104600	-1.18999600	2.11812000
H	-1.44985100	-0.98531200	2.06148800
H	2.09714200	-2.08912700	-0.99244200
H	0.21000700	1.38749900	-0.77499600
H	0.59367900	0.45659700	1.73278700
O	0.64439100	2.96802400	0.12108100
H	-0.12284700	3.27636100	0.61173400
H	0.94513700	3.72409100	-0.39024700
C	-2.60115500	-0.84844800	-0.66788200
H	-3.01755300	-0.17762600	-1.42079200
H	-2.25515500	-1.75604600	-1.16087600
H	-3.39056400	-1.11383500	0.03906600
S	0.01418600	0.08835500	-1.16278000
H	-2.45599300	1.48085700	0.06944700

52-cis_gas

0 1			
C	-1.73905500	-0.38182200	-0.02800200
C	-0.62995800	-1.35559800	0.37041800
C	0.51822800	-0.58308500	0.97585300
C	0.81376800	0.56683900	0.03393900
H	1.41781400	-1.19035500	1.11104700
H	-0.28268000	-1.87219300	-0.52840600
H	0.24459700	-0.17002100	1.95095900
H	-1.03381000	-2.11465700	1.04567800
O	1.44594800	0.00172200	-1.11368400
H	1.41341100	0.64481400	-1.82686100
C	1.68700400	1.64457300	0.62793900
H	2.65982400	1.21774800	0.88469800
H	1.84565300	2.45663400	-0.08598800
H	1.23073400	2.06486900	1.52442300
O	3.77382400	-1.11408500	0.09323900
H	4.32251800	-1.72665900	-0.39618400
H	3.09005400	-0.81413400	-0.52329500
S	-0.84328900	1.22937000	-0.39879000
O	-2.46867900	-0.81823500	-1.13484800
H	-1.87149600	-0.90963500	-1.88295800
C	-2.74295900	-0.14625700	1.07252100
H	-3.43749000	0.64732600	0.79564900
H	-3.31309700	-1.06375900	1.23834000
H	-2.24432800	0.13699000	1.99987700

52-trans_gas

0 1			
C	-1.76870300	-0.33823500	0.04342400

C	-0.69675000	-1.39335900	0.22630200
C	0.48654000	-0.71339200	0.87914500
C	0.81767000	0.50069000	0.03584500
H	1.37023400	-1.35254100	0.95162800
C	-2.80745800	-0.67509600	-0.99907000
H	-3.53015400	0.13737100	-1.10920400
H	-2.34546200	-0.85445300	-1.97013800
H	-3.35086300	-1.57057700	-0.68707200
H	-0.41144200	-1.79472400	-0.74888200
H	0.21968400	-0.38457800	1.88605000
H	-1.10394600	-2.20870300	0.82939100
O	1.50726200	0.02109900	-1.11488500
H	1.47050200	0.69143600	-1.80217500
O	-2.36660400	-0.15190800	1.30288000
H	-2.89834800	0.64758500	1.28789300
C	1.64689500	1.54646300	0.73916200
H	2.61206500	1.11571000	1.01785600
H	1.83043800	2.40323200	0.08613500
H	1.13903200	1.90297000	1.63538300
O	3.93362300	-0.98131800	0.00260300
H	4.36617000	-1.69105600	-0.47160200
H	3.18970200	-0.70542000	-0.55268700
S	-0.82631400	1.18739600	-0.46413700

53_gas

1 1			
C	1.20767200	0.09371800	0.04905800
C	0.55317700	1.30261800	-0.57881100
C	-0.87567600	1.38104600	-0.08449800
C	-1.42122300	0.00600500	-0.03445400
H	-1.52247100	2.03138800	-0.67867100
C	2.38545600	-0.48748700	-0.67177600
H	2.74905600	-1.39335500	-0.18198100
H	2.14388200	-0.72724600	-1.70692200
H	3.19250400	0.24919300	-0.66713700
H	0.56835500	1.19532800	-1.66541500
H	-0.92658900	1.76939000	0.94366500
H	1.13638500	2.18669900	-0.31505700
O	1.40355100	0.32542800	1.37583100
H	2.05896200	-0.26968800	1.75625700
C	-2.86301800	-0.24299000	0.05361200
H	-3.34358700	0.14630400	-0.85075800
H	-3.12055900	-1.29153600	0.17751400
H	-3.27733200	0.34314700	0.88049100
S	-0.30033300	-1.19753100	-0.06858900

53_sol

1 1			
C	1.19496300	0.08916200	0.04558600
C	0.54509000	1.31289200	-0.55686100
C	-0.88560800	1.38204100	-0.06971800
C	-1.42037600	0.00574900	-0.03147900
H	-1.53312900	2.02776100	-0.66613700
C	2.36620100	-0.47576000	-0.70013400
H	2.74345300	-1.38026300	-0.21993600
H	2.10255900	-0.70977700	-1.73075400
H	3.16323400	0.27068100	-0.70341500
H	0.56148500	1.22402300	-1.64416600
H	-0.95093300	1.76218300	0.95975200
H	1.12894400	2.19041400	-0.27617100
O	1.42935800	0.30878600	1.37672500
H	2.03492500	-0.34972800	1.73540100
C	-2.85797900	-0.25624400	0.04286200
H	-3.32160900	0.10835200	-0.87938800
H	-3.10327100	-1.30477300	0.18427300
H	-3.28610000	0.34628000	0.84874700
S	-0.28926000	-1.18765500	-0.06272100

TS(1-11)_gas

0 1			
C	-1.12593000	-0.61849000	0.07073800
C	0.11831100	-1.47400800	-0.16237400
C	1.36293200	-0.96175400	0.53278600
C	2.09277000	0.16155700	-0.13357900
O	1.60886600	0.83234600	-1.02201000
H	1.07213500	-0.58579000	1.52388200
C	-2.39108100	-1.33400300	-0.34841900
H	-2.59208100	-2.12705500	0.37365600
H	-3.23319300	-0.64040300	-0.33370400
H	-2.30605800	-1.76636500	-1.34667100
O	-1.16053100	-0.02669500	1.23083700
H	-0.12030700	-2.45821300	0.25118800
H	2.07958000	-1.76771200	0.71975700
H	-0.10384200	0.75962900	-1.19572300
H	0.27708500	-1.61919700	-1.23494500
C	3.47772200	0.42956600	0.36338200
H	3.50545000	0.41523200	1.45449000
H	4.13936700	-0.37095300	0.02175400
H	3.84409600	1.38128700	-0.01388200
H	-1.56852600	1.36074900	-0.55650200
O	-2.07059800	2.02987500	0.48092300
H	-1.76449100	1.10733500	1.05270200
H	-3.01918800	2.15569800	0.50264300
O	-1.05503300	0.53179300	-1.08398100

TS(1-21)_gas

0 1			
C	-1.24431800	-0.55617800	0.22212100
C	-0.11228300	-1.57281500	-0.00089700
C	1.27255200	-1.16875700	0.45734700
C	2.02917000	-0.25052500	-0.46342000
O	1.63975800	0.01944400	-1.57977800
H	1.24539900	-0.70465400	1.44765800
C	-2.55163600	-1.17056300	-0.23243100
H	-3.38794200	-0.50249300	-0.03038400
H	-2.53833200	-1.43353100	-1.29379300
H	-2.71598500	-2.08064600	0.34480100
O	-1.33762600	-0.10666900	1.48908900
H	-0.42024700	-2.45135000	0.57165100
H	1.90019400	-2.06183000	0.56923300
H	-0.40390300	0.40070900	-1.51143600
H	-0.08775500	-1.87642800	-1.05335800
C	3.29085100	0.31795100	0.09428600
H	2.98830100	1.07781100	0.82142400
H	3.86721800	-0.43595700	0.63358200
H	3.89227700	0.77453200	-0.68849800
N	-0.92036300	0.68521700	-0.67796200
C	-2.04105200	1.58454200	-0.96089600
H	-1.65875600	2.50770000	-1.39385700
H	-2.75192000	1.13141900	-1.64883900
H	-2.53640900	1.81481900	-0.01851300
H	-0.23818000	1.23114300	-0.03299100
O	0.40802400	1.54429700	1.33426900
H	-0.54241500	0.66144200	1.62536100
H	0.29004500	2.39228400	1.75838500

TS(3-4)_gas

0 1			
C	1.32175600	-0.00957800	-0.12377900
C	0.87246100	1.23813500	0.03731900

C	-0.61493100	1.38878100	0.02342500
C	-1.23658500	0.03131700	0.14966700
H	-0.95905700	1.95724700	0.89643800
C	2.74323900	-0.43483800	-0.15396300
H	2.96614600	-0.93347400	-1.09990200
H	3.41534400	0.41401100	-0.03290300
H	2.94075300	-1.15777200	0.64101700
H	1.52649600	2.08646300	0.18293000
H	-0.98263100	1.90381100	-0.87019500
H	-0.23751200	-1.10085200	0.86299500
O	-1.18241300	-0.59188600	1.28496300
O	0.40538500	-0.98196900	-0.25938100
C	-2.23928900	-0.39847900	-0.85274300
H	-2.42175500	-1.46789700	-0.77236800
H	-3.17327600	0.12882300	-0.62779400
H	-1.93819100	-0.13155200	-1.86443800

TS(4-2)_gas

O 1			
C	-1.37075100	0.02081200	-0.07846700
C	-0.94534400	-1.03566500	-0.76430400
C	0.51481600	-0.93364600	-0.89477200
C	0.79793100	0.34277100	-0.29371000
O	-0.30020500	0.89197900	0.16703300
H	1.04453500	-1.22021700	-1.79812400
C	-2.66239300	0.45652100	0.47029800
H	-2.62404300	0.52275400	1.55968400
H	-2.94219400	1.44172500	0.09015800
H	-3.43899300	-0.25538800	0.19524200
H	-1.56083200	-1.86414300	-1.07538000
O	1.53466700	-0.94028000	1.29844300
H	1.72495000	-1.07790500	2.23003100
H	1.00928700	-1.49862300	0.05787400
C	2.00061200	1.17720100	-0.39159200
H	2.88006200	0.54373300	-0.46801400
H	1.93005800	1.80963100	-1.28340400
H	2.09225300	1.81688300	0.48340300

TS(5-6)_gas

O 1			
C	1.42630400	-0.19642000	0.13787300
C	1.14735700	-1.36027500	-0.44870200
C	-0.29615700	-1.75786400	-0.39677600
C	-1.10650600	-0.52517300	-0.09047500
O	-1.40682800	0.21667400	-1.08161000
H	-0.64390700	-2.14423700	-1.35934800
C	2.75822100	0.45078600	0.23872700
H	3.52962500	-0.15140200	-0.23988800
H	2.74199900	1.43681000	-0.23544100
H	3.02724100	0.60659800	1.28607000
O	0.40275000	0.45487100	0.71144100
H	1.89811500	-1.98540700	-0.91094300
H	0.00806500	1.57845300	0.24642000
H	-0.48176600	-2.52961800	0.35936200
H	-1.25142500	1.35448600	-0.78650900
O	-0.70433900	2.30839700	-0.26189400
H	-0.25243400	2.85582200	-0.90579200
C	-1.97503400	-0.50210000	1.12142900
H	-2.29391800	0.51527400	1.34727500
H	-2.86693100	-1.09614400	0.89851400
H	-1.47243700	-0.93389100	1.98432700

TS(7-8)_gas

1	1			
C		1.47565200	-0.25970800	0.10852000
C		1.20495100	-1.45061600	-0.39090200
C		-0.22816500	-1.87476600	-0.32200700
C		-1.08047100	-0.66990700	-0.06605800
H		-0.55921300	-2.32043600	-1.26388100
C		2.74153700	0.48562000	0.21912800
H		2.98995100	0.67507100	1.26546100
H		3.55314200	-0.07675900	-0.23779200
H		2.67294600	1.45530600	-0.28284500
H		1.96469800	-2.10007600	-0.79884400
H		-0.39097400	-2.61206500	0.46931700
H		0.23161000	1.29630900	0.36905800
O		-1.37689300	-0.01160700	-1.15106200
O		0.35155200	0.36138600	0.66166500
O		-0.62230100	2.71053100	-0.22821000
H		-0.83003800	3.42840700	0.37748700
H		-1.97316200	0.73367200	-0.98220700
H		-0.33702300	3.13458200	-1.04323200
C		-2.00791300	-0.60849700	1.08189900
H		-2.39672200	0.40038600	1.23171500
H		-2.84842200	-1.27317700	0.85919100
H		-1.52920200	-0.95645800	1.99394300

TS(7-8)_sol

1	1			
C		1.41821600	-0.39857600	0.12682500
C		1.04409000	-1.57781600	-0.33549400
C		-0.42181200	-1.85644500	-0.23204500
C		-1.13677900	-0.54805400	-0.07473800
H		-0.80990400	-2.34097000	-1.13066500
C		2.74189100	0.24544800	0.19143000
H		3.01331100	0.47053200	1.22478200
H		3.49849200	-0.40713300	-0.23948400
H		2.74161900	1.18960900	-0.36005100
H		1.73926200	-2.30069100	-0.73397100
H		-0.65389000	-2.50173100	0.61881800
H		0.31935500	1.27719300	0.37841000
O		-1.30231300	0.07907500	-1.20663200
O		0.35848500	0.32334900	0.66840200
O		-0.28335700	2.70126200	-0.21500000
H		-0.44506500	3.41799900	0.40510300
H		-1.82283200	0.89109100	-1.10614500
H		0.15865700	3.09967900	-0.97041800
C		-2.11199200	-0.32586100	1.01124600
H		-2.38407300	0.72680000	1.09579500
H		-3.01099100	-0.89481600	0.75961000
H		-1.72814100	-0.68922700	1.96071400

TS(8-10)_gas

1	1			
C		1.46802100	-0.13741900	0.06580900
C		1.36325500	-1.33076200	-0.48502500
C		-0.04409500	-1.81565900	-0.39447000
C		-0.79201900	-0.57539900	0.08162800
O		0.22179900	0.32269100	0.54587100
H		-0.15067700	-2.63256600	0.32537600
C		2.58781600	0.78093800	0.31294100
H		2.43583600	1.74542900	-0.18207700
H		2.70816900	0.97209300	1.38160900
H		3.51322000	0.35374300	-0.06776100
H		2.18780800	-1.88886400	-0.89901200
O		-1.36279100	0.13309700	-1.04209200
H		-2.06960800	-0.38125700	-1.44538300

H	-0.45004000	-2.17149800	-1.34474000
O	-0.91359600	2.41345200	-0.17000500
H	-0.52886800	3.16576900	-0.64107800
H	-0.22855800	1.79599100	0.28723100
H	-1.34225500	1.71792500	-0.77618300
C	-1.81752500	-0.77641800	1.15463700
H	-2.26897000	0.17288900	1.44860600
H	-2.60598300	-1.44302300	0.80002000
H	-1.35609600	-1.23223200	2.03008200

TS(8-10)_sol

1 1			
C	1.41763600	-0.30325000	0.07224100
C	1.19006700	-1.50975200	-0.41091300
C	-0.26258600	-1.83559300	-0.32917800
C	-0.89092400	-0.49515300	0.04500900
O	0.22735400	0.30976800	0.50469200
H	-0.46904400	-2.59218100	0.43314000
C	2.63480100	0.49323700	0.28107500
H	2.61457600	1.41794100	-0.30085900
H	2.74407600	0.76704700	1.33254400
H	3.50662800	-0.08241300	-0.02323100
H	1.95883800	-2.17282400	-0.77500000
O	-1.33428100	0.20986400	-1.09520000
H	-2.18237600	-0.13928500	-1.38747300
H	-0.68812400	-2.19483400	-1.26816100
O	-0.50143500	2.55061300	-0.13185300
H	0.11546800	3.24616100	-0.40272000
H	-0.03467300	1.64083100	0.20854400
H	-1.04813500	2.25873000	-0.88795900
C	-1.93263400	-0.52951200	1.12229100
H	-2.27783400	0.47937500	1.35303000
H	-2.78442100	-1.12467300	0.78967200
H	-1.52624900	-0.98568900	2.02420600

TS(9-2)_gas

0 1			
C	-1.65244100	-0.26484200	-0.07219200
C	-0.96140000	-1.04939400	-0.89173500
C	0.34700000	-0.41888300	-1.14219600
C	0.25066400	0.79140800	-0.37034100
O	-0.92648400	0.90982200	0.18507700
H	0.67373200	-0.26057400	-2.17232800
C	-2.94846000	-0.35116100	0.61335600
H	-2.81591100	-0.35752900	1.69726500
H	-3.58502800	0.50053900	0.36338100
H	-3.46132300	-1.26607000	0.32112000
H	-1.28588800	-2.01283600	-1.25054400
O	1.22679800	0.01576600	1.48162100
H	1.75433900	0.64471400	1.97446500
H	1.27799400	-1.04042000	-0.69294400
O	2.48118300	-1.43944800	0.08129200
H	1.92171000	-0.72524700	0.94501000
H	2.48389200	-2.36277300	0.33393500
C	1.10409200	1.98241600	-0.46744400
H	0.99471800	2.61138000	0.41349500
H	2.14328300	1.67955700	-0.58541800
H	0.80976900	2.56287300	-1.34803400

TS(11-12)-cis_gas

0 1			
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C	-1.19108800	0.00827300	-0.08750000
C	-0.66410600	-0.41659600	1.27821500
C	0.73612200	0.15626300	1.36436500
C	1.38798200	-0.10588400	0.02411800
O	1.57829800	-1.34580200	-0.32529300
H	0.72043800	1.22737900	1.58355900
H	-1.31908900	-0.07897600	2.08224500
H	1.33855300	-0.33460100	2.13169800
O	-0.08011900	-0.04970000	-0.97510100
H	0.50293100	-1.10232500	-0.92105000
H	-0.63228500	-1.50756600	1.30122800
C	2.30601400	0.93657000	-0.51718000
H	3.22511000	0.91284000	0.07533600
H	2.55915000	0.70780600	-1.55076000
H	1.87495300	1.93542100	-0.44479000
O	-2.15840500	-0.91187700	-0.47919600
H	-2.52108900	-0.63855900	-1.32656500
C	-1.72436000	1.42209400	-0.11402800
H	-2.02344900	1.68517700	-1.13122700
H	-2.58664500	1.51256900	0.54792000
H	-0.96013700	2.13554900	0.20118900

TS(11-12)-trans_gas

O 1			
C	1.17913700	-0.06668000	-0.09438300
C	0.66292500	-0.01353700	1.33680200
C	-0.76571300	-0.52085900	1.26049200
C	-1.40228600	0.14251700	0.06507500
O	-1.51474900	1.43950600	0.06775900
H	-0.78709500	-1.60670100	1.15221400
C	2.36988800	0.82572300	-0.34700100
H	2.69336100	0.73572200	-1.38600300
H	2.11770200	1.86976700	-0.15352400
H	3.19514400	0.53377000	0.30386600
O	1.47797300	-1.41104400	-0.36247300
H	1.29267300	-0.61214500	1.99500200
H	-1.34764300	-0.24598200	2.14332800
H	1.63502500	-1.49518000	-1.30730200
O	0.11084600	0.31811800	-0.92702400
H	-0.45882200	1.32411100	-0.56785900
H	0.68064100	1.02074700	1.68723900
C	-2.34655700	-0.65818700	-0.76081500
H	-3.28036000	-0.75981700	-0.19994800
H	-2.56313900	-0.13617600	-1.69120300
H	-1.95440800	-1.65461800	-0.96292800

TS(12-4)-cis_gas

O 1			
C	1.23756600	0.05664700	-0.05887000
C	0.77889000	0.22310600	1.38251800
C	-0.72778100	0.09844100	1.27899900
C	-0.95466500	-0.56847200	0.04021600
H	-1.29627600	-0.25487300	2.13408800
H	1.11686900	1.18940000	1.75545700
H	-1.25910200	1.10437600	0.84200900
H	1.21515700	-0.55891000	2.00970200
C	-2.13647000	-1.33230900	-0.37917600
H	-1.98823100	-2.38184600	-0.09937000
H	-3.02106500	-0.94377100	0.11730100
H	-2.26752500	-1.27413000	-1.45708500
O	-1.95824500	1.43950300	-0.36693700
H	-2.16948400	2.17670900	-0.94281900
O	0.10873100	-0.64782300	-0.70623500
C	2.44816200	-0.80573500	-0.28437500
H	2.65553700	-0.89804200	-1.35261500
H	3.30883100	-0.34230600	0.19896600

H	2.30248600	-1.80375200	0.12936600
O	1.35811300	1.30115900	-0.63035500
H	1.45979400	1.21435500	-1.58265100

TS(12-4)-trans_gas

O 1			
C	1.24478000	-0.03924400	-0.04802600
C	0.77468200	-0.09385300	1.39700600
C	-0.73479200	-0.15970300	1.27952100
C	-0.96557700	-0.62996300	-0.05225600
H	-1.30560800	-0.65895500	2.05870100
H	1.12624600	0.78299600	1.94056100
H	-1.21558200	0.90466900	1.07963300
H	1.19774500	-0.98436600	1.86751400
C	-2.21732400	-1.17046500	-0.59319200
H	-2.21912300	-2.25747600	-0.45876700
H	-3.05985400	-0.73996600	-0.05786900
H	-2.30128300	-0.94866900	-1.65448400
O	-1.67244500	1.70743800	-0.10956900
H	-2.16484900	2.48196600	-0.38462800
O	0.07851700	-0.63463000	-0.79839800
O	2.31483800	-0.86936400	-0.23851400
H	2.73826700	-0.66353300	-1.07712800
C	1.41293200	1.33563300	-0.62325300
H	2.22506400	1.84654400	-0.10369600
H	1.65245000	1.26848600	-1.68811100
H	0.47103700	1.88632800	-0.50868800

TS(13-14)-cis_gas

O 1			
C	-1.31162600	0.05200200	0.04578000
C	-0.95630400	-0.88294000	-1.11300500
C	0.26870200	-1.64842900	-0.66519700
C	1.19174400	-0.59267500	-0.10014400
O	1.68231600	0.23272900	-0.96091000
H	0.01993700	-2.38778700	0.10126400
H	-1.80182100	-1.52195100	-1.37079200
H	0.77199000	-2.15824700	-1.48827300
H	0.33042700	1.32341200	0.59794100
H	-0.70709800	-0.28419000	-1.99272000
O	1.03451700	2.24763700	0.06208000
H	1.56840500	1.39826200	-0.49856200
H	1.61310800	2.75251800	0.63311100
C	2.06466100	-0.98036100	1.05760400
H	2.87114600	-1.60998000	0.67468100
H	2.51689600	-0.09094600	1.49903400
H	1.51531700	-1.52748800	1.82288000
C	-2.29545300	-0.54784300	1.01481000
H	-2.43348800	0.12779200	1.85861000
H	-3.25595900	-0.70302600	0.52249300
H	-1.92471700	-1.50404100	1.38721500
O	-1.84400700	1.26441100	-0.37360900
H	-1.24289800	1.68205400	-1.00002700
O	-0.07427500	0.26836000	0.74919700

TS(13-14)-trans_gas

O 1			
C	1.31478100	-0.02907900	-0.08606300
C	0.92794800	-0.81040600	1.15815400
C	-0.31722600	-1.57615100	0.75751100
C	-1.23426200	-0.56062700	0.12340900
O	-1.77335100	0.28530100	0.92712800
H	-0.06856300	-2.36905900	0.04983900

C	2.17238000	1.18268000	0.19309400
H	2.41612900	1.69698600	-0.73988900
H	1.65156600	1.88310500	0.84827100
H	3.10269000	0.87203700	0.67020000
O	1.97573000	-0.93339400	-0.93444900
H	1.74856000	-1.45129600	1.48098300
H	-0.83049200	-2.01178200	1.61646000
H	2.06891100	-0.51699300	-1.79541900
O	0.10748700	0.35888000	-0.70231000
H	-0.30825200	1.44256600	-0.46826800
H	0.68926300	-0.11005100	1.96211400
O	-1.02609500	2.30864000	-0.00199800
H	-1.60881700	1.42416400	0.51171300
H	-1.55551700	2.77045300	-0.65294200
C	-2.01314600	-0.96839000	-1.08877600
H	-2.83575900	-1.60945500	-0.76108700
H	-2.44595400	-0.09056300	-1.57086000
H	-1.39677200	-1.51369100	-1.80205300

TS(15-16)-cis_gas

1 1			
C	0.96968300	-0.99035400	-0.09638500
C	-0.24362800	-1.72020100	-0.55384100
C	-1.24141400	-0.69532000	-1.06496500
C	-1.42819400	0.35763600	0.01800300
O	-0.11921900	0.45062400	0.68296300
H	-2.19531000	-1.15460100	-1.32307100
C	1.69651700	-1.37429500	1.12932200
H	2.41416100	-0.61080400	1.43033300
H	1.01054700	-1.57940100	1.94749200
H	2.24992900	-2.29151500	0.90204700
H	-0.64690900	-2.30934300	0.27147400
H	-0.85734200	-0.20380500	-1.96074600
H	0.05648200	-2.41115300	-1.34571600
O	1.60237800	-0.38382900	-1.05037900
H	2.32452400	0.18375700	-0.71730700
O	2.27124300	1.98868300	0.07708700
H	2.32767500	2.66899800	-0.60123300
H	2.77547900	2.33044800	0.82127800
H	0.32841500	1.26804500	0.39913600
C	-2.42201800	-0.01960400	1.08161900
H	-2.44644500	0.74004900	1.86531500
H	-3.41458800	-0.11712000	0.64109900
H	-2.15515000	-0.96862700	1.54855800
O	-1.69787900	1.56632600	-0.58048400
H	-2.20932700	2.13346600	0.00532300

TS(15-16)-cis_sol

1 1			
C	1.06340200	-0.93879300	-0.09165300
C	-0.10470900	-1.77407700	-0.47329100
C	-1.18483100	-0.84889700	-1.00222100
C	-1.40129800	0.26180600	0.02063800
O	-0.13152700	0.40296900	0.72024500
H	-2.11438300	-1.38528200	-1.18892900
C	1.87997500	-1.23214000	1.09872500
H	2.52321500	-0.39388300	1.36442600
H	1.25610200	-1.51083600	1.94324500
H	2.51853200	-2.08254600	0.84121200
H	-0.43913100	-2.34537800	0.39340100
H	-0.86600400	-0.39575200	-1.94202200
H	0.22080500	-2.48345000	-1.23750700
O	1.58612700	-0.28732200	-1.08225500
H	2.26879400	0.34761800	-0.79034100
O	1.89683200	2.14915000	0.06675300
H	1.83285800	2.83708500	-0.60231300

H	2.38916500	2.54081500	0.79402000
H	0.30613900	1.24633600	0.47804200
C	-2.43643000	-0.06565600	1.06277200
H	-2.49391200	0.73585800	1.80157600
H	-3.40974500	-0.19078600	0.58839200
H	-2.17889200	-0.98861600	1.58338600
O	-1.67630400	1.43426300	-0.66007400
H	-2.11122400	2.06288200	-0.07376600

TS(15-16)-trans_gas

1 1			
C	1.01507400	-0.96866700	-0.10754800
C	-0.16351600	-1.70931100	-0.63303900
C	-1.19745700	-0.69258200	-1.09460400
C	-1.41411300	0.24942300	0.07368100
O	-0.07306200	0.48088700	0.61083700
H	-2.13550700	-1.16915800	-1.37596200
C	1.68208400	-1.35787200	1.14989000
H	2.37808500	-0.59025400	1.49191300
H	0.95124800	-1.56624900	1.92766800
H	2.24898200	-2.27297700	0.95017400
H	-0.57190800	-2.35175900	0.14658500
H	-0.82415000	-0.13334700	-1.95542900
H	0.17773300	-2.33464500	-1.46118100
O	-2.10100500	-0.44895700	1.03665800
H	-2.36338000	0.12905400	1.75982800
O	1.70372000	-0.36576100	-1.03348200
H	2.44837200	0.14088900	-0.67060200
C	-2.04819400	1.56596900	-0.28489800
H	-3.03682800	1.38330500	-0.70576800
H	-2.16018100	2.19476800	0.60085800
H	-1.45681000	2.10495200	-1.02760900
O	2.00283900	2.22533300	0.04421200
H	2.14331600	2.84258300	-0.67995400
H	2.34895800	2.66790700	0.82498900
H	0.34886400	1.30115000	0.28779400

TS(15-16)-trans_sol

1 1			
C	1.08181000	-0.90398300	-0.11707900
C	-0.06306000	-1.77159400	-0.49908800
C	-1.17808400	-0.86553700	-0.99386200
C	-1.40886900	0.18008100	0.08589900
O	-0.11061700	0.39247500	0.69657700
H	-2.09851400	-1.41540100	-1.18255800
C	1.92362200	-1.18668700	1.06011400
H	2.53406700	-0.32556400	1.33151400
H	1.31950700	-1.49939200	1.90713600
H	2.59357300	-2.00620000	0.78505500
H	-0.37702800	-2.35938100	0.36344100
H	-0.87940100	-0.37525800	-1.92142800
H	0.27485400	-2.45702700	-1.27896600
O	-2.21869100	-0.39552700	1.04970000
H	-2.41033500	0.24897300	1.73911900
O	1.58594400	-0.24102600	-1.11499700
H	2.26555900	0.39771100	-0.83071700
C	-1.94576100	1.48955100	-0.42763300
H	-2.90361700	1.31683600	-0.91806600
H	-2.09445600	2.19340800	0.39360200
H	-1.26061500	1.93043800	-1.15440000
O	1.78465400	2.22963300	0.05414700
H	1.69971900	2.90324900	-0.62724300
H	2.25013600	2.65415400	0.78074200
H	0.29828200	1.25803000	0.47924900

TS(16-18)-cis_gas

1	1			
C		-0.97249700	-0.64597700	-0.05352000
C		-0.17964600	-1.57459900	0.84863700
C		0.99652100	-0.71651200	1.26249200
C		1.31975700	0.06085500	0.00417100
O		-0.01544400	0.22076400	-0.63111100
H		1.85658100	-1.28509600	1.61268000
C		-1.78943700	-1.30538700	-1.12449200
H		-2.31211300	-0.56099900	-1.72659500
H		-1.13987400	-1.88933400	-1.77694900
H		-2.52516300	-1.98115200	-0.68307200
H		0.14128700	-2.44792300	0.27551400
H		0.71566900	-0.00532100	2.04210200
H		-0.78475200	-1.93300900	1.68120900
O		-1.81069300	0.22158000	0.74972700
H		-2.56575800	-0.26185200	1.09824200
O		-1.05436000	2.43724300	-0.09355300
H		-1.49536300	2.99269700	-0.75062700
H		-1.68218400	1.80149100	0.37812800
H		-0.42052700	1.73071100	-0.49739400
C		2.20604500	-0.64937200	-0.97942700
H		2.26710000	-0.08608200	-1.91294600
H		3.20687500	-0.76376700	-0.56072200
H		1.81590900	-1.64074800	-1.21225500
O		1.75699400	1.33203700	0.30130300
H		2.42586900	1.62334500	-0.32541400

TS(16-18)-cis_sol

1	1			
C		0.95182400	-0.66909000	0.05155500
C		0.08011900	-1.78085700	-0.49128700
C		-1.12712200	-1.02622400	-1.00451800
C		-1.31490200	0.09836600	-0.00120200
O		0.02489300	0.25358300	0.60716500
H		-2.02521900	-1.63699900	-1.08069100
C		1.95354500	-1.06530400	1.09591000
H		2.49353800	-0.19098400	1.46183500
H		1.44910500	-1.54824700	1.93232200
H		2.67364600	-1.76715700	0.67196700
H		-0.18498400	-2.45625300	0.32573000
H		-0.92480100	-0.58444800	-1.98109400
H		0.60109700	-2.35982800	-1.25305200
O		1.57931700	0.04814600	-1.01568100
H		2.30567200	-0.46884200	-1.37872600
O		1.19860400	2.36996100	0.05461100
H		1.73739500	2.82280600	0.72050500
H		1.76355800	1.83330600	-0.55526400
H		0.59065300	1.61820800	0.45645800
C		-2.26342400	-0.19941200	1.12564800
H		-2.22998300	0.59969300	1.86925100
H		-3.27844600	-0.28556200	0.73732000
H		-1.99373600	-1.13498600	1.61636400
O		-1.62743500	1.26929400	-0.66303900
H		-2.06077100	1.88655900	-0.06401300

TS(16-18)-trans_gas

1	1			
C		0.86374600	-0.69910800	0.03988400
C		-0.03437500	-1.63285100	-0.74552500
C		-1.16872600	-0.72222500	-1.17507300
C		-1.36200000	0.14221000	0.05146100
O		0.02889300	0.32610900	0.52770800
H		-2.08546200	-1.25070900	-1.42722700
C		1.65742400	-1.31408700	1.15265300

H	2.26420700	-0.56228300	1.66162200
H	0.97475700	-1.75938800	1.87643900
H	2.31528800	-2.09883800	0.77341400
H	-0.39969400	-2.41904500	-0.08272800
H	-0.87428400	-0.09850900	-2.02164100
H	0.50127700	-2.10391600	-1.56937600
O	-2.04150600	-0.59587100	0.98959400
H	-2.32015100	-0.04885000	1.73005000
O	1.76399000	0.00182300	-0.88211700
H	2.45753000	-0.58289800	-1.20454400
C	-1.93976100	1.51056300	-0.16597900
H	-2.96520700	1.41829100	-0.52326700
H	-1.95706500	2.07724500	0.76925200
H	-1.36753300	2.06868800	-0.90887800
O	1.55550500	2.24248100	0.02969500
H	2.17212200	2.68709400	0.62638100
H	1.93807000	1.40026400	-0.46502600
H	0.79324300	1.76950900	0.50196600

TS(16-18)-trans_sol

1 1			
C	0.91184500	-0.68862200	0.01961400
C	0.00225000	-1.72438600	-0.61023100
C	-1.17786700	-0.89132400	-1.06961200
C	-1.34062600	0.10373100	0.05972600
O	0.03127600	0.31084300	0.52410000
H	-2.09313900	-1.46034100	-1.21835300
C	1.80615900	-1.17919800	1.12044900
H	2.39677900	-0.35720500	1.52794600
H	1.20384200	-1.61464200	1.91762600
H	2.48636200	-1.94399700	0.74153800
H	-0.30001000	-2.44987500	0.14702300
H	-0.94249400	-0.35844900	-1.99261600
H	0.51289300	-2.25659800	-1.41153900
O	-2.05272000	-0.50997500	1.07745100
H	-2.21863600	0.12084200	1.78572900
O	1.66912900	-0.00415500	-0.98611600
H	2.39141200	-0.56156700	-1.29381700
C	-1.90536100	1.44430100	-0.31493100
H	-2.92296300	1.31653100	-0.68324200
H	-1.93205900	2.10917500	0.55199100
H	-1.30614600	1.90964500	-1.09884600
O	1.39697900	2.33079900	0.03248700
H	1.94893300	2.76916300	0.69771300
H	1.92550400	1.69818900	-0.52595200
H	0.71399700	1.67203200	0.44134200

TS(17-9)-cis_gas

0 1			
C	-1.38072600	-0.39001400	0.07361900
C	-0.58423400	-0.28560300	1.38372200
C	0.52534000	0.71491100	1.13222000
C	0.20325400	1.33354900	-0.10555100
H	0.79101200	1.41164000	1.92661700
C	-2.84765800	-0.10821100	0.18372400
H	-3.29457400	-0.08975400	-0.80937600
H	-3.31157900	-0.91046100	0.75939200
H	-3.03277100	0.83941400	0.69042500
H	-0.18725900	-1.27071300	1.63384200
H	1.56784500	0.12591300	0.96079200
H	3.49300800	-0.53504900	0.62332100
O	2.62672500	-0.89717900	0.80888900
H	-1.24621800	0.02830900	2.19288600
O	-1.14873400	-1.44058500	-0.69386200
H	-0.14386600	-1.57756200	-0.84372200
C	1.02334400	2.35528500	-0.77425600

H	1.74578600	1.80761700	-1.38963500
H	0.42595600	2.98328300	-1.43198800
H	1.57933200	2.95441900	-0.05575400
O	1.35323000	-1.52204100	-1.11725500
H	1.68412600	-2.26918900	-1.61253200
H	2.05401600	-1.29757100	-0.23527400
O	-0.80131200	0.86983100	-0.71900600

TS(17-9)-trans_gas

O 1			
C	-1.47844500	-0.23671800	-0.04418300
C	-0.92076500	-0.45614800	1.35172500
C	0.44807500	0.20230500	1.30995100
C	0.38067900	1.07621900	0.17350800
O	-0.66888300	0.93354000	-0.54314600
H	1.27679500	-0.60141800	1.09846800
C	-1.23420700	-1.34200800	-1.02956900
H	-1.56027300	-1.03318100	-2.02613500
H	-0.16927800	-1.57122200	-1.09167000
H	-1.79717300	-2.22409900	-0.72124300
H	-0.86381600	-1.52248300	1.57373600
H	0.78719200	0.71391900	2.21096700
H	-1.59288700	0.01285700	2.07237500
O	1.74000800	-0.32702400	-1.33283700
H	2.48898200	-0.05973800	-1.86393400
O	-2.78082800	0.17445900	0.01655500
H	-3.18562100	0.10801700	-0.85345400
C	1.26384200	2.21817800	-0.09192800
H	2.27396000	1.98775000	0.23994700
H	1.25987900	2.47377400	-1.14816900
H	0.89478000	3.07353500	0.48456600
O	2.35652800	-1.60447000	0.60188500
H	2.14450500	-2.53733700	0.59103300
H	2.11327700	-1.00338500	-0.52316900

TS(21-30)-cis_gas

O 1			
C	-1.20747600	-0.16735800	-0.02018200
C	-0.68028900	-1.58980300	-0.10793300
C	0.71211600	-1.52182100	0.48492600
C	1.32263600	-0.23213400	-0.08170400
O	1.72212800	-0.30884300	-1.35592800
H	0.67320500	-1.49563100	1.57949200
H	-1.35163700	-2.28712500	0.39447300
H	1.34409800	-2.35916300	0.18889600
H	0.50214800	0.32334500	-1.41864200
H	-0.63296600	-1.86293500	-1.16449800
N	-0.00669100	0.62738300	-0.38096500
C	-0.01197500	2.05158200	-0.12276200
H	0.87612000	2.49044400	-0.57835500
H	-0.88879100	2.51374300	-0.58319300
H	-0.01022600	2.28081400	0.94582900
C	2.27579900	0.45191400	0.86639000
H	1.82421200	0.68412800	1.83583900
H	3.11228400	-0.22864100	1.03867100
H	2.67929200	1.36079200	0.41890800
C	-1.71760600	0.18095600	1.36243000
H	-2.10608400	1.20227300	1.40131100
H	-2.52754800	-0.50091500	1.62434700
H	-0.93434200	0.09243200	2.11743600
O	-2.21240500	0.00678300	-0.97703200
H	-2.74994200	0.77122400	-0.75706400

TS(21-30)-trans_gas

O 1			
C	-1.19345500	-0.16924000	0.05531900
C	-0.67106600	-1.59088500	-0.05393000
C	0.74577200	-1.51057500	0.47781700
C	1.32648500	-0.23366100	-0.13491400
O	1.65746900	-0.31383800	-1.42825100
H	0.73833100	-1.45581000	1.56985000
H	-1.32129800	-2.26978300	0.49799900
H	1.36612400	-2.35279600	0.17082800
H	0.44499900	0.34720700	-1.42931500
H	-0.66537500	-1.88827200	-1.10548600
N	-0.02702600	0.63274800	-0.37744900
C	-0.02503600	2.04438200	-0.05202300
H	0.83952900	2.51057400	-0.52431500
H	-0.92376100	2.52998300	-0.43973000
H	0.03367700	2.20454600	1.02687600
C	2.31115900	0.46674500	0.76650500
H	1.88016700	0.71293000	1.74121400
H	3.15084300	-0.21220000	0.92932800
H	2.70393900	1.36618200	0.29131500
C	-2.40496900	0.10445900	-0.80055000
H	-3.20951800	-0.57431600	-0.51381200
H	-2.76541500	1.12979700	-0.67574400
H	-2.17498200	-0.05074200	-1.85538200
O	-1.46209300	0.07000300	1.41577900
H	-2.00442500	0.85678900	1.50894500

TS(22-23)_gas

O 1			
C	-1.28617200	-0.34621400	-0.04544600
C	-0.77520100	-1.52948100	-0.36009100
C	0.70934000	-1.55084100	-0.38938800
C	1.15383000	-0.18433100	0.16276500
H	1.12570600	-2.31453200	0.27357700
C	-2.70710500	0.04147400	0.11031900
H	-3.00439800	0.80598000	-0.61304500
H	-3.35174900	-0.82449500	-0.03487000
H	-2.89778800	0.44916900	1.10746200
H	-1.39376700	-2.39968400	-0.54159400
H	1.09419400	-1.74502700	-1.39686000
H	0.18107400	0.52649700	1.34212800
O	1.39965700	-0.13864000	1.47064400
N	-0.26383700	0.61577500	0.24781300
C	-0.40890200	1.94501400	-0.32008900
H	0.42895900	2.56308200	0.00012400
H	-0.43161800	1.90267500	-1.41250900
H	-1.33068500	2.40856400	0.03368600
C	2.14446600	0.52180200	-0.72945100
H	2.42686600	1.48683100	-0.30787400
H	3.04426700	-0.09565900	-0.77001800
H	1.77699400	0.65075700	-1.75177400

TS(23-20)_gas

O 1			
C	-1.34175500	-0.33043300	-0.14017100
C	-0.85227500	-1.55543200	-0.34819100
C	0.60676500	-1.45628700	-0.50391600
C	0.86349800	-0.02810400	-0.48980300
H	1.13954700	-2.06270200	-1.23251500
C	-2.70626200	0.11502600	0.20876700
H	-2.73634800	0.59548300	1.19065300
H	-3.11270600	0.82274400	-0.51922600
H	-3.36860400	-0.74889200	0.24131500
H	-1.42455900	-2.46865600	-0.30696700

O	1.51711100	-0.50792900	1.64555700
H	1.84085500	-0.28236800	2.51939700
H	1.08080000	-1.61047400	0.55298900
C	2.13390600	0.63759900	-0.82230400
H	2.95031000	-0.06764300	-0.68644000
H	2.11968600	0.96999000	-1.86758700
H	2.32534900	1.49414900	-0.17986100
N	-0.28148300	0.60590500	-0.28091900
C	-0.35125300	1.98137800	0.14742600
H	0.01656700	2.04991500	1.17684900
H	0.26367600	2.60986100	-0.49465300
H	-1.37682400	2.33819700	0.09717200

TS(24-25)_gas

O 1			
C	1.40216000	-0.20676800	-0.30510500
C	0.96518600	-1.09599000	-1.18487800
C	-0.52001700	-1.17727200	-1.21428300
C	-0.98516800	-0.53008000	0.10725300
H	-0.93192200	-0.59878800	-2.04818500
C	2.78474900	0.23316700	-0.01689700
H	3.06642800	0.06093900	1.02540700
H	3.48526600	-0.31141700	-0.64891000
H	2.90852400	1.30247800	-0.21298900
H	1.62458200	-1.65307900	-1.83717000
H	-0.07738800	1.31097900	-0.27155300
H	-0.90340100	-2.19696400	-1.29904200
H	-1.78212100	1.14204600	-0.56718600
O	-1.01871100	1.99585600	-1.10331900
H	-1.27464000	2.89997500	-0.92800700
O	-2.07924400	0.21890300	0.06014900
N	0.29173400	0.44418700	0.35032200
C	0.46389500	0.90933100	1.72122700
H	0.82126200	0.11082000	2.37254000
H	1.16942000	1.74009700	1.75215000
H	-0.50497300	1.26406400	2.07456800
C	-1.04391400	-1.54508500	1.22521700
H	-1.30353700	-1.06990800	2.17098400
H	-1.84409400	-2.24527700	0.98237500
H	-0.11325900	-2.10716200	1.33292600

TS(26-20)_gas

O 1			
C	-1.52969400	-0.67421400	-0.08023800
C	-0.74458700	-1.64758700	-0.53870100
C	0.52168800	-1.05568300	-1.01004700
C	0.33319700	0.37506400	-0.77825500
H	0.82367500	-1.27920800	-2.03785200
C	-2.84189900	-0.72343700	0.59394000
H	-2.78137100	-0.31996600	1.60821900
H	-3.60920900	-0.16050600	0.05571700
H	-3.17170700	-1.75874100	0.66393500
H	-0.97806000	-2.70001800	-0.51298000
O	1.17128400	0.41011600	1.56452200
H	1.56683800	1.12543400	2.06213800
H	1.42389400	-1.33309700	-0.39011000
O	2.90066000	-0.92369400	0.56116200
H	2.13044400	-0.29574100	1.14590500
H	3.32404800	-1.54003900	1.15597400
N	-0.87032200	0.57544100	-0.29658800
C	-1.31508100	1.81774100	0.29042000
H	-2.40056700	1.83818000	0.34314700
H	-0.87924300	1.88731100	1.29099900
H	-0.98314000	2.65904300	-0.31326200
C	1.30324900	1.40710600	-1.17031600
H	1.18243500	1.63806100	-2.23492900

H	1.20181600	2.32076900	-0.59077200
H	2.30561500	1.00512400	-1.01629900

TS(28-29)_gas

1	1		
C	1.40145000	-0.31984200	-0.20756600
C	1.07971500	-1.45429700	-0.81028900
C	-0.34752200	-1.80450200	-0.55581000
C	-0.90288300	-0.49815700	-0.01070300
H	-0.44749300	-2.60697600	0.18385100
C	2.69845100	0.38666900	-0.14844800
H	2.59757300	1.43711700	-0.43898300
H	3.13113700	0.37114500	0.85469500
H	3.41429500	-0.08380000	-0.82017100
H	1.76169900	-2.05320400	-1.39554200
O	-1.35521400	0.29480200	-1.18568200
H	-2.19798000	-0.02789700	-1.52373000
H	-0.90001100	-2.12487900	-1.44224700
O	-0.65492500	2.45411100	-0.55636000
H	-0.20654100	3.06993000	-1.14788100
H	-0.00992900	1.87102200	-0.01886900
H	-1.14050700	1.54943600	-1.03249700
C	-2.06133800	-0.61235500	0.93547500
H	-2.42860400	0.36899200	1.24277700
H	-2.87652100	-1.14891500	0.44434300
H	-1.79234200	-1.18424000	1.82290700
N	0.25958900	0.26351000	0.48252000
C	0.44125600	0.27666300	1.94336900
H	-0.39980900	0.76437000	2.43256800
H	0.56780100	-0.73373000	2.34649200
H	1.33643900	0.85067500	2.17481600

TS(28-29)_sol

1	1		
C	1.41420900	-0.28208100	-0.20319800
C	1.13681000	-1.43072800	-0.80508900
C	-0.27916500	-1.82773800	-0.55389500
C	-0.88018600	-0.53494100	-0.01681800
H	-0.35548600	-2.63018900	0.18811400
C	2.68567000	0.47120200	-0.15473100
H	2.53744600	1.50958200	-0.46473100
H	3.11076800	0.49381900	0.85152300
H	3.41993600	0.01217800	-0.81509500
H	1.84173100	-2.00120400	-1.39226600
O	-1.35793500	0.23336600	-1.17395300
H	-2.19406900	-0.11676100	-1.50216000
H	-0.82087900	-2.16216300	-1.44086000
O	-0.78830400	2.47001800	-0.55531300
H	-0.38630400	3.06630400	-1.20191300
H	-0.08429700	1.98345900	-0.02842200
H	-1.21065800	1.56600800	-0.99989600
C	-2.02095100	-0.69992300	0.94483200
H	-2.42666000	0.26607200	1.25040300
H	-2.81491600	-1.26932700	0.45773700
H	-1.71508100	-1.25694100	1.82957200
N	0.26006300	0.26317600	0.47534800
C	0.43775600	0.31248100	1.93141500
H	-0.42354100	0.77696100	2.40739900
H	0.59888500	-0.68405800	2.35848700
H	1.30774500	0.92731800	2.15370800

TS(30-23)-cis_gas

0	1		
C	1.24457500	-0.18659200	0.00362000
C	0.76001500	-1.50972900	-0.59122100
C	-0.74501600	-1.36355300	-0.67715400

C	-0.99104400	0.04484300	-0.62301400
H	-1.28103400	-1.92665700	-1.43687700
H	1.08742400	-2.32685500	0.05090000
H	-1.26734000	-1.51633200	0.39479200
H	1.20649800	-1.65428300	-1.57903800
C	-2.26949000	0.69509600	-0.96551000
H	-2.18405400	1.15924800	-1.95528500
H	-3.05881700	-0.05183900	-0.98594600
H	-2.54586000	1.45602200	-0.23985400
O	-1.89283700	-0.69431300	1.47235300
H	-2.15431600	-0.74961900	2.39184000
C	2.49236000	0.35820500	-0.65348500
H	2.81557300	1.29615000	-0.19295200
H	3.29880600	-0.36756600	-0.53815800
H	2.32902400	0.53659600	-1.71691700
O	1.43974400	-0.36492900	1.37265500
H	1.88143100	0.39901100	1.75136200
N	0.08489500	0.71597300	-0.25498400
C	0.00188700	1.99887200	0.40139900
H	-0.57406900	2.70321900	-0.19662600
H	-0.48235700	1.86641300	1.37646200
H	0.99985800	2.41576500	0.53330200

TS(30-23)-trans_gas

O 1			
C	1.21984600	-0.14323100	-0.12850800
C	0.72332900	-1.22088800	-1.08927400
C	-0.78744700	-1.09972700	-1.04074000
C	-1.02668500	0.24545700	-0.59807500
H	-1.36322700	-1.42422900	-1.90462400
H	1.09163100	-2.20218200	-0.78997700
H	-1.21753400	-1.58511800	-0.04630700
H	1.11921900	-0.99365000	-2.08250800
C	-2.34085600	0.91254000	-0.58886500
H	-2.32242000	1.80614100	-1.22015600
H	-3.10480300	0.23028900	-0.95409800
H	-2.60415400	1.20352600	0.42778400
O	-1.53156000	-1.28088800	1.43369400
H	-2.01614700	-1.74028700	2.11900700
O	2.32872300	0.51794100	-0.66509800
H	2.95645700	0.70819400	0.03540400
C	1.47397800	-0.64652200	1.27109100
H	2.25816600	-1.40551200	1.24000500
H	1.80396300	0.16663600	1.92631700
H	0.54146800	-1.07319300	1.67032600
N	0.05328100	0.79696900	-0.11303900
C	0.05806900	1.96091500	0.73556000
H	-0.58296400	2.73732200	0.32104100
H	-0.30276200	1.69151000	1.73426900
H	1.07142200	2.35407400	0.79888900

TS(31-32)-cis_gas

O 1			
C	1.25914500	-0.19133400	0.21659700
C	0.67799200	0.17387700	1.57952100
C	-0.68860700	-0.46715000	1.60086400
C	-1.30035000	-0.14980700	0.23362600
O	-1.83747200	1.08070800	0.14838400
H	-0.61016200	-1.55040100	1.74355500
H	1.34180600	-0.16734600	2.37466600
H	-1.34858900	-0.07252400	2.37319700
H	0.02047200	0.85986700	-0.99155200
H	0.59337300	1.26031400	1.64571800
O	0.07138900	2.43331200	-0.45544400
H	-1.05309300	1.84374900	-0.04697500
H	-0.08747400	3.24251900	-0.93693900

C	-2.28866300	-1.19926700	-0.20961200
H	-3.09975600	-1.20046300	0.52037600
H	-2.71902100	-0.94929100	-1.17963500
H	-1.85778200	-2.20254300	-0.23853500
N	0.00339100	-0.14981000	-0.68836200
C	0.02978800	-0.97929600	-1.89059900
H	0.94729000	-0.77123400	-2.44215900
H	-0.01493000	-2.03870200	-1.64528500
H	-0.82169200	-0.72136500	-2.51822900
C	1.89918300	-1.55587200	0.21596500
H	2.29930600	-1.80842200	-0.76564600
H	2.73330600	-1.53233100	0.91701400
H	1.20214500	-2.33362800	0.53380800
O	2.16674900	0.71293100	-0.28130600
H	1.71480900	1.58796500	-0.29609300

TS(31-32)-trans_gas

O 1			
C	1.25914500	-0.19133400	0.21659700
C	0.67799200	0.17387700	1.57952100
C	-0.68860700	-0.46715000	1.60086400
C	-1.30035000	-0.14980700	0.23362600
O	-1.83747200	1.08070800	0.14838400
H	-0.61016200	-1.55040100	1.74355500
H	1.34180600	-0.16734600	2.37466600
H	-1.34858900	-0.07252400	2.37319700
H	0.02047200	0.85986700	-0.99155200
H	0.59337300	1.26031400	1.64571800
O	0.07138900	2.43331200	-0.45544400
H	-1.05309300	1.84374900	-0.04697500
H	-0.08747400	3.24251900	-0.93693900
C	-2.28866300	-1.19926700	-0.20961200
H	-3.09975600	-1.20046300	0.52037600
H	-2.71902100	-0.94929100	-1.17963500
H	-1.85778200	-2.20254300	-0.23853500
N	0.00339100	-0.14981000	-0.68836200
C	0.02978800	-0.97929600	-1.89059900
H	0.94729000	-0.77123400	-2.44215900
H	-0.01493000	-2.03870200	-1.64528500
H	-0.82169200	-0.72136500	-2.51822900
C	1.89918300	-1.55587200	0.21596500
H	2.29930600	-1.80842200	-0.76564600
H	2.73330600	-1.53233100	0.91701400
H	1.20214500	-2.33362800	0.53380800
O	2.16674900	0.71293100	-0.28130600
H	1.71480900	1.58796500	-0.29609300

TS(33-26)-cis_gas

O 1			
C	1.28194300	-0.54319600	-0.06633000
C	0.56610200	-1.19052300	-1.26672900
C	-0.64519100	-0.31830500	-1.53119900
C	-0.39316700	0.89672900	-0.82810200
H	-0.98344000	-0.20030200	-2.55972500
C	2.77715500	-0.46586400	-0.24575000
H	3.25550700	-0.00477200	0.61912400
H	3.16577200	-1.48141200	-0.33369200
H	3.03752600	0.08788000	-1.14877500
H	0.29804700	-2.21561100	-1.00742300
H	-1.60914600	-0.77524400	-0.93864000
H	-3.46499000	-1.26365700	-0.20854000
O	-2.54042900	-1.41299700	-0.01417400
N	0.66218300	0.83275300	-0.05771200
C	0.94076600	1.74808400	1.02823700
H	0.22023800	1.58481200	1.83424500
H	1.94330800	1.56011300	1.40484500

H	0.88375000	2.77928500	0.68120200
H	1.23897100	-1.22130300	-2.12745900
O	1.03539800	-1.13805100	1.14964600
H	0.09752600	-0.98130700	1.42693500
C	-1.32285600	2.03940200	-0.79762700
H	-0.80829000	3.00086300	-0.81055500
H	-2.02619000	1.98701400	-1.62602200
H	-1.88603400	1.96898800	0.14012000
O	-1.42478300	-0.24853500	1.80862000
H	-1.75457800	-0.48979900	2.67319600
H	-2.03325700	-0.76610900	1.07741100

TS(33-26)-trans_gas

O 1			
C	-1.42096800	-0.42044700	-0.09833900
C	-1.00104200	-1.27567500	1.10161200
C	0.35379700	-0.71242000	1.49072900
C	0.35672000	0.63825400	0.98682800
H	0.66187400	-0.78414300	2.55006900
H	-0.97733300	-2.33952900	0.84024400
H	1.24232300	-1.23673600	0.91590100
H	2.75043600	0.64542600	-1.92165100
O	1.93091200	0.31806400	-1.53409800
N	-0.60388600	0.83493800	0.13095600
C	-0.66682100	1.92684700	-0.82671700
H	-0.57480500	2.88893400	-0.31461900
H	0.16880400	1.77970900	-1.52937000
H	-1.63817500	1.88303600	-1.32670800
H	-1.73497800	-1.15148400	1.91545700
C	1.42321700	1.61773700	1.24984700
H	2.38118200	1.08591300	1.21549200
H	1.45357600	2.42471200	0.51617700
H	1.29957300	2.02894600	2.26441300
O	2.42998000	-1.62191700	-0.15913000
H	2.42585000	-2.40155800	-0.73128200
H	2.18217100	-0.65863100	-0.84186000
C	-1.05473100	-1.00880300	-1.44040800
H	-1.65250800	-1.91477900	-1.59427200
H	-1.27928000	-0.30354700	-2.24843100
H	0.01773900	-1.22885200	-1.48981300
O	-2.77941100	-0.10256100	-0.14086900
H	-3.09213800	0.09637200	0.75502500

TS(34-35)-cis_gas

1 1			
C	1.08964300	-0.53706800	-0.11835100
C	0.50931600	-1.06900100	-1.42658300
C	-0.79136200	-0.31374900	-1.60377800
C	-1.29284500	-0.12957800	-0.17525900
H	-1.51411500	-0.83375800	-2.23185800
C	1.84012200	-1.58470700	0.66378200
H	2.32481400	-1.16857400	1.54677900
H	1.17083000	-2.38915400	0.97322400
H	2.60888500	-2.03103400	0.02824900
H	0.32759800	-2.14132500	-1.32091000
H	-0.62206900	0.67475000	-2.03873600
H	1.21144300	-0.94593000	-2.25166900
O	2.02421300	0.56750800	-0.37841700
H	2.85633900	0.24778100	-0.73938800
O	0.58870300	2.54662500	-0.19072200
H	0.71707000	3.29488400	0.40696900
H	1.42249600	1.95981800	-0.33721700
H	-0.02670100	1.82137900	0.18828200
C	-2.12017300	-1.29108000	0.32665900

H	-2.41380900	-1.14782400	1.36688900
H	-3.02792200	-1.38854100	-0.27258200
H	-1.57302900	-2.23261800	0.24619600
O	-1.98369300	1.09112400	0.00308800
H	-2.91595100	1.00190300	-0.21090300
N	-0.03450500	0.08157600	0.55815000
C	-0.07878900	0.06352300	2.01288300
H	-0.16090200	-0.94278000	2.43356700
H	0.82385800	0.52894600	2.41427900
H	-0.93655500	0.64895300	2.34407500

TS(34-35)-cis_sol

1 1			
C	1.06489100	-0.57353900	-0.11854600
C	0.46174100	-1.08650800	-1.42526700
C	-0.80512200	-0.27766200	-1.60088400
C	-1.29639700	-0.08222000	-0.17196400
H	-1.55154400	-0.76249500	-2.22943800
C	1.75727100	-1.65798200	0.66911400
H	2.26164100	-1.25819700	1.54854400
H	1.04395000	-2.42177300	0.98286300
H	2.50249400	-2.14188700	0.03419300
H	0.23272700	-2.14912200	-1.31621600
H	-0.59093100	0.70596600	-2.02676600
H	1.17017100	-0.99224700	-2.24814700
O	2.04385000	0.47606700	-0.37629800
H	2.83114200	0.12646600	-0.80506000
O	0.72414600	2.55278700	-0.19288700
H	0.94812700	3.25726100	0.43331900
H	1.51121100	1.91720200	-0.36429100
H	0.08658500	1.87929600	0.21418500
C	-2.14636700	-1.23069200	0.32656100
H	-2.44166700	-1.07694700	1.36483500
H	-3.05054400	-1.31346100	-0.27974700
H	-1.60804800	-2.17760500	0.25413000
O	-1.97853100	1.14599200	0.00120800
H	-2.90567400	1.04730600	-0.23208600
N	-0.03539700	0.09331400	0.55720400
C	-0.07681500	0.07861400	2.00995200
H	-0.20105500	-0.92340200	2.43195800
H	0.84474800	0.50941800	2.40510700
H	-0.90649200	0.70219200	2.34220700

TS(34-35)-trans_gas

1 1			
C	0.99497100	-0.58760000	-0.10240000
C	0.43246200	-0.94922200	-1.47614000
C	-0.83928700	-0.13323900	-1.60870200
C	-1.33218500	-0.05240800	-0.17573700
H	-1.58719900	-0.59740800	-2.24871600
C	1.51309300	-1.77657000	0.65929400
H	2.00306800	-1.49197100	1.58959000
H	0.69153300	-2.45959200	0.87615800
H	2.23492800	-2.31628500	0.04175200
H	0.19971300	-2.01462500	-1.48623900
H	-0.64247100	0.87270100	-1.98870000
H	1.16084700	-0.76884500	-2.26768400
O	2.14785000	0.35155500	-0.23456700
H	2.86724300	-0.03183000	-0.74779000
O	1.03963000	2.42131800	-0.23379900
H	1.29891200	3.15324300	0.33756000
H	1.78501600	1.57684000	-0.33590700
H	0.35529100	1.78166800	0.20165800
N	-0.04953500	0.20863500	0.54663200
C	-0.10582800	0.14474000	2.00431500
H	-0.38081200	-0.84654200	2.37192400

H	0.86446600	0.41606900	2.42258000
H	-0.83574600	0.86676300	2.36979400
C	-2.35009000	1.03147700	0.06787800
H	-3.22254300	0.84338900	-0.55894400
H	-2.68417900	1.05314000	1.10802400
H	-1.96103200	2.01775200	-0.19158300
O	-1.83013200	-1.31460700	0.17453800
H	-2.53788000	-1.24410400	0.81967400

TS(34-35)-trans_sol

1 1			
C	0.96223100	-0.64023900	-0.09889400
C	0.39233400	-0.96815500	-1.48145400
C	-0.85617600	-0.11424700	-1.60691100
C	-1.33099700	0.00390800	-0.17251500
H	-1.62562800	-0.55460500	-2.23898600
C	1.37159200	-1.87000900	0.67077900
H	1.84980200	-1.61667000	1.61626200
H	0.49785300	-2.49379800	0.86128500
H	2.07729900	-2.45005900	0.07259900
H	0.13494100	-2.02723800	-1.51468500
H	-0.62844300	0.88233100	-1.99298000
H	1.12980300	-0.78651200	-2.26286600
O	2.15446500	0.21045100	-0.20010700
H	2.85758600	-0.22035800	-0.69796100
O	1.22494100	2.40743900	-0.26991500
H	1.55840300	3.09697900	0.32078800
H	1.87251500	1.54016200	-0.33325300
H	0.46202200	1.90478200	0.15376700
N	-0.04998600	0.20725100	0.53356100
C	-0.09142700	0.20206500	1.98937200
H	-0.41160100	-0.75803100	2.40463800
H	0.89767100	0.43792900	2.38284800
H	-0.77310100	0.97796800	2.33603800
C	-2.30373100	1.13119100	0.06640000
H	-3.18155400	0.97672700	-0.56162500
H	-2.63665000	1.16653900	1.10578400
H	-1.86779600	2.09842500	-0.18858100
O	-1.91768500	-1.23607600	0.17180100
H	-2.41994800	-1.14692100	0.98709800

TS(36-46)_gas

0 1			
C	-0.94140800	-0.63694400	-0.25970500
C	0.34701800	-1.43882800	-0.43484100
C	1.57308200	-0.98478700	0.33455500
C	2.25492300	0.26031300	-0.12993900
O	1.72981200	1.06777400	-0.87229200
H	1.27744000	-0.78914700	1.37714600
C	-2.10222100	-1.41021700	-0.84234500
H	-2.28828400	-2.30164400	-0.24428300
H	-3.00978700	-0.80435800	-0.82208200
H	-1.89788900	-1.70161900	-1.87807200
H	0.11455500	-2.45421200	-0.10359200
H	2.31865100	-1.78521100	0.38156900
H	0.09784400	0.87947700	-1.10531300
H	0.56504700	-1.50413300	-1.50841300
C	3.63946700	0.48438000	0.38468600
H	4.31918800	-0.22012900	-0.10187000
H	3.96701600	1.50003700	0.17643700
H	3.68833300	0.27946400	1.45568900
H	-1.59756200	1.39858700	-0.67872400
O	-2.28000000	2.03038600	0.05881600
H	-2.05707900	1.30140200	0.85741400

H	-3.21402700	1.96851500	-0.16017900
O	-0.84069200	0.56153800	-1.13418700
S	-1.23634900	-0.16800700	1.47631900

TS(38-39)_gas

O 1			
C	1.45648000	0.24938300	-0.05159800
C	0.66750700	1.33921400	-0.02146700
C	-0.77636300	1.27456500	-0.33953000
C	-1.57910700	0.15319000	0.17253800
H	-1.30554500	2.14509400	0.09172900
C	2.92432000	0.35967300	0.20014700
H	3.21591900	-0.26963500	1.04362700
H	3.48092700	-0.00514800	-0.66576000
H	3.22504700	1.38915900	0.40820200
H	1.09502300	2.31980200	0.16266700
H	-0.97822300	1.35088900	-1.41733100
H	-0.33252100	-0.74336600	1.21212400
O	-1.31194600	-0.48182800	1.25420000
S	0.81708900	-1.33178900	-0.40360700
C	-2.90711600	-0.10954500	-0.41003100
H	-2.79609300	-0.93757400	-1.11731300
H	-3.60275300	-0.43422600	0.36282300
H	-3.29395100	0.74936700	-0.95701000

TS(39-37)_gas

O 1			
C	1.50280400	0.12911800	-0.10798200
C	0.90340700	1.18110400	-0.67084700
C	-0.55053200	1.07773200	-0.78174600
C	-0.98201000	-0.22259400	-0.32253800
H	-1.05843400	1.47327100	-1.66085500
C	2.92389300	-0.06380500	0.26727200
H	3.04651500	-0.14511100	1.34980500
H	3.34288000	-0.97032800	-0.17641600
H	3.51613200	0.78554500	-0.07486300
H	1.44912000	2.07490400	-0.94852900
O	-1.70740800	0.98854000	1.35614000
H	-2.06988100	1.04630100	2.24495300
H	-1.04174200	1.61168800	0.17073300
C	-2.28970600	-0.83632800	-0.62548000
H	-3.05530100	-0.06308700	-0.64468900
H	-2.24634900	-1.32167600	-1.60683600
H	-2.56821400	-1.58402600	0.11527200
S	0.33108700	-1.15044700	0.23938900

TS(40-41)_gas

O 1			
C	1.53536100	-0.33019000	0.00285300
C	0.98596300	-1.40919600	-0.55517600
C	-0.42032900	-1.80539700	-0.23775700
C	-1.32941800	-0.61225500	-0.18091000
O	-1.42350300	0.09431700	-1.20957200
H	-0.82018400	-2.46183300	-1.02050000
C	2.93913200	0.09711600	-0.25276100
H	3.44074100	-0.57679800	-0.95063900
H	2.96937500	1.11006800	-0.66376600
H	3.50935400	0.12549800	0.67883100
H	1.56515100	-2.02676700	-1.23545100
H	-0.11738700	1.83110100	0.07387300
H	-0.47596000	-2.35551500	0.70802600
H	-1.26037900	1.35819200	-1.01975300
O	-0.81404200	2.31795600	-0.65737200

H	-0.29883500	2.72374600	-1.36107900
C	-2.37890100	-0.52208500	0.87392700
H	-2.73118700	0.50407000	0.97732800
H	-3.22798500	-1.13122600	0.54005800
H	-2.03370200	-0.89868800	1.83360300
S	0.58690700	0.62450000	1.15462300

TS(41-43)_gas

1	1		
C	1.31903400	0.05768700	-0.06265500
C	1.21371200	-1.35047100	-0.64308600
C	-0.22627100	-1.70983300	-0.75377200
C	-1.08751700	-1.05395500	0.00796700
O	1.07291900	1.04497200	-1.01177800
H	1.73047000	-1.37044500	-1.60883500
S	-0.21149000	0.11864900	1.06147900
H	1.53409400	0.83885400	-1.83176900
H	1.74492200	-2.06449600	-0.00435700
H	-0.75898400	1.28778700	0.54491500
H	-0.56320200	-2.50192700	-1.41335200
O	-1.60633500	2.42105000	-0.42773900
H	-2.13104900	3.17853900	-0.15520500
H	-1.06434900	2.70992000	-1.16713900
C	-2.55214700	-1.16607500	0.16595800
H	-2.93729300	-1.93322200	-0.50522900
H	-2.82822700	-1.43498200	1.18790100
H	-3.04336600	-0.21980200	-0.07375200
C	2.55508600	0.33418300	0.74588600
H	3.42475700	0.22669400	0.09254600
H	2.54945300	1.35360200	1.13046800
H	2.66256500	-0.36631100	1.57449400

TS(41-43)_sol

1	1		
C	1.30193600	-0.01926900	-0.05496300
C	1.08801300	-1.37429200	-0.72391500
C	-0.37344100	-1.62417500	-0.82604100
C	-1.17021100	-0.96219700	-0.00272200
O	1.12701600	1.04297600	-0.94035900
H	1.58449100	-1.36504800	-1.69859800
S	-0.20180100	0.08781100	1.09414100
H	1.62364400	0.87615400	-1.74975800
H	1.57357400	-2.16262400	-0.13991400
H	-0.68189600	1.30149400	0.62253600
H	-0.77746400	-2.34399100	-1.52843700
O	-1.39090900	2.46945300	-0.46464400
H	-1.61683500	3.33763400	-0.11854800
H	-0.63270600	2.60285700	-1.04460500
C	-2.63602000	-0.98911700	0.17874300
H	-3.07993400	-1.67706800	-0.54010800
H	-2.90901000	-1.31344300	1.18488700
H	-3.06689900	0.00291600	0.02443700
C	2.56490900	0.10643800	0.74899600
H	3.41260400	-0.02388100	0.07250300
H	2.63650900	1.09339500	1.20448700
H	2.62276000	-0.65711800	1.52430000

TS(43-45)_gas

1	1		
C	-1.65293500	0.01235400	0.14636800
C	-1.21691800	-0.60674700	1.23488000
C	0.24960600	-0.82131100	1.35216600
C	0.86197200	-0.69092400	-0.03811100

H	0.50932500	-1.79609000	1.77446400
C	-3.02863200	0.41058100	-0.22492900
H	-3.10445200	1.48919800	-0.38208800
H	-3.34530900	-0.07248800	-1.15156200
H	-3.72450200	0.13287600	0.56632500
H	-1.89502500	-0.89971900	2.02771900
O	2.12937400	-0.01437900	0.07601500
H	2.75594200	-0.33562100	-0.58268300
H	0.69322500	-0.07209700	2.02086700
O	1.40717200	2.29057900	0.42334100
H	1.85923000	3.09328400	0.12718100
H	0.57766600	2.07673600	-0.11656000
H	1.94752500	1.38224500	0.31139400
C	1.05114500	-2.00406000	-0.74115200
H	1.41350100	-1.86823000	-1.76268600
H	1.75347700	-2.62755000	-0.18152800
H	0.09618700	-2.52816200	-0.79336100
S	-0.33841100	0.37604200	-1.01422900

TS(43-45)_sol

1 1			
C	-1.58660200	-0.32731400	0.09298300
C	-1.08202900	-1.03723500	1.09591000
C	0.40219300	-1.10201400	1.25412900
C	1.10251500	-0.56365300	-0.00975300
H	0.74529500	-2.11940500	1.44907200
C	-3.01163100	-0.06321100	-0.25739900
H	-3.22952500	1.00638200	-0.24620300
H	-3.24923000	-0.43335300	-1.25600100
H	-3.66563400	-0.55480300	0.46091800
H	-1.72658700	-1.53196500	1.81105400
O	2.08644300	0.36343900	0.36542400
H	2.76106000	0.42995700	-0.32205100
H	0.71670600	-0.49746400	2.10864600
O	0.45899000	2.69400500	0.48005600
H	0.58613300	3.50730900	-0.03272600
H	0.02177400	1.78615100	-0.20316200
H	1.33579100	2.36357400	0.75193200
C	1.64974800	-1.64409600	-0.92160300
H	2.07098800	-1.21854700	-1.83217100
H	2.42993200	-2.19042000	-0.38977700
H	0.86483100	-2.34476500	-1.20011500
S	-0.30438400	0.36018400	-0.96180400

TS(44-37)_gas

0 1			
C	-1.73542900	-0.40507600	-0.08921400
C	-0.91180500	-1.15696400	-0.82147300
C	0.40891600	-0.57368800	-1.07428700
C	0.48564300	0.71741900	-0.43120800
H	0.74147100	-0.53375600	-2.11721700
C	-3.09498600	-0.69874100	0.42173600
H	-3.11375100	-0.73341000	1.51334600
H	-3.81848900	0.05751500	0.10769900
H	-3.43201800	-1.66569700	0.04704600
H	-1.18588400	-2.14859600	-1.16130800
O	1.54171300	0.03265900	1.47959200
H	2.16600500	0.66546300	1.83753800
H	1.29100100	-1.21688600	-0.60941400
O	2.56875000	-1.64421000	0.14744900
H	2.13948700	-0.83233600	0.94327700
H	2.52529100	-2.52973200	0.50833200
C	1.53055600	1.71207900	-0.74872100
H	1.60514400	2.48895600	0.01042900
H	2.49199700	1.20708300	-0.84665200
H	1.29431900	2.18904400	-1.70589800

S	-0.98035300	1.14841100	0.30721900
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TS(46-47)-cis_gas

O	1			
C		-1.77491200	0.11130400	-0.15254000
C		-0.84234600	1.26186000	-0.26081200
C		0.50016900	1.00276000	-0.89431700
C		1.39660400	0.13340900	-0.02513100
H		0.99996300	1.95543100	-1.10241000
C		-2.94728900	0.26071200	0.73227000
H		-2.61363200	0.07122100	1.75625500
H		-3.33211600	1.28245500	0.70728400
H		-3.72447100	-0.45537000	0.47739900
H		-0.75164500	1.72976600	0.72407800
H		0.37770000	0.49928500	-1.85762100
H		-1.41375800	1.98610100	-0.86835500
O		-1.79591100	-0.85057300	-0.99517300
H		-0.80491800	-1.22715500	-0.93825300
S		0.44999600	-1.33410300	0.53464300
O		2.47412900	-0.23151500	-0.86325100
H		2.87075300	-1.02575800	-0.49544100
C		1.92723100	0.89018000	1.17785700
H		2.58145100	0.24151900	1.76223600
H		2.50327500	1.75909400	0.84470600
H		1.12497600	1.22441500	1.83926600

TS(46-47)-trans_gas

O	1			
C		-1.79108700	0.11287600	-0.18208100
C		-0.85809700	1.26122500	-0.15789400
C		0.49632400	1.07557900	-0.79357300
C		1.38811900	0.16327900	0.03386300
H		0.98517300	2.05147300	-0.88700200
C		-3.00114400	0.18053600	0.65934100
H		-3.81216200	-0.39597100	0.21931400
H		-2.74206700	-0.27611800	1.61961800
H		-3.30427300	1.20856900	0.85843100
H		-0.75968200	1.61539600	0.87203800
H		0.40154500	0.66834700	-1.80450100
H		-1.42542200	2.04899900	-0.68509500
O		1.68808700	0.89333700	1.21404500
H		1.90881100	0.25389000	1.89693600
O		-1.75654700	-0.80271600	-1.07316000
H		-0.76032400	-1.16727000	-0.99129400
C		2.66538500	-0.15155400	-0.71454000
H		3.18653800	0.77741800	-0.96824900
H		3.32275600	-0.75992000	-0.09181700
H		2.45709500	-0.70769100	-1.63022000
S		0.48079300	-1.36835900	0.46212900

TS(47-39)-cis_gas

O	1			
C		1.36967700	0.11461000	0.02353500
C		0.77736700	0.41711000	1.38376700
C		-0.72277300	0.50147500	1.22566000
C		-1.17088800	-0.42372600	0.23337600
H		-1.31922300	0.51381100	2.13753300
H		1.22287800	1.34633100	1.74725400
H		-1.09979900	1.43267500	0.55098000
H		1.05242200	-0.38441700	2.07751400
C		-2.51613300	-1.02442800	0.19449600
H		-2.51060000	-1.92484200	0.82266200
H		-3.24524500	-0.31921800	0.58618500

H	-2.80392100	-1.31082600	-0.81539400
O	-1.90581300	1.50053900	-0.71030400
H	-2.11441100	2.01497300	-1.49347100
S	0.08532800	-1.04715000	-0.73866700
O	1.41955700	1.31315100	-0.65379600
H	1.55465300	1.17484800	-1.59460500
C	2.70361500	-0.58985700	0.03816200
H	3.05213800	-0.79137800	-0.97855000
H	3.43846900	0.05847000	0.52084400
H	2.65225800	-1.53664900	0.57655700

TS(47-39)-trans_gas

O 1			
C	1.37429200	0.02495900	0.06790200
C	0.75891400	0.15699700	1.44648300
C	-0.73812800	0.26843000	1.29147400
C	-1.17255900	-0.50897900	0.16321700
H	-1.33610700	0.09707100	2.18796800
H	1.19845600	1.02380800	1.94712100
H	-1.08713500	1.30052100	0.85337400
H	1.03438800	-0.73448900	2.01876400
C	-2.56332700	-0.96190000	-0.01219400
H	-2.70627700	-1.89048900	0.55253000
H	-3.23548900	-0.20229800	0.38448700
H	-2.80891700	-1.14930600	-1.05559200
O	-1.65087400	1.80984600	-0.48183500
H	-2.07763800	2.52685100	-0.95480200
O	2.56534700	-0.67357100	0.15513100
H	3.12792200	-0.44537800	-0.58955500
C	1.50089000	1.32341700	-0.68437600
H	2.20791200	1.96860100	-0.15419800
H	1.87618400	1.14736000	-1.69709900
H	0.52379200	1.81859900	-0.75655800
S	0.06291400	-1.02303700	-0.85986500

TS(48-49)-cis_gas

O 1			
C	1.45815300	-0.17145300	0.07090900
C	0.65773900	-0.38345600	1.35641700
C	-0.59496000	-1.18165900	1.09991300
C	-1.56859900	-0.44319300	0.21094600
O	-2.04034000	0.66569500	0.60082900
H	-0.35658100	-2.15289000	0.65893900
H	1.30268300	-0.86948400	2.09552600
H	-1.12967200	-1.37351400	2.03860600
H	-0.12810500	1.59522500	-0.67858800
O	0.38586600	0.59143100	1.77376100
O	-0.52439400	2.43192200	0.13081700
H	-1.29207400	1.70363300	0.50142100
H	-0.95900800	3.16318700	-0.31569600
C	-2.44130300	-1.27614600	-0.67347500
H	-3.21933300	-1.72156800	-0.04306200
H	-2.93328300	-0.65043800	-1.41610100
H	-1.89003800	-2.07537800	-1.16519700
S	0.23110000	0.14246500	-1.30749500
O	2.36087000	0.88595900	0.21475900
H	1.88160700	1.68184500	0.46541200
C	2.28480100	-1.37917900	-0.29796800
H	2.81187200	-1.19747400	-1.23436400
H	3.02198900	-1.56588700	0.48735000
H	1.66240700	-2.26623400	-0.41976400

TS(48-49)-trans_gas

0	1			
C		1.45181600	-0.26077800	0.06484300
C		0.63212800	-0.37688300	1.33941100
C		-0.64290700	-1.14672700	1.08649400
C		-1.63587200	-0.43645600	0.21133000
O		-2.11188000	0.67853300	0.54806800
H		-0.40083000	-2.11852700	0.65336400
C		2.61283900	0.69480900	0.23933300
H		3.21118400	0.73910400	-0.67242000
H		2.26853500	1.70406500	0.47096100
H		3.25163100	0.34388700	1.05560800
O		1.93246700	-1.56234900	-0.20476000
H		1.24276200	-0.88942900	2.09024600
H		-1.17123100	-1.32629200	2.03188700
H		2.22925400	-1.58762000	-1.11814200
H		-0.08569300	1.74898700	-0.52002000
H		0.41480100	0.61999000	1.73097400
O		-0.58269300	2.46248800	0.22923300
H		-1.35811600	1.69267000	0.53635400
H		-1.00639200	3.18168700	-0.24755200
C		-2.43969500	-1.27013500	-0.72851500
H		-3.21283700	-1.77818200	-0.13995300
H		-2.93734200	-0.64117600	-1.46385700
H		-1.83351000	-2.02531700	-1.22397000
S		0.35092400	0.28023700	-1.31507400

TS(50-51)-cis_gas

1	1			
C		0.91257000	0.65354400	0.06598600
C		-0.18744700	1.47909700	0.68731300
C		-1.27165700	0.58250500	1.23677100
C		-1.86488500	-0.25249800	0.11061700
O		1.57886700	-0.04212600	0.97125600
H		0.27621500	2.07933800	1.47499200
S		-0.37637100	-0.75642100	-0.94304400
H		2.45613800	-0.36807700	0.65424200
H		-0.58313900	2.17310300	-0.05799400
H		-0.01743100	-1.76357600	-0.12118700
H		-0.85039100	-0.09135600	1.98822800
O		-2.40638400	-1.45476900	0.53771300
H		-2.95279100	-1.32029300	1.31924300
H		-2.06898100	1.16098600	1.71275800
C		-2.80553500	0.49886600	-0.79952900
H		-3.66262600	0.83605400	-0.21164900
H		-2.34275100	1.37638200	-1.25515100
H		-3.16949800	-0.15653500	-1.58988800
C		1.70835400	1.27862000	-1.03294200
H		2.29255500	2.09324700	-0.59372300
H		2.40045800	0.57016800	-1.48771900
H		1.06455500	1.69980800	-1.80403900
O		3.98081300	-0.91970400	0.11647500
H		4.22266600	-1.84896100	0.09484300
H		4.78218200	-0.44556300	0.35290400

TS(50-51)-cis_sol

1	1			
C		-0.97673300	0.81203700	-0.08341900
C		0.21799600	1.59427000	-0.53478200
C		1.28294300	0.70707900	-1.13633900
C		1.82976400	-0.26276400	-0.10249500
O		-1.63368900	0.25564100	-1.05719400
H		-0.15024100	2.31132700	-1.27495800
S		0.28849900	-0.96163000	0.79412500
H		-2.46789500	-0.19771500	-0.75086600

H	0.60962200	2.17199500	0.30313100
H	-0.10546200	-1.74528100	-0.22839200
H	0.86347200	0.14246600	-1.97561100
O	2.57708500	-1.27539900	-0.65845800
H	2.20803700	-1.55180900	-1.50470100
H	2.11394400	1.29891300	-1.52832100
C	2.65786700	0.37968500	0.97984400
H	3.49643000	0.90085000	0.51403100
H	2.08699500	1.09622900	1.57016900
H	3.04830800	-0.38502000	1.65058200
C	-1.72287100	1.25291400	1.12100700
H	-2.25202100	2.17139700	0.84464000
H	-2.45853200	0.51388000	1.43362000
H	-1.04868600	1.48240400	1.94338000
O	-3.69123500	-1.09646400	-0.10968000
H	-4.59183900	-0.77124300	-0.19480900
H	-3.71921100	-2.02185000	-0.36813000

TS(50-51)-trans_gas

1 1			
C	-0.99071100	0.66219200	-0.03663700
C	0.12534900	1.51776900	-0.54952500
C	1.23268900	0.69576400	-1.16999400
C	1.90007700	-0.13915400	-0.09675100
O	-1.63694600	0.02808700	-0.97376200
H	-0.32464400	2.18870400	-1.28852300
S	0.45003400	-0.96361100	0.84748800
H	-2.51071800	-0.34201500	-0.68431200
H	0.51836200	2.13094600	0.26267300
H	0.10294200	-1.83393300	-0.12192800
H	0.83870700	0.04358800	-1.95373000
H	1.99477100	1.33603900	-1.62148900
C	-1.73598700	1.09195000	1.17443100
H	-2.34323900	1.95845500	0.88845300
H	-2.40690400	0.31634200	1.54140700
H	-1.05853000	1.40327100	1.96686500
O	-4.03154500	-0.90151000	-0.23054500
H	-4.82393500	-0.42882800	-0.49846000
H	-4.27539600	-1.82982100	-0.19630200
C	2.83637000	-1.19259200	-0.62087000
H	3.65193800	-0.69512000	-1.15170700
H	3.26199100	-1.78763900	0.18905900
H	2.33688500	-1.86639500	-1.31734300
O	2.48132600	0.71720700	0.81219700
H	3.12781000	0.25833300	1.35849300

TS(50-51)-trans_sol

1 1			
C	0.99254900	0.79500000	0.08172700
C	-0.18678200	1.60400800	0.51758300
C	-1.26163700	0.73024700	1.12480000
C	-1.82959900	-0.19798000	0.07048900
O	1.60339500	0.19198800	1.06054400
H	0.19083100	2.32742500	1.24689600
S	-0.32332000	-0.88532800	-0.86576000
H	2.43843700	-0.26864400	0.77098600
H	-0.57775800	2.16409300	-0.33265200
H	0.08126900	-1.76316300	0.07334000
H	-0.85502100	0.13701300	1.94674500
H	-2.08278600	1.32981100	1.52457300
C	1.79481400	1.23571900	-1.08733100
H	2.36373100	2.11496900	-0.76705600
H	2.50100700	0.46938100	-1.40300100
H	1.15791500	1.52388300	-1.92021000
O	3.68830600	-1.16674500	0.17070900
H	4.58233000	-0.83656000	0.29653800

H	3.70962600	-2.09070800	0.43479900
C	-2.65429400	-1.32363900	0.63257300
H	-3.50558200	-0.88963500	1.16254900
H	-3.03071700	-1.97336000	-0.15862200
H	-2.08001300	-1.92560100	1.33626100
O	-2.51787600	0.57186300	-0.85187200
H	-3.04105000	0.00936200	-1.43308800

TS(51-53)-cis_gas

1	1		
C	1.49366400	-0.20241900	0.08993200
C	0.76353500	-0.42686900	1.39769300
C	-0.49057500	-1.22091900	1.13147300
C	-1.30556500	-0.51859800	0.05323200
O	-1.98536900	0.60464100	0.58199700
H	-0.24886700	-2.23235100	0.79301800
H	1.43706000	-0.93181300	2.09481200
H	-1.11418000	-1.32397300	2.02240200
H	-0.15480600	1.64639700	-0.58210500
H	0.52637800	0.55074000	1.82594600
O	-0.42059800	2.69866700	0.07257200
H	-1.27483100	2.46110100	0.47503900
H	-0.49757100	3.52883900	-0.41271800
C	-2.25241100	-1.42642700	-0.68443100
H	-2.81369100	-0.88270500	-1.44511900
H	-1.71710100	-2.24432600	-1.16645300
H	-2.95759700	-1.86553000	0.02874400
S	-0.00658200	0.15820200	-1.12390200
H	-2.90054000	0.36710000	0.76332300
O	2.27102900	0.91865100	0.17048300
H	3.01066200	0.87588900	-0.44423700
C	2.22776100	-1.39722100	-0.45541500
H	2.64761800	-1.18591400	-1.44112700
H	3.04342800	-1.64713600	0.22776800
H	1.58038600	-2.26850100	-0.55218000

TS(51-53)-cis_sol

1	1		
C	1.46593800	-0.24575400	0.08111500
C	0.74382700	-0.45419900	1.39545100
C	-0.53364700	-1.21194600	1.13537000
C	-1.34487000	-0.48870100	0.07317300
O	-2.00623300	0.58565500	0.66018400
H	-0.31809200	-2.22433400	0.78604800
H	1.40610200	-0.98355400	2.08488500
H	-1.15380200	-1.30320200	2.02866300
H	-0.11617400	1.64071400	-0.56219000
H	0.53381300	0.52792500	1.82843200
O	-0.27694400	2.74858300	0.07532900
H	-1.08572300	2.61086600	0.59252500
H	-0.42251400	3.50522500	-0.50733300
C	-2.27844800	-1.37879600	-0.69962600
H	-2.82987300	-0.81774600	-1.45631500
H	-1.73053300	-2.17878300	-1.19687700
H	-2.99302800	-1.82377700	-0.00294100
S	0.00519700	0.17798500	-1.11728200
H	-2.79576900	0.80252000	0.15190000
O	2.30688800	0.83617900	0.18545100
H	2.97156600	0.81523300	-0.51116800
C	2.15524600	-1.46535800	-0.47051300
H	2.59202900	-1.25342000	-1.44836500
H	2.95279100	-1.75689700	0.21672600
H	1.46808900	-2.30334100	-0.58501900

TS(51-53)-trans_gas

1	1		
C	1.53793500	-0.11032800	0.05268200
C	0.86304400	-0.43656000	1.36910000
C	-0.30765700	-1.33944600	1.05682500
C	-1.17035600	-0.64978100	0.01575300
O	-1.98203700	0.37263600	0.65284400
H	0.05104100	-2.28619700	0.64623200
C	2.43395500	1.09934700	0.06024300
H	2.81164900	1.32446400	-0.93996700
H	1.92141900	1.98214000	0.44413000
H	3.29065700	0.89245400	0.70542000
O	2.17647900	-1.24932000	-0.38219700
H	1.59366600	-0.91185400	2.02673700
H	-0.91613100	-1.57252700	1.93473400
H	2.75013800	-1.06700600	-1.13276000
H	-0.49813200	2.00757900	-0.49629200
H	0.52941700	0.48744400	1.85017600
O	-1.05920100	2.61228800	0.14903000
H	-1.66120600	1.87115500	0.52052000
H	-1.55044800	3.30908300	-0.30928500
C	-2.06545800	-1.57146900	-0.76590100
H	-2.66480100	-1.02402700	-1.49373200
H	-1.47228000	-2.31805800	-1.29254800
H	-2.73918100	-2.09904300	-0.08295800
S	0.02931500	0.22509800	-1.09678700
H	-2.74556400	-0.03258700	1.07855200

TS(51-53)-trans_sol

1	1		
C	1.44292600	-0.36323100	0.04888800
C	0.73514500	-0.50513300	1.37911900
C	-0.57721400	-1.20856800	1.12319600
C	-1.35608900	-0.44265000	0.06838300
O	-1.99138500	0.64210000	0.66669500
H	-0.39090000	-2.22042300	0.75818700
H	1.38200900	-1.06292100	2.05977400
H	-1.20089600	-1.28287900	2.01539700
H	-0.07543000	1.68026900	-0.51438300
H	0.57246700	0.48590900	1.81113700
O	-0.21285900	2.76560800	0.13981400
H	-1.01667700	2.62568700	0.66531700
H	-0.35159000	3.53887800	-0.42277400
C	-2.30741300	-1.28587100	-0.73439900
H	-2.82893900	-0.69186900	-1.48715800
H	-1.77806400	-2.09329600	-1.23903800
H	-3.04664500	-1.72046100	-0.05727000
S	0.02534600	0.21448200	-1.10060500
H	-2.77150100	0.88824400	0.15716200
C	2.56098400	0.64272400	0.01357900
H	3.34903800	0.29575700	0.68569500
H	2.98163600	0.73376800	-0.98957200
H	2.23196900	1.62634400	0.34588700
O	1.84486400	-1.62079900	-0.36179300
H	2.42299100	-1.55361000	-1.12899800

TS(52-44)-cis_gas

0	1			
C	-1.41328400	-0.46844800	0.14981900	
C	-0.61698800	-0.34346100	1.45238200	
C	0.66793100	0.41586400	1.23377800	
C	0.54305000	1.32491600	0.14492800	
H	1.09878200	0.88453100	2.12313900	
C	-2.90593100	-0.39944000	0.33101100	
H	-3.40619200	-0.42862600	-0.63684600	

H	-3.21939900	-1.28175600	0.89506300
H	-3.21212500	0.49295300	0.87659000
H	-0.42968800	-1.35775400	1.81626400
H	1.56901500	-0.33041100	0.96041900
H	3.44144700	-1.15052400	0.62469500
O	2.53506300	-1.45271800	0.68791700
H	-1.24016400	0.16924000	2.19141500
O	-1.09710500	-1.47648900	-0.65888900
H	-0.09387000	-1.52713800	-0.91294500
C	1.64921800	2.22753800	-0.23128400
H	2.38090700	1.61561400	-0.77251900
H	1.33653400	3.03735800	-0.88736600
H	2.15014900	2.62855500	0.65079000
O	1.31941000	-1.46195600	-1.36126800
H	1.53370800	-2.14579400	-1.99371900
H	2.00724900	-1.53819100	-0.42880800
S	-0.84495400	1.21996500	-0.77075300

TS(52-44)-trans_gas

O 1			
C	-1.56175400	-0.33744000	0.04149300
C	-0.90959400	-0.48878200	1.40137600
C	0.52461300	-0.01891500	1.31460600
C	0.63848100	1.01493200	0.31631800
H	1.25757400	-0.86577000	1.00645800
C	-1.25069600	-1.43631900	-0.94144200
H	-1.72399700	-1.23034800	-1.90624900
H	-0.17710700	-1.52449300	-1.12280500
H	-1.64483300	-2.37856700	-0.55009900
H	-0.98803700	-1.53232700	1.71808200
H	0.96025700	0.31566600	2.26102000
H	-1.48397000	0.11833300	2.10707700
O	1.78004600	-0.43915900	-1.40044000
H	2.50993900	-0.16978800	-1.95710700
O	-2.91928000	-0.13223200	0.20121300
H	-3.38426200	-0.39439300	-0.59780300
C	1.78182900	1.94453400	0.28836100
H	2.69048100	1.40262500	0.55208900
H	1.90676700	2.42092600	-0.68135800
H	1.61630400	2.71955400	1.04554900
O	2.42863000	-1.81658500	0.43657600
H	2.24708800	-2.75005600	0.33128200
H	2.17598200	-1.17613300	-0.60325300
S	-0.72591400	1.25503300	-0.62662200

Coordinates of all the species optimized using B3LYP method

1_gas

```
0 1
C      1.55719000   -0.27283600   -0.11541500
C      0.71007100    0.06691200    1.10278500
C     -0.71257400   -0.45786900    1.00311300
C     -1.55563600    0.29569100   -0.01552700
O     -1.20716400    1.36577900   -0.46077000
H      0.71647900    1.14795900    1.24794000
H     -0.71844300   -1.51904500    0.75050800
C      2.84170400    0.50354800   -0.27865300
H      3.46706800    0.04182600   -1.03805700
H      2.59717800    1.52331000   -0.58597300
H      3.38390200    0.57557000    0.66570400
O      1.21933500   -1.12507600   -0.90552100
H      1.21671500   -0.36387500    1.97273300
H     -1.22247200   -0.36825800    1.96800300
C     -2.85006900   -0.35989400   -0.43315400
H     -3.46968100    0.34502600   -0.98098300
H     -2.61934600   -1.21150000   -1.07791700
H     -3.39288500   -0.74994600    0.42948300
```

1_sol

```
0 1
C      1.57337200   -0.06026200    0.27473400
C      0.71216700    1.04061100   -0.31170300
C     -0.71557200    1.06405200    0.20594900
C     -1.57170700   -0.09474100   -0.26488300
O     -1.20035600   -0.85431800   -1.13927200
H      0.73801600    0.95953500   -1.39947700
H     -0.73985700    1.09120500    1.29657500
C      2.90394200   -0.29526000   -0.39204200
H      3.52252100   -0.95625200    0.20932400
H      2.73402100   -0.75231900   -1.36983600
H      3.42261600    0.64756400   -0.56968000
O      1.21514900   -0.71243000    1.23691500
H      1.21079900    1.98585000   -0.07574500
H     -1.21784900    1.97911300   -0.12221500
C     -2.91379700   -0.24886600    0.40267500
H     -3.52254900   -0.97809700   -0.12531200
H     -2.76237300   -0.58401300    1.43152600
H     -3.43412000    0.70818600    0.45531200
```

2_gas

```
0 1
C     -2.42703700   -0.68135300    0.00000100
C     -1.10767100   -0.00379100    0.00000100
C     -0.71709100    1.29460100    0.00000200
C      0.71707200    1.29460900   -0.00000100
C      1.10766600   -0.00377800   -0.00000400
O      0.00000200   -0.80955200   -0.00000300
H     -2.55065500   -1.31545400    0.88065500
H     -3.22310600    0.06082700    0.00000800
H     -1.36904200    2.15142800    0.00000300
H     -2.55066100   -1.31544300   -0.88066000
H      1.36901400    2.15144400    0.00000000
C      2.42705300   -0.68134600    0.00000300
H      2.55074000   -1.31531600    0.88072900
H      2.55062300   -1.31555000   -0.88057200
H      3.22312100    0.06083600   -0.00014900
```

2_sol

```
0 1
C     -2.43088500   -0.68046200    0.00001800
C     -1.11069400   -0.00412000    0.00000300
```

C	-0.71794900	1.29399400	-0.00001800
C	0.71794900	1.29399400	-0.00002200
C	1.11069400	-0.00412000	-0.00000300
O	0.00000000	-0.81070000	0.00001200
H	-2.55595500	-1.31392700	0.88081900
H	-3.22515500	0.06329100	0.00000700
H	-1.37024500	2.15091500	-0.00002900
H	-2.55595900	-1.31395600	-0.88076100
H	1.37024500	2.15091500	-0.00003800
C	2.43088500	-0.68046200	0.00000400
H	2.55596200	-1.31392400	0.88080600
H	2.55595300	-1.31396000	-0.88077400
H	3.22515500	0.06329100	-0.00001500

3_gas

O 1			
C	1.53003300	-0.07754100	-0.00179300
C	0.59637400	-1.00229000	0.27007500
C	-0.72768400	-0.70733300	0.94525600
C	-1.60051200	0.16049500	0.05406900
O	-1.36778000	1.35231300	-0.04930300
H	-1.23232800	-1.64155900	1.18628400
C	2.88017000	-0.39185600	-0.56053500
H	3.65465300	-0.02752400	0.11743500
H	3.01282000	-1.46174100	-0.70243700
H	3.02419300	0.11732700	-1.51525400
O	1.37736100	1.25036700	0.22385300
H	0.81453100	-2.03079800	0.02417800
H	0.43203600	1.48078100	0.31268500
H	-0.57182500	-0.15704000	1.87823800
C	-2.71686700	-0.49492300	-0.71186600
H	-3.18203100	0.21176100	-1.39356800
H	-2.33424700	-1.35529600	-1.26428500
H	-3.46353800	-0.87666600	-0.01091000

4_gas

O 1			
C	1.32463700	0.00416000	-0.05643800
C	0.97950600	1.28865900	-0.08115300
C	-0.51833600	1.40285600	-0.13419100
C	-0.96427500	-0.06608700	0.03604900
O	0.24649300	-0.85389800	-0.08955800
H	-0.87504700	1.82186900	-1.07854000
C	2.65034300	-0.66126200	-0.01205400
H	2.74156700	-1.27635700	0.88543900
H	2.77931500	-1.32097000	-0.87254700
H	3.44888400	0.07751400	-0.01423200
H	1.66657600	2.11822100	-0.06794200
O	-1.45466100	-0.20236000	1.35047600
H	-1.62010500	-1.13646700	1.52000900
H	-0.94139100	2.00160600	0.67305100
C	-1.95815000	-0.58345500	-0.98764300
H	-2.16347400	-1.64098600	-0.81353300
H	-2.89213100	-0.02808600	-0.91052400
H	-1.56120400	-0.47549100	-1.99594300

4_sol

O 1			
C	1.32999600	0.00144100	-0.05337500
C	0.98405800	1.28647900	-0.07299200
C	-0.51331200	1.40111800	-0.14021500
C	-0.96633300	-0.06459400	0.03401000
O	0.24798700	-0.85576100	-0.09319300
H	-0.85941400	1.81165800	-1.09138400
C	2.65619000	-0.66396200	-0.01133000
H	2.74754900	-1.28925200	0.87917900
H	2.79072900	-1.31285000	-0.87925500
H	3.45334700	0.07604800	-0.00280100

H	1.67170600	2.11591800	-0.05959600
O	-1.44987100	-0.20297900	1.35378300
H	-1.74798500	-1.11134800	1.48292700
H	-0.94368100	2.01280600	0.65331600
C	-1.96574200	-0.57903400	-0.98313200
H	-2.18446800	-1.63247800	-0.80189000
H	-2.89271700	-0.01158300	-0.91110900
H	-1.56914100	-0.47767800	-1.99190400

5_gas

O 1			
C	-1.70181800	-0.38570500	0.01792400
C	-0.61706600	-1.03871800	0.46667500
C	0.63896000	-0.41946900	1.03221700
C	1.73733300	-0.34409600	-0.01747900
O	2.03699000	0.70352400	-0.56430000
H	0.45657000	0.58171200	1.41858900
C	-2.93008100	-1.09807800	-0.46007400
H	-3.14216000	-0.82751800	-1.49615300
H	-2.82072100	-2.17746800	-0.38935700
H	-3.79212000	-0.78997900	0.13466400
O	-1.87278400	0.95132200	-0.04567500
H	-0.65928600	-2.11850400	0.44229200
H	-1.06301700	1.48628700	0.09721600
H	0.99615600	-1.03471700	1.86258000
H	1.02404100	2.13115800	-0.21257900
O	0.27359800	2.67635200	0.10455700
H	0.17935300	3.40916000	-0.50939300
C	2.44687600	-1.62515400	-0.37054800
H	1.72999100	-2.42597800	-0.55293500
H	3.08030600	-1.48177800	-1.24153100
H	3.06322900	-1.93463900	0.47765500

5_sol

O 1			
C	-1.70197800	-0.41293600	0.02038600
C	-0.59856000	-1.05527600	0.43139900
C	0.64571600	-0.43478800	1.02142300
C	1.75272300	-0.32647700	-0.01481800
O	2.02195500	0.73844900	-0.55289800
H	0.44941900	0.55561600	1.42792600
C	-2.91886000	-1.12781700	-0.48071500
H	-3.14433800	-0.82178300	-1.50436500
H	-2.78507000	-2.20625200	-0.45632800
H	-3.78543500	-0.86822200	0.13118700
O	-1.89951700	0.93181100	0.02495200
H	-0.61022600	-2.13320500	0.35270700
H	-1.08434000	1.46917000	0.12971000
H	1.00223200	-1.06529200	1.83901800
H	0.96522300	2.12713500	-0.20901400
O	0.21809600	2.69236400	0.08382900
H	0.08928900	3.35177000	-0.60548800
C	2.50424600	-1.57921700	-0.35898200
H	1.81734600	-2.40872600	-0.52725800
H	3.13299200	-1.42690100	-1.23181400
H	3.12891100	-1.85522900	0.49448800

6_gas

O 1			
C	1.44804300	0.42363000	0.06815700
C	1.85247700	-0.77259900	-0.34574800
C	0.69988800	-1.73581700	-0.32329100
C	-0.49792300	-0.82574700	0.02346300
O	0.10928700	0.45991100	0.40803700
H	0.83068400	-2.52685800	0.41951800
C	2.17293500	1.70782700	0.23669900
H	1.74380800	2.48106000	-0.40433500
H	2.10232000	2.06035700	1.26796700

H	3.22343000	1.58805600	-0.01900000
H	2.85695700	-1.01443300	-0.65101800
O	-1.24361900	-0.63722700	-1.14155000
H	-1.89696400	0.06378700	-0.98997200
H	0.51349200	-2.21335100	-1.28556200
C	-1.35637500	-1.28271900	1.18942700
H	-2.14706200	-0.55785600	1.38347500
H	-1.81654200	-2.24002900	0.94700100
H	-0.75606900	-1.39501400	2.09123000
O	-2.18519500	1.97821600	-0.30390000
H	-2.69979500	2.44288500	0.36079400
H	-1.31231400	1.81674600	0.08696900

6_sol

0 1			
C	1.44843200	0.43868500	0.06761200
C	1.85753500	-0.74116800	-0.39002800
C	0.72040200	-1.72376700	-0.35123600
C	-0.47946800	-0.83339300	0.03146600
O	0.11529500	0.44277000	0.44106200
H	0.87939000	-2.51544200	0.38442800
C	2.15881400	1.72702400	0.26252300
H	1.69705800	2.51839100	-0.33159500
H	2.11569800	2.03785300	1.30843600
H	3.20205400	1.63339700	-0.03045100
H	2.85891200	-0.96319000	-0.72024200
O	-1.24205800	-0.60653500	-1.12892100
H	-1.87114400	0.11159600	-0.94282700
H	0.52400600	-2.20462200	-1.30997100
C	-1.33323700	-1.33211800	1.18166900
H	-2.12621500	-0.61804100	1.40480500
H	-1.78824800	-2.28424700	0.91120400
H	-0.72791200	-1.47393200	2.07564800
O	-2.21979500	1.97233900	-0.31973200
H	-2.85190700	2.22517300	0.36089600
H	-1.37409200	1.85289000	0.13835900

7_gas

1 1			
C	-1.70805600	-0.47107800	0.01930200
C	-0.56346800	-1.10726400	0.28127100
C	0.62372700	-0.51019100	1.01311900
C	1.73320600	-0.33632300	0.02530700
O	1.89963700	0.74056000	-0.60378400
H	0.36583700	0.44266200	1.47092600
C	-2.90576300	-1.10114100	-0.60884400
H	-3.16905400	-0.58776000	-1.53629300
H	-2.72839400	-2.14927100	-0.83235500
H	-3.76592500	-1.04124300	0.06365100
O	-1.84789900	0.86097900	0.34748500
H	-0.49295600	-2.14458500	-0.00910200
H	-0.60448700	2.22301200	0.03177900
H	0.95397800	-1.19539800	1.79528700
H	1.23826100	1.52600300	-0.37451800
O	0.30454000	2.56757000	-0.03543200
H	0.29498300	3.41702800	-0.48921700
H	-2.77859900	1.11150300	0.32378600
C	2.66935800	-1.43930300	-0.26530100
H	3.23960200	-1.25718200	-1.17112100
H	3.35896600	-1.51298200	0.58435800
H	2.14355000	-2.39286400	-0.31246500

7_sol

1 1			
C	-1.69347000	-0.49786800	0.02701000
C	-0.54044900	-1.13098000	0.25341800
C	0.63961800	-0.54218600	1.00025200
C	1.74885600	-0.29892200	0.02599400

O	1.87643300	0.79851900	-0.57295100
H	0.36686500	0.38516800	1.49870400
C	-2.87798500	-1.10591400	-0.64646900
H	-3.13952600	-0.53983100	-1.54305800
H	-2.67785600	-2.13539300	-0.92986200
H	-3.74461100	-1.09316700	0.01906400
O	-1.85309500	0.80600700	0.44016600
H	-0.44705500	-2.14788900	-0.09575000
H	-0.66018000	2.12094700	0.06665400
H	0.99086000	-1.25066600	1.75037600
H	1.16283900	1.55727000	-0.34094700
O	0.20878600	2.55768900	-0.04465400
H	0.11118300	3.23024100	-0.72935300
H	-2.77030600	1.08398200	0.33529700
C	2.72721600	-1.35938500	-0.27372300
H	3.32255400	-1.12376500	-1.14972200
H	3.38030200	-1.45248600	0.60074000
H	2.22521800	-2.32059800	-0.38152500

8_gas

1 1			
C	1.06270700	-0.96377900	0.02610300
C	0.25374300	-1.76496700	-0.64090800
C	-1.13728100	-1.23695500	-0.82086900
C	-1.25029800	0.04091400	0.00551600
O	0.36490000	0.20438700	0.48470000
H	-1.88956700	-1.95158500	-0.48435000
C	2.48521200	-1.04786500	0.42770800
H	3.06667900	-0.22158500	0.01356900
H	2.58664000	-1.01945200	1.51373500
H	2.91221800	-1.97856900	0.06159100
H	0.56395000	-2.71913400	-1.03592200
O	-1.52105600	1.11333800	-0.75558700
H	-1.86048900	1.85155900	-0.23160100
H	-1.34954900	-1.00853500	-1.86677800
O	1.35048300	2.48299300	-0.24642300
H	1.97674400	3.00042600	0.27165800
H	0.77288900	1.07448600	0.16218300
H	1.39228500	2.80713400	-1.15278500
C	-1.96046200	-0.03709800	1.32563100
H	-1.83882900	0.88431300	1.89528700
H	-3.02235400	-0.19818000	1.13374300
H	-1.58696400	-0.86813100	1.91907400

8_sol

1 1			
C	1.05228800	-0.96456200	0.06268500
C	0.22597700	-1.87734900	-0.41096900
C	-1.19979300	-1.42207000	-0.46650200
C	-1.20907300	0.04105300	-0.01120800
O	0.33615800	0.21296600	0.44492500
H	-1.83901800	-2.01933100	0.18394600
C	2.50905900	-0.93312200	0.32139300
H	2.99920200	-0.14330000	-0.25024400
H	2.71168900	-0.75599600	1.37878300
H	2.94510900	-1.88684000	0.03454300
H	0.54080100	-2.86130400	-0.71736200
O	-1.39937900	0.87193500	-1.06669700
H	-1.66973000	1.75343700	-0.77705900
H	-1.61105000	-1.48058500	-1.47416000
O	1.29158400	2.44064400	-0.21887800
H	1.94132800	2.81428200	0.38900100
H	0.76209600	1.11461700	0.13680800
H	1.65791600	2.53490300	-1.10674000
C	-1.99150900	0.38011700	1.22795900
H	-1.83354300	1.41827000	1.51833800
H	-3.04980100	0.22955100	1.01642300
H	-1.70359200	-0.26646900	2.05278100

9_gas

0 1			
C	1.86266200	-0.27165000	-0.05895100
C	1.29488600	-1.19202200	0.71446100
C	-0.11180700	-0.77286800	1.03940000
C	-0.29219100	0.46756100	0.14025400
O	1.02446300	0.78953400	-0.34718300
H	-0.24099000	-0.51919800	2.09426900
C	3.22019600	-0.16892400	-0.64786000
H	3.16529400	-0.13073200	-1.73764200
H	3.71560900	0.74542400	-0.31509800
H	3.82821900	-1.02250600	-0.35643400
H	1.77239100	-2.09163400	1.06493900
O	-1.08249200	0.06616500	-0.97536700
H	-1.05288100	0.77044200	-1.63345100
H	-0.86510600	-1.52057900	0.79099100
O	-3.80734900	-0.70594400	-0.34246000
H	-2.90044600	-0.51416300	-0.62690000
H	-4.05144200	-1.51718700	-0.79484100
C	-0.87312200	1.70073700	0.80272500
H	-0.91467900	2.52776100	0.09231000
H	-1.88185500	1.49146200	1.15631900
H	-0.25482500	2.00586800	1.64544200

10_gas

1 1			
C	-2.39708300	-0.75338900	0.00004900
C	-1.07797200	-0.11431000	-0.00012600
C	-0.72767300	1.32393600	-0.00007100
C	0.76548200	1.28281600	0.00010700
C	1.16938200	0.02000300	0.00002500
O	-0.02209900	-0.82775600	-0.00015700
H	-2.96231600	-0.42098000	0.87567000
H	-2.96513200	-0.41658700	-0.87198300
H	-1.16833400	1.82569400	-0.87067100
H	-2.31544300	-1.83626300	-0.00253900
H	1.40632600	2.14816300	0.00021300
C	2.44077500	-0.72138400	0.00004200
H	2.52206400	-1.35704800	0.88293000
H	2.52220200	-1.35685500	-0.88297300
H	3.26862500	-0.01595200	0.00018200
H	-1.16866300	1.82584600	0.87026300

10_sol

1 1			
C	-2.39254200	-0.75180900	0.00001600
C	-1.07596300	-0.11496100	-0.00003600
C	-0.72898100	1.31935900	0.00019200
C	0.76177900	1.28115100	0.00019700
C	1.16288400	0.01876600	-0.00003500
O	-0.01851800	-0.83042500	-0.00019200
H	-2.95195900	-0.41259000	0.87520100
H	-2.95321400	-0.41060200	-0.87355300
H	-1.17149800	1.81718300	-0.86985900
H	-2.31002600	-1.83358000	-0.00116900
H	1.40174200	2.14587800	0.00034100
C	2.43923500	-0.71535200	-0.00018400
H	2.52271900	-1.34995600	0.88277000
H	2.52270600	-1.34962300	-0.88337800
H	3.26075300	-0.00320000	-0.00005500
H	-1.17155000	1.81696700	0.87033800

11-cis_gas

0 1			
C	-1.48230500	-0.02258000	-0.02422100
C	-0.41673600	0.44108000	0.98229000
C	0.89153500	0.94552200	0.37396300

C	1.91307400	-0.13182300	0.04946000
O	1.63942300	-1.31387800	0.06061300
H	0.71949600	1.50590500	-0.55067700
H	-0.85998300	1.22247700	1.59939100
H	1.37546700	1.65805800	1.04794100
O	-0.95171200	-0.86827100	-1.01830300
H	-0.27068200	-1.42983900	-0.61907500
H	-0.20933000	-0.40082300	1.64343800
C	3.30898800	0.34395500	-0.27690300
H	3.28417500	1.17082300	-0.98829800
H	3.78453700	0.72007100	0.63231700
H	3.90090800	-0.47554400	-0.67503900
C	-2.16392300	1.12675000	-0.76002000
H	-2.88042900	0.72402700	-1.47672200
H	-2.69153000	1.76557600	-0.05404000
H	-1.44377000	1.72552300	-1.31714900
O	-2.43128100	-0.72608900	0.77226600
H	-3.06409600	-1.13777700	0.17389000

12-cis_gas

O 1			
C	1.17286100	0.01459400	-0.08089200
C	0.78116400	-0.94236500	1.06469900
C	-0.75277700	-0.83679600	1.15253200
C	-1.14966100	-0.00793300	-0.08577600
H	-1.22486400	-1.81660600	1.12093300
C	2.35181500	-0.42480100	-0.92026000
H	2.50948400	0.28746000	-1.72804400
H	3.25012700	-0.45557800	-0.30503500
H	2.17276600	-1.41184600	-1.34218500
H	1.28940000	-0.66383100	1.98474000
H	-1.09534900	-0.33317700	2.05326400
H	-1.61848900	1.87380400	-0.36845000
O	-1.44179000	1.31339100	0.39607300
H	1.08284200	-1.95722900	0.80845000
O	1.46511300	1.31552900	0.38948600
H	0.65164600	1.68952000	0.75235500
C	-2.30786600	-0.54337800	-0.90512800
H	-3.21294200	-0.56633700	-0.29995400
H	-2.48176300	0.09355100	-1.77370300
H	-2.08915800	-1.54903500	-1.26068100
O	0.00081300	0.02775400	-0.90965200

13-cis_gas

O 1			
C	1.48394600	-0.26121600	-0.05828900
C	0.55124900	-0.48743200	1.14415100
C	-0.74204800	-1.23471600	0.82025300
C	-1.84990500	-0.41103500	0.18703600
O	-2.04010200	0.75340900	0.47835700
H	-0.55603200	-2.12023100	0.21233200
H	1.10998100	-1.03806900	1.90133300
H	-1.18070600	-1.60788500	1.75367300
O	0.84490000	0.43364000	-1.10407000
H	0.55545500	1.30951800	-0.78291100
H	0.31809100	0.48657200	1.57443700
O	-0.30066200	2.84910700	-0.12042400
H	-1.04801100	2.33156100	0.22105000
H	-0.67923000	3.50446600	-0.71209100
C	-2.75312300	-1.12695200	-0.78367800
H	-3.61879500	-0.51561700	-1.02358400
H	-2.18689800	-1.33133500	-1.69593300
H	-3.06996100	-2.09164800	-0.38299100
C	2.02154200	-1.55283600	-0.66851600
H	2.73204300	-1.30660700	-1.45815300
H	2.53039900	-2.14665800	0.08900500
H	1.22733300	-2.14682800	-1.11793300
O	2.55438500	0.50867900	0.47526100
H	3.12821100	0.75919600	-0.25696000

13-cis_sol

```
0 1
C      1.51110400   -0.33463300   -0.05199200
C      0.47708700   -0.52968200    1.06910900
C     -0.83147400   -1.20094200    0.65622100
C     -1.94362500   -0.31097500    0.14529700
O     -1.97447400    0.89362300    0.33673200
H     -0.67481500   -2.00561800   -0.06324000
H      0.95199300   -1.12746700    1.84662300
H     -1.27196900   -1.69876900    1.52815000
O      1.00659000    0.43388300   -1.12448100
H      0.71726800    1.30297300   -0.78605800
H      0.26890100    0.44589400    1.50987800
O     -0.06179500    2.85447800   -0.06725300
H     -0.83553900    2.31436000    0.17511500
H     -0.38511800    3.51383200   -0.68939600
C     -3.06141100   -1.00483500   -0.58413300
H     -3.92317900   -0.35005800   -0.68034800
H     -2.70610000   -1.27873500   -1.58092200
H     -3.34112100   -1.93143000   -0.08257400
C      2.01690300   -1.64031200   -0.65288400
H      2.80692600   -1.42569000   -1.37356600
H      2.41872700   -2.28518200    0.12661900
H      1.22438400   -2.17131600   -1.17690600
O      2.58586000    0.36128100    0.58296500
H      3.28867900    0.47936100   -0.06679000
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14-cis_gas

```
0 1
C     -1.26672500    0.31633400    0.04703700
C     -1.53406500   -1.09038600   -0.55532200
C     -0.26256000   -1.90175300   -0.26677500
C      0.77782900   -0.82845800    0.04751800
O      0.01303000    0.19483800    0.69992000
H      0.05444200   -2.52505300   -1.09969200
H     -1.72373400   -0.99273800   -1.62207300
H     -0.39265900   -2.53620900    0.60892600
H     -2.41789500   -1.54227200   -0.10905600
O      1.26881800   -0.34536100   -1.19560700
H      1.83434500    0.42305600   -1.01089200
C      1.90911300   -1.23876900    0.96989600
H      2.47911900   -2.04456100    0.50944100
H      2.57845900   -0.39681500    1.14533400
H      1.51910400   -1.57891100    1.92785700
O      2.04792200    2.12802100    0.08713900
H      1.20146700    1.83693400    0.46309600
H      1.89558600    3.01484000   -0.25006800
C     -2.27564000    0.78289200    1.07477600
H     -2.35647800    0.05697900    1.88186800
H     -1.96449000    1.74051100    1.48948100
H     -3.25060700    0.90775200    0.60595500
O     -1.20398900    1.31789300   -0.94694300
H     -0.55062200    1.03419000   -1.59902800
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14-cis_sol

```
0 1
C     -1.26840000    0.32551300    0.04667700
C     -1.51762100   -1.04664400   -0.63186100
C     -0.28252800   -1.89062900   -0.29486900
C      0.77456900   -0.84364100    0.04170800
O      0.02288700    0.19859100    0.67972000
H      0.03895500   -2.53544400   -1.10944400
H     -1.62647600   -0.90287300   -1.70504700
H     -0.45909500   -2.50917800    0.58366500
H     -2.43774900   -1.49891300   -0.26892800
O      1.30539100   -0.36140100   -1.18927700
H      1.85343700    0.41558400   -0.98874500
```

C	1.87717000	-1.28456100	0.98409200
H	2.43734600	-2.10139000	0.53135500
H	2.56369600	-0.46096100	1.18017000
H	1.46000800	-1.62513500	1.93019500
O	2.07806800	2.14767100	0.10869000
H	1.22375900	1.84019300	0.45243500
H	1.89258500	2.98030500	-0.33742400
C	-2.27377500	0.71336700	1.11010800
H	-2.33961700	-0.06683300	1.86603400
H	-1.97075700	1.64483000	1.58705600
H	-3.25614300	0.85214700	0.66110800
O	-1.23409600	1.38779300	-0.89010100
H	-0.61444900	1.14599500	-1.58981700

15-cis_gas

1 1			
C	-1.56859300	-0.34795100	-0.08202500
C	-0.46679900	-0.71265100	0.92470800
C	0.43526400	0.48757200	1.25484100
C	1.16092800	1.04617500	0.07307100
O	2.00883100	0.35622900	-0.57344400
H	-0.13295900	1.28791200	1.72389400
H	-0.90658200	-1.09174700	1.84570700
H	1.19898500	0.17029600	1.97257300
O	-0.95805400	0.51501900	-1.07239700
H	-0.89149600	0.00940900	-1.89145200
H	0.12001000	-1.52565400	0.50011400
O	2.61703400	-2.08097000	0.04787500
H	2.15796300	-0.60768400	-0.29464600
H	2.36933600	-2.82617600	-0.51181100
C	1.10319500	2.48049400	-0.26490700
H	1.57053600	2.68369300	-1.22373500
H	0.07848200	2.84148700	-0.24108400
H	1.65540800	3.01568200	0.51793400
H	3.52678900	-2.23966000	0.32582800
C	-2.74612100	0.39462400	0.52600600
H	-3.47006100	0.63967900	-0.25158700
H	-3.22834900	-0.21677200	1.28715900
H	-2.43050600	1.33209900	0.98122300
O	-1.95085600	-1.54884700	-0.69244000
H	-2.86043200	-1.49359400	-1.00703500

15-cis_sol

1 1			
C	-1.59042800	-0.31963000	-0.08290600
C	-0.46621300	-0.70473700	0.88736700
C	0.46795500	0.46851100	1.23413600
C	1.24037500	1.01997300	0.08201100
O	2.07304000	0.32058800	-0.55928900
H	-0.08251800	1.27952600	1.70341200
H	-0.89738700	-1.07904600	1.81430200
H	1.20588400	0.12044100	1.96322900
O	-1.02779500	0.33749300	-1.22608300
H	-0.65095600	-0.34216600	-1.79917100
H	0.09912700	-1.52437300	0.44646800
O	2.53403600	-2.09452200	0.03579500
H	2.21687800	-0.66603600	-0.27302900
H	2.65849000	-2.65414700	-0.74054400
C	1.16002600	2.44613400	-0.27758500
H	1.71207200	2.66255800	-1.18624500
H	0.11948700	2.75305800	-0.36325800
H	1.58562900	3.01473700	0.55650800
H	3.30692200	-2.23241800	0.59699200
C	-2.62118100	0.63233000	0.50221800
H	-3.40449300	0.81706600	-0.23319200
H	-3.06670500	0.19900800	1.39547400
H	-2.17707300	1.59141400	0.76156700
O	-2.17519800	-1.54244300	-0.47245300
H	-3.00121800	-1.36404800	-0.93771400

16-cis_gas

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1 1
C      -1.26589400   -0.37547800   -0.01632700
C      -0.75161900   -1.80112600   -0.11894200
C       0.68861100   -1.74529700    0.40497000
C       1.27436300   -0.38004500    0.01799700
O      -0.03284500    0.34394500   -0.54683000
H       1.30127500   -2.54399600   -0.00557700
C      -2.43362100    0.00930600   -0.89086100
H      -2.67323000    1.06855000   -0.78338700
H      -2.22257700   -0.19638000   -1.93728900
H      -3.30468200   -0.57123200   -0.58922700
H      -0.77871000   -2.11644500   -1.16049800
H       0.70589900   -1.84713100    1.48941400
H      -1.37908300   -2.47282700    0.46083000
O      -1.41720700   -0.04115800    1.31594200
H      -2.01206700    0.71004200    1.42551400
O       0.01632800    2.88562500   -0.03089600
H       0.71816800    3.19485000    0.55373300
H      -0.13514100    3.58333900   -0.67846100
H      -0.01130900    1.33876200   -0.35259100
C      2.24949300   -0.34716900   -1.12756400
H      2.49933000    0.67864700   -1.39189700
H      3.16314600   -0.85162300   -0.81556300
H      1.84321600   -0.85659100   -1.99802100
O      1.73942400    0.38014800    1.04912300
H      1.27216400    0.17240900    1.86866400

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16-cis_sol

```

1 1
C       1.27467600   -0.36124900    0.00754300
C       0.74603200   -1.78449100    0.07502900
C      -0.66997600   -1.70435700   -0.49826200
C      -1.26798500   -0.37790000   -0.01797700
O       0.01977800    0.37490400    0.45264300
H      -1.29325300   -2.53431000   -0.17641900
C      2.37799500    0.01214600    0.96694300
H      2.63736200    1.06693900    0.87429200
H      2.08106100   -0.18926900    1.99277500
H      3.25879100   -0.58278300    0.73024000
H       0.73175800   -2.11362700    1.11207300
H      -0.64164400   -1.71279300   -1.58704600
H      1.38977200   -2.45229900   -0.49045400
O      1.53515400   -0.03414400   -1.30870400
H      2.09076800    0.75273300   -1.36503500
O      -0.02130800    2.87733200    0.00699300
H      -0.73438400    3.17301100   -0.57192400
H      -0.06325400    3.43320300    0.79458500
H      -0.00904500    1.38884700    0.25591900
C      -2.15068700   -0.43939600    1.20269600
H      -2.40899900    0.56436900    1.53490300
H      -3.06523800   -0.97056000    0.94403300
H      -1.65052400   -0.96803100    2.01039700
O      -1.87480400    0.38450400   -0.98020900
H      -1.45406200    0.25528800   -1.83996900

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17-cis_gas

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0 1
C      -1.60682100   -0.29013900   -0.04938900
C      -0.82975600   -0.86032200    1.17046200
C       0.41119700    0.03104300    1.31020600
C       0.50224100    0.70768800   -0.05626200
O      -0.83197100    0.85155700   -0.47457200
H       1.32108400   -0.51042600    1.55827400
H      -0.56590100   -1.89753100    0.97407100
H       0.25845500    0.80112900    2.06536900
H      -1.44762200   -0.84823300    2.06607700

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O	1.18160300	-0.22691400	-0.93367000
H	1.18315800	0.15578600	-1.81890300
C	1.18705100	2.05770800	-0.09910900
H	2.22219600	1.96109500	0.22446500
H	1.17101100	2.45891600	-1.11359400
H	0.67193500	2.76236200	0.55115600
O	3.75838600	-0.97705300	0.15914000
H	4.06008900	-1.83948100	-0.13662200
H	2.92295500	-0.81713400	-0.30644500
C	-3.01318900	0.18824200	0.24275600
H	-3.43580800	0.64487400	-0.65052900
H	-3.63841600	-0.65433300	0.53441600
H	-3.00359100	0.92247700	1.04649900
O	-1.70874000	-1.22564100	-1.09905900
H	-0.81811100	-1.52040900	-1.32094000

18_gas

1 1			
C	1.10701500	-0.00783700	0.04666400
C	0.53541900	1.31890400	-0.42965300
C	-0.95367800	1.29662700	-0.06566500
C	-1.30078400	-0.15349100	-0.03551200
O	-0.31411700	-0.91854800	-0.04308300
H	-1.59439600	1.84969300	-0.75189200
C	2.06323400	-0.76308800	-0.82487500
H	2.28113500	-1.74560300	-0.40614700
H	1.67012200	-0.88884600	-1.83053900
H	2.99332200	-0.19557900	-0.88490300
H	0.66280700	1.40790800	-1.50616800
H	-1.15248900	1.70081000	0.93309100
H	1.07022000	2.13426500	0.05049600
O	1.38496300	0.03240400	1.35786600
H	1.90685600	-0.72819500	1.64711400
C	-2.67094600	-0.69589800	0.01000300
H	-3.17428800	-0.44988200	-0.93025600
H	-2.67325100	-1.77138300	0.15751000
H	-3.23837800	-0.19534000	0.79767100

18_sol

1 1			
C	1.08389900	-0.01596300	0.04436700
C	0.52860500	1.33510200	-0.38808300
C	-0.96794800	1.30020100	-0.06506300
C	-1.29655500	-0.14673300	-0.02181300
O	-0.29643600	-0.90148600	-0.00400700
H	-1.59747800	1.82708100	-0.77983800
C	2.01455300	-0.74626900	-0.87900000
H	2.24609200	-1.73727100	-0.48996000
H	1.58293100	-0.84263100	-1.87179700
H	2.93870300	-0.17315200	-0.95326200
H	0.68127100	1.46789100	-1.45550100
H	-1.20632000	1.71451100	0.91975900
H	1.05225500	2.12613300	0.13987000
O	1.43695000	-0.00069100	1.34890000
H	1.94185600	-0.78967000	1.58655000
C	-2.65400000	-0.71043900	0.00415300
H	-3.12147400	-0.50228400	-0.96277500
H	-2.64227000	-1.77970800	0.18715500
H	-3.25100200	-0.18887100	0.75329100

19_gas

0 1			
C	-1.25591200	-0.40503100	-0.07588600
C	-0.15078000	-1.41504500	-0.28984500
C	1.14522800	-0.85821600	-0.87531900
C	1.94347700	0.13639700	-0.04101900
H	1.82635700	-1.69751100	-1.05811100
C	-2.59639400	-0.96129700	0.35264200

H	-3.35036300	-0.77800400	-0.41653300
H	-2.55002400	-2.03377200	0.53164300
H	-2.94919200	-0.47379400	1.26322600
H	0.03245700	-1.92674200	0.66170200
H	0.96355300	-0.38394500	-1.83789800
O	2.64208000	0.96218200	-0.58202500
N	-1.00557700	0.82380000	-0.26087500
C	-2.04935400	1.81654800	-0.06677100
H	-1.64975700	2.80281700	-0.29207500
H	-2.91009500	1.64084700	-0.72025600
H	-2.41743900	1.82747100	0.96467700
H	-0.53362700	-2.19705100	-0.95393000
C	1.91781500	-0.00153100	1.46658600
H	2.63701200	0.68486900	1.90515500
H	0.92136800	0.22480800	1.84756900
H	2.15765500	-1.02499500	1.76482800

19_sol

0 1			
C	-1.24133400	-0.40736300	-0.09475900
C	-0.13272100	-1.39970200	-0.35458100
C	1.16404700	-0.81771500	-0.91267200
C	1.92789500	0.15575000	-0.03621600
H	1.85542300	-1.64867800	-1.09426200
C	-2.55403100	-0.99136700	0.37033300
H	-3.35524500	-0.73950600	-0.32742100
H	-2.50270800	-2.07419500	0.45807800
H	-2.83648500	-0.57883500	1.34091200
H	0.05108000	-1.95323000	0.57158300
H	0.99323100	-0.33113800	-1.87129600
O	2.55641700	1.07326300	-0.53368000
N	-1.02070800	0.83253200	-0.26701000
C	-2.08937500	1.78965900	-0.00896500
H	-1.72266800	2.79722300	-0.19494000
H	-2.95446900	1.61919900	-0.65698900
H	-2.44087000	1.74192700	1.02613200
H	-0.51115600	-2.15132000	-1.05360400
C	1.96396700	-0.09599700	1.45020400
H	2.66777000	0.58081300	1.92728500
H	0.97178600	0.05442800	1.87782100
H	2.24724500	-1.13010600	1.65515200

20_gas

0 1			
C	2.51214200	0.26361200	-0.01090100
C	1.13023700	-0.29725700	-0.00653000
C	0.71005700	-1.60503100	0.01418900
C	-0.71007800	-1.60502200	0.01417800
C	-1.13024100	-0.29724200	-0.00654500
H	2.70964300	0.90208100	0.85476100
H	3.23101000	-0.55320200	0.01410900
H	1.35798800	-2.46570100	0.02294500
H	2.72199400	0.85627000	-0.90615600
H	-1.35802100	-2.46568300	0.02293300
N	0.00000300	0.50051200	-0.02724100
C	0.00002500	1.94756600	0.02650100
H	0.88006100	2.33948400	-0.47812300
H	-0.87987900	2.33951800	-0.47832100
H	-0.00008100	2.31684000	1.05580700
C	-2.51215300	0.26363900	-0.01089500
H	-2.70968300	0.90197300	0.85485500
H	-2.72195500	0.85642800	-0.90606900
H	-3.23102200	-0.55317600	0.01396000

20_sol

0 1			
C	2.51220400	0.26584100	-0.00714500
C	1.13032000	-0.29732100	-0.00650400
C	0.71136500	-1.60839400	0.01115900
C	-0.71135900	-1.60839600	0.01115300
C	-1.13031800	-0.29732500	-0.00651400
H	2.70216800	0.90428300	0.85933800
H	3.23376800	-0.54875300	0.01717300
H	1.36195400	-2.46793200	0.01918000
H	2.71852800	0.86344600	-0.89898400
H	-1.36194600	-2.46793700	0.01916800
N	0.00000000	0.49796400	-0.02486100
C	-0.00000600	1.94979600	0.02172800
H	0.88006900	2.33702200	-0.48463700
H	-0.88004200	2.33701900	-0.48470800
H	-0.00004800	2.31794100	1.04978200
C	-2.51220300	0.26583400	-0.00716600
H	-2.70217500	0.90427300	0.85931800
H	-2.71851900	0.86344400	-0.89900400
H	-3.23376700	-0.54876000	0.01714200

21_gas

0 1			
C	-1.22498800	-0.42991800	-0.03733600
C	-0.02567600	-1.14154600	-0.70402800
C	1.32423500	-1.06201600	0.01669300
C	2.13880700	0.20618400	-0.12351300
O	1.71236000	1.21976700	-0.63606200
H	1.18484500	-1.23420200	1.08727400
C	-2.52950100	-1.12763500	-0.43600800
H	-3.39592400	-0.62109600	-0.00872300
H	-2.64322300	-1.12217100	-1.51946700
H	-2.52977600	-2.15749600	-0.08122500
O	-1.02697700	-0.60673300	1.39253300
H	-0.27835700	-2.19971200	-0.77710400
H	1.96224100	-1.88445600	-0.32279000
H	-1.83574400	-0.36124900	1.85027600
H	-0.31438600	1.32426500	-0.50682100
H	0.06212600	-0.76319300	-1.72256200
C	3.55289800	0.14352100	0.41284000
H	3.57488100	-0.30083100	1.40888800
H	4.15923800	-0.49472800	-0.23456000
H	3.98690400	1.13941300	0.43685600
N	-1.25477200	0.95357700	-0.45306800
C	-2.14593600	1.86370700	0.24710700
H	-2.01080000	2.86358100	-0.16316700
H	-3.19070900	1.59233500	0.08775400
H	-1.97001000	1.92644500	1.33055800

22_gas

0 1			
C	1.14101500	-0.62585800	0.06369500
C	-0.01631500	-1.26602800	0.34456900
C	-1.20068700	-0.61537500	1.02299200
C	-1.88650500	0.33517600	0.05534400
O	-1.54420300	1.50076800	-0.01862200
H	-1.89808900	-1.38379200	1.35728900
C	2.30572100	-1.37478300	-0.52200600
H	3.16866800	-1.34536900	0.14694800
H	2.03996100	-2.41626900	-0.68300300
H	2.62266900	-0.95012700	-1.47667400
H	-0.08994800	-2.31535500	0.10218600
H	0.48900300	1.24749600	0.46528900
H	-0.88630800	-0.03389100	1.89465300
C	-2.96589300	-0.22991500	-0.83574100
H	-2.64507300	-1.17351400	-1.27839400

H	-3.85146000	-0.44398800	-0.23094400
H	-3.22790500	0.48168700	-1.61441000
N	1.33763600	0.71068800	0.35199300
C	2.45593600	1.48308600	-0.15661500
H	3.40787500	1.03969000	0.13307800
H	2.44937800	1.59688300	-1.24742800
H	2.41177100	2.47776400	0.28301100

23_gas

O 1			
C	-1.28743900	-0.34352400	-0.09515800
C	-0.83738900	-1.60209000	0.01513200
C	0.65348400	-1.60758400	-0.18776100
C	1.02637000	-0.11780200	0.00150200
H	1.21951900	-2.22508100	0.51081800
C	-2.70497500	0.12233400	-0.06935000
H	-2.97166800	0.61930800	-1.00531100
H	-3.37257600	-0.72558700	0.06773800
H	-2.88840000	0.83436400	0.73792200
H	-1.45797900	-2.47831100	0.10557200
H	0.91506500	-1.93861400	-1.19847300
N	-0.24007700	0.56682400	-0.32673000
C	-0.37868400	1.96990400	0.02221000
H	0.47665200	2.52383900	-0.35888700
H	-1.26934200	2.38011900	-0.45004900
H	-0.43954300	2.14893300	1.10192400
C	2.19712900	0.35528700	-0.84038900
H	3.07671800	-0.24633400	-0.61441700
H	1.96405700	0.26278600	-1.89917200
H	2.44124900	1.39360600	-0.61929000
O	1.40371300	0.13700400	1.36197700
H	0.74611000	-0.27197500	1.93580500

24_gas

O 1			
C	1.24198400	-0.89145400	0.10922200
C	0.05877200	-1.33670600	0.59567400
C	-1.07970600	-0.46589300	1.06936300
C	-2.03787500	-0.14311600	-0.06601600
H	-1.63549800	-0.99287400	1.85012800
C	2.30289800	-1.88112400	-0.29398100
H	3.21790700	-1.74554200	0.28589700
H	1.95123400	-2.89725200	-0.13726200
H	2.56853200	-1.76719900	-1.34720300
H	-0.08851000	-2.40554800	0.64257900
H	-0.72453800	0.47481900	1.49200300
O	-2.09511100	0.96447700	-0.57274700
N	1.55413300	0.43084000	-0.07389200
C	2.89307800	0.94230700	-0.28566500
H	3.55695500	0.78633500	0.57280400
H	3.36441400	0.49774500	-1.16319100
H	2.81607100	2.01310300	-0.45994200
H	0.88110800	1.13322800	0.19475100
O	-0.21539100	2.88236600	0.14437300
H	-0.98348400	2.34584200	-0.13345800
H	-0.56195800	3.57112400	0.71613200
C	-2.92764500	-1.25717900	-0.55903000
H	-3.40928800	-0.97281700	-1.49063900
H	-2.36197000	-2.17878600	-0.69081500
H	-3.69492500	-1.45381700	0.19504800

24_sol

O 1

C	1.25591900	-0.88466200	0.07945000
C	0.08419000	-1.33038900	0.58929100
C	-1.05896900	-0.46686500	1.07098300
C	-2.01810300	-0.18036500	-0.06837600
H	-1.60064900	-0.99259800	1.86004700
C	2.32238100	-1.86875500	-0.32255500
H	3.23085100	-1.73735800	0.26802800
H	1.97053700	-2.88691000	-0.17905400
H	2.59952100	-1.74216800	-1.37127900
H	-0.06204800	-2.39961200	0.63783900
H	-0.71097500	0.48313700	1.47825700
O	-2.03581900	0.90323000	-0.63808500
N	1.54721300	0.44453100	-0.14707600
C	2.90730000	0.96199700	-0.19155200
H	3.44514800	0.84532700	0.75602600
H	3.48929000	0.47860100	-0.97455700
H	2.85821400	2.02363500	-0.42351800
H	0.87215300	1.12392000	0.17313000
O	-0.33173500	2.96728700	0.10474000
H	-1.01995800	2.31305000	-0.13088400
H	-0.66186200	3.41891500	0.88728600
C	-2.94755000	-1.28511200	-0.48744500
H	-3.38492900	-1.07561300	-1.46004700
H	-2.43849600	-2.24772800	-0.49838700
H	-3.74786300	-1.35553600	0.25463900

25_gas

O 1			
C	0.93895600	-0.96764500	-0.28395400
C	0.53490800	-0.84637700	-1.55410200
C	-0.90906100	-0.42947000	-1.57451100
C	-1.17103700	-0.01431200	-0.10469300
H	-1.56560300	-1.25792900	-1.85962400
C	2.26510900	-1.43068900	0.21655400
H	2.76024600	-0.66406300	0.81550200
H	2.16153200	-2.31932800	0.84383600
H	2.91191200	-1.67971500	-0.62182300
H	1.11810300	-1.10470800	-2.42233500
O	-0.97271300	1.41978800	0.05177500
H	-1.68904200	1.88966400	-0.38683300
H	-1.13087500	0.40259100	-2.24619800
O	1.64678200	2.66466900	-0.15607200
H	2.08412800	2.18135700	-0.86216100
H	0.77318400	2.24866400	-0.08727300
N	-0.09345500	-0.66235700	0.62496200
C	0.19547000	-0.24751600	1.98952500
H	0.81144100	-1.00095300	2.47705100
H	0.70588100	0.71808700	2.04888600
H	-0.73429100	-0.17605300	2.54969000
C	-2.55737400	-0.37709900	0.41179400
H	-3.32614900	0.10042400	-0.19922800
H	-2.70865000	-1.45407200	0.36644500
H	-2.69201000	-0.04447300	1.44003200

25_sol

O 1			
C	-1.06533800	-0.69373000	0.49719100
C	-0.79009000	0.03687700	1.58635600
C	0.67993100	0.35671300	1.60747700
C	1.13632400	-0.01918400	0.17590500
H	1.21400100	-0.24901600	2.34614900
C	-2.36774600	-1.30914700	0.10951100
H	-2.71808500	-0.94430000	-0.85791500
H	-2.28286900	-2.39553600	0.03209100
H	-3.12427000	-1.07778200	0.85609000
H	-1.48691100	0.26338000	2.37680800

O	1.08629300	1.16238100	-0.68396200
H	1.84544000	1.72154000	-0.48378100
H	0.91822000	1.40048700	1.81735600
O	-1.32487200	2.66887500	-0.75888400
H	-1.86096400	2.23025000	-0.08977300
H	-0.49003200	2.16483800	-0.74567800
N	0.08536700	-0.91498500	-0.28469900
C	-0.00627500	-1.24908700	-1.69748300
H	-0.65048700	-2.11595900	-1.82868500
H	-0.39451400	-0.43024500	-2.31144400
H	0.97947400	-1.51590600	-2.07163900
C	2.53141800	-0.62122300	0.09623300
H	3.26707000	0.08131500	0.49070500
H	2.58276600	-1.53379200	0.68721600
H	2.80286600	-0.85173700	-0.93296700

26_gas

O 1			
C	1.54774700	-0.74541600	0.07198800
C	0.72887200	-1.55840400	0.74513000
C	-0.47261200	-0.78727600	1.21336100
C	-0.36098700	0.54403500	0.43750700
H	-0.43742400	-0.59842400	2.29051600
C	2.88230300	-1.06644000	-0.51185000
H	2.90310600	-0.91576300	-1.59336700
H	3.66491100	-0.43714900	-0.08051900
H	3.13331200	-2.10575000	-0.31160200
H	0.93451600	-2.58709900	0.99058500
O	-1.24121300	0.41779100	-0.70985400
H	-1.35202900	1.27935500	-1.12420800
H	-1.43029100	-1.26280100	1.00212000
O	-3.77493700	-0.96209500	-0.81242000
H	-2.89869100	-0.54574800	-0.79709900
H	-3.69233300	-1.70140700	-1.41986400
N	1.04464800	0.57369900	0.01672900
C	1.42826700	1.46797400	-1.05862700
H	2.51275800	1.53153200	-1.11919400
H	1.04779300	1.16029900	-2.04102400
H	1.06406900	2.47328800	-0.84779600
C	-0.76071900	1.77688100	1.23605200
H	-1.79347500	1.68279500	1.57011000
H	-0.11540100	1.89078700	2.10479300
H	-0.68137900	2.68649600	0.63626300

26_sol

O 1			
C	1.55272700	-0.73418700	0.06676500
C	0.75410600	-1.55121600	0.76471900
C	-0.44057300	-0.78058200	1.25609700
C	-0.36396200	0.53462500	0.45100200
H	-0.37480600	-0.56834000	2.32725200
C	2.87721800	-1.04768600	-0.54457200
H	2.87103600	-0.90101600	-1.62646100
H	3.66253400	-0.40648800	-0.13736900
H	3.14317600	-2.08314600	-0.34322600
H	0.97871300	-2.57382500	1.02074300
O	-1.25506600	0.35910500	-0.68799300
H	-1.33367400	1.19377900	-1.16339000
H	-1.40004200	-1.26902300	1.08587500
O	-3.76693400	-0.95565200	-0.83977300
H	-2.88895000	-0.53826600	-0.77457300
H	-3.64360000	-1.70995100	-1.42363200
N	1.03453400	0.57649700	0.01181400
C	1.40923700	1.48516500	-1.05931200
H	2.49269300	1.55411200	-1.12312800
H	1.02760600	1.18136500	-2.04129100

H	1.03635500	2.48411300	-0.83955800
C	-0.78257100	1.77831500	1.22047800
H	-1.80990300	1.66970400	1.56639100
H	-0.13537900	1.92473700	2.08318200
H	-0.72858600	2.67252500	0.59755300

27_gas

1 1			
C	-1.27684300	-0.88581800	-0.25864800
C	-0.07666600	-1.18520500	0.22620200
C	0.90831000	-0.31220700	0.95193800
C	2.15378400	-0.04667000	0.08538200
O	2.19672100	0.93914700	-0.62251100
H	0.49146500	0.65321100	1.23053400
C	-2.19557200	-1.83318200	-0.96207100
H	-2.39445700	-1.50498600	-1.98633500
H	-1.75748800	-2.82617200	-1.01091200
H	-3.15786800	-1.91785000	-0.45085500
H	0.23330200	-2.21265900	0.07716100
H	-1.12144300	1.23715400	-0.27586700
H	1.21444900	-0.82501400	1.86616500
H	0.86841200	2.04754400	-0.67347500
O	-0.03627300	2.41670600	-0.55043500
H	-0.07276300	3.28708500	-0.95671700
H	-2.51299000	0.61069200	-0.88126400
C	3.28201100	-1.02719800	0.15747500
H	4.02242300	-0.81548100	-0.60805100
H	3.74978100	-0.95635600	1.14356700
H	2.91786400	-2.05178500	0.05988500
C	-2.56785800	0.73474200	1.17556700
H	-1.85451600	0.65719700	1.98841700
H	-2.99103700	1.73517900	1.14495600
H	-3.35443100	-0.00332500	1.29917300
N	-1.84675600	0.48171100	-0.11969700

27_sol

1 1			
C	-1.27802500	-0.88358100	-0.26310800
C	-0.07987200	-1.18925100	0.22062200
C	0.89823900	-0.30715600	0.94693500
C	2.15074600	-0.05483900	0.10432600
O	2.26674000	0.97573000	-0.53628900
H	0.47521000	0.65573300	1.22016100
C	-2.20206100	-1.83677400	-0.94894700
H	-2.41471600	-1.50930300	-1.96937900
H	-1.75739300	-2.82687900	-0.99360000
H	-3.15638100	-1.91455100	-0.42377100
H	0.22865500	-2.21781200	0.08395400
H	-1.09890900	1.22574500	-0.26347700
H	1.19603800	-0.81374700	1.86717200
H	0.88340400	2.09661500	-0.61967900
O	-0.00298700	2.50525800	-0.52062900
H	-0.15709000	3.03380600	-1.31056100
H	-2.48454800	0.63560600	-0.90170300
C	3.21640200	-1.10617900	0.10729200
H	3.98053100	-0.88257900	-0.63133500
H	3.66728900	-1.14513500	1.10198500
H	2.78768100	-2.09169100	-0.07929400
C	-2.57180400	0.73327900	1.15545800
H	-1.87271300	0.63596500	1.97809900
H	-2.98097300	1.73816300	1.12277600
H	-3.36981500	0.00507100	1.25173900
N	-1.83400600	0.48487100	-0.13045900

28_gas

```
1 1
C      1.28754800   -0.72719800   -0.14804500
C      0.70623100   -1.81933800   -0.61569200
C     -0.78252700   -1.81257600   -0.46848000
C     -1.11945500   -0.35205200   -0.13886700
H     -1.11653400   -2.49400000    0.31677200
C      2.71196400   -0.30026400   -0.12858200
H      2.84549300    0.66174300   -0.62852100
H      3.10689600   -0.20392800    0.88437400
H      3.31826300   -1.03713600   -0.65004800
H      1.25071100   -2.63329900   -1.06969000
O     -1.28849700    0.32160400   -1.34280400
H     -1.71805500   1.17383500   -1.20135500
H     -1.29804700   -2.09437300   -1.38559000
O      0.23644600    2.90775700   -0.56307600
H      0.34811200    3.74173700   -0.09358500
H      0.37019900    1.13724600    0.05450000
H      0.44851200    3.09899000   -1.48366000
C     -2.27575900   -0.13384100    0.81386400
H     -2.44112100    0.92608200    1.01438400
H     -3.17152300   -0.52876200    0.33634100
H     -2.14628700   -0.65576300    1.75882000
C      0.38763000    0.28511000    1.92858200
H     -0.35919800    0.97395400    2.30980400
H      0.25816200   -0.69885700    2.36898000
H      1.37730400    0.66184800    2.16930800
N      0.26424600    0.18524800    0.44136200
```

28_sol

```
1 1
C      1.51900300    0.20211000   -0.18592400
C      1.68005400   -1.04361100   -0.60081300
C      0.46906500   -1.89862000   -0.39163600
C     -0.64653200   -0.88630500   -0.10976900
H      0.60199900   -2.59687500    0.43634400
C      2.42279300    1.38048600   -0.23223100
H      1.96387000    2.20721300   -0.77860800
H      2.67824000    1.74575500    0.76347100
H      3.34604600    1.10675700   -0.73735800
H      2.59084200   -1.40536500   -1.05231200
O     -1.16641900   -0.48729300   -1.33939000
H     -1.80316900    0.23553800   -1.21124300
H      0.20490400   -2.48219800   -1.27226900
O     -1.91522300    2.13332000   -0.59015100
H     -2.57009800    2.48381100    0.02396500
H     -0.31643000    1.18890400    0.05383400
H     -1.82378000    2.79709000   -1.28294900
C     -1.72634900   -1.33592500    0.85228200
H     -2.47532300   -0.56015200    1.00884400
H     -2.21990900   -2.19406900    0.39894900
H     -1.32611200   -1.64767000    1.81357800
C      0.24803600    0.52917700    1.91502600
H     -0.74945200    0.67929600    2.31229000
H      0.70858700   -0.35108100    2.35064800
H      0.85313100    1.40424100    2.12766100
N      0.17048100    0.36238800    0.42855400
```

29_gas

```
1 1
C      2.49761000    0.35875800    0.00003000
C      1.11788200   -0.18379700   -0.00001900
C      0.74650200   -1.62259700   -0.00019300
C     -0.74207700   -1.59491300   -0.00019100
C     -1.15902500   -0.32710100   -0.00003400
H      2.67721900    0.97922700    0.88051800
```

H	3.22068800	-0.45207000	0.00006400
H	1.17966700	-2.12800100	-0.87166400
H	2.67727400	0.97918300	-0.88048200
H	-1.37360900	-2.46707300	-0.00029700
C	-2.52003900	0.26731900	0.00003700
H	-2.69425200	0.88533500	0.88243500
H	-2.69426000	0.88552800	-0.88222400
H	-3.25839400	-0.53049300	-0.00004700
H	1.17965800	-2.12820300	0.87116600
N	0.02091000	0.52207000	0.00006900
C	-0.06923700	1.98306900	0.00023800
H	0.92466400	2.41471500	0.00027600
H	-0.60736600	2.31157200	-0.88620900
H	-0.60734900	2.31137000	0.88677100

29_sol

1 1			
C	2.49191100	0.35982000	0.00005800
C	1.11527900	-0.18365900	-0.00002000
C	0.74741100	-1.62125400	-0.00019800
C	-0.74039100	-1.59483400	-0.00018900
C	-1.15520800	-0.32685900	-0.00003300
H	2.66390300	0.98022600	0.88097900
H	3.21227300	-0.45245400	0.00005100
H	1.18226700	-2.12207600	-0.87190500
H	2.66396600	0.98028900	-0.88080600
H	-1.37259400	-2.46581100	-0.00029000
C	-2.51617700	0.26623300	0.00004800
H	-2.68549200	0.88604300	0.88162000
H	-2.68549100	0.88628600	-0.88135200
H	-3.25210700	-0.53370200	-0.00006200
H	1.18227500	-2.12230100	0.87137500
N	0.01987600	0.52218900	0.00005900
C	-0.06969600	1.98117800	0.00020800
H	0.92473400	2.40962700	0.00012600
H	-0.60591800	2.30748100	-0.88729600
H	-0.60572500	2.30731900	0.88789100

30-cis_gas

0 1			
C	1.16987400	-0.14466100	-0.06638800
C	0.77196500	-1.57116800	-0.46350700
C	-0.74751100	-1.61871800	-0.23299400
C	-1.18989200	-0.14658600	-0.01251200
H	-1.26472700	-2.05395600	-1.08633400
C	2.45072400	0.34846600	-0.72455400
H	2.73524800	1.32926500	-0.34801600
H	3.26874500	-0.34250500	-0.51187500
H	2.32720600	0.40430300	-1.80527700
H	1.32161000	-2.31158800	0.11747800
H	-1.02020100	-2.20074600	0.64441700
H	-0.74277800	-0.04204800	1.88358500
O	-1.54270700	0.08941400	1.35798500
N	-0.00076900	0.61167500	-0.41894900
C	0.00236200	2.04419300	-0.15298900
H	-0.91713800	2.48220900	-0.53409000
H	0.08276300	2.28942800	0.90936800
H	0.82870700	2.51428500	-0.68356700
H	1.01401200	-1.72941600	-1.51434200
O	1.33008900	-0.07167300	1.39429400
H	2.12153300	-0.55227900	1.65540200
C	-2.42804600	0.22868800	-0.81322000
H	-3.25490200	-0.41885600	-0.52351400
H	-2.72955200	1.25525200	-0.61234300
H	-2.24106400	0.11170600	-1.87949900

31_gas

O 1			
C	-1.75726000	-0.13777800	-0.09163500
C	-0.91687300	-1.13473500	-0.92537500
C	0.32142600	-1.72758500	-0.24939400
C	1.51903400	-0.83037200	-0.04422000
O	1.58865600	0.28677900	-0.52693300
H	0.06038600	-2.16470600	0.71572400
C	-3.23785600	-0.25847700	-0.46344800
H	-3.84728700	0.45368800	0.09439500
H	-3.37717400	-0.05669100	-1.52487100
H	-3.59916700	-1.26116700	-0.23929900
O	-1.59145400	-0.55519100	1.29050000
H	-1.56016900	-1.97490600	-1.18863800
H	0.68791800	-2.56537700	-0.85501100
H	-2.23148400	-0.08782200	1.83457600
H	-0.27790900	1.21800500	-0.39196100
H	-0.64233400	-0.64191800	-1.85747400
C	2.64013000	-1.39112600	0.79372600
H	2.34441000	-1.32467100	1.84426800
H	2.80926700	-2.44608600	0.57699700
H	3.55385700	-0.82000700	0.65091700
N	-1.28800700	1.20709000	-0.34922300
C	-1.78750900	2.28277200	0.49349200
H	-1.28338600	3.20564300	0.21038900
H	-2.85507000	2.44097900	0.33602500
H	-1.61660700	2.13291200	1.56898800
O	4.08879100	1.64853400	-0.16299400
H	3.20363000	1.29854000	-0.35749600
H	4.27267300	2.28677900	-0.85642100

31_sol

O 1			
C	-1.34520000	-0.37264800	-0.32879500
C	-0.18244400	-0.51774500	-1.32463200
C	1.03739900	-1.27671700	-0.80722100
C	2.04627300	-0.48234800	-0.00535300
O	2.21252100	0.71668200	-0.15799800
H	0.75590900	-2.16526600	-0.24272900
H	-0.57250700	-1.02432800	-2.20661400
H	1.61410500	-1.65471900	-1.66041800
H	-0.44106800	1.18199800	0.58211200
H	0.11629000	0.48084800	-1.64644800
O	0.79004800	3.12957000	-0.26719600
H	1.31733200	2.32154300	-0.38882500
H	0.50360800	3.38290800	-1.14985600
C	2.89852400	-1.26482800	0.95497700
H	3.27192000	-2.17532500	0.48422800
H	3.72557400	-0.66186800	1.31990200
H	2.27729700	-1.57820200	1.79757700
N	-0.86911000	0.30601900	0.85988200
C	-1.83000700	0.55601600	1.93338700
H	-2.74456900	1.06837400	1.60796700
H	-2.11703700	-0.37439900	2.42109700
H	-1.35169500	1.18440400	2.68306400
C	-1.98203000	-1.71865900	0.01887200
H	-2.89979400	-1.58029300	0.59029900
H	-2.23349800	-2.25277400	-0.89578800
H	-1.31221100	-2.33629500	0.61470500
O	-2.31768300	0.41737400	-1.07122800
H	-3.16005400	0.39381700	-0.60548100

32-cis_gas

O 1			
C	1.29985100	0.00925000	0.17450400

C	0.81808700	0.13785200	1.63033500
C	-0.71047700	0.02813500	1.56506500
C	-1.02679700	-0.65159200	0.21580000
H	-1.11808200	-0.54574100	2.39515400
C	2.68700500	-0.61503600	0.06911400
H	3.03046300	-0.62485300	-0.96426300
H	3.39507500	-0.01704300	0.64154500
H	2.68263100	-1.63257200	0.45642200
H	1.16291500	1.07328800	2.06590800
H	-1.18636300	1.00562100	1.58669400
H	-2.20089700	-0.13335100	-1.32286800
O	-1.87460200	0.29752900	-0.52689100
N	0.26608800	-0.86286900	-0.39465500
C	0.31649500	-1.13203200	-1.81900300
H	-0.42067100	-1.89087600	-2.08327300
H	0.14139800	-0.24195300	-2.43381100
H	1.29229800	-1.53273300	-2.08692500
H	1.23655300	-0.67970500	2.21725600
O	1.42004300	1.26858600	-0.48296400
H	0.64431500	1.83317900	-0.32774400
C	-1.82056600	-1.94894300	0.35240800
H	-2.78053100	-1.75183700	0.82831000
H	-2.01126300	-2.40970700	-0.61893100
H	-1.26366600	-2.66349700	0.95655500
O	-0.95936400	2.89338300	-0.26404300
H	-1.46632200	2.09417500	-0.49870000
H	-1.07066400	3.51590500	-0.98689200

33-cis_gas

0 1			
C	-1.54915800	-0.41635600	-0.05511500
C	-0.99077500	-1.40409300	0.97838300
C	0.46895300	-0.96264400	1.18748800
C	0.61399000	0.37631200	0.42407000
H	0.68797600	-0.82103000	2.24421500
C	-3.05345700	-0.20667100	0.03489900
H	-3.41340300	0.42549700	-0.77454300
H	-3.56722600	-1.16700800	-0.03640400
H	-3.31819400	0.24867900	0.98823600
H	-1.08503200	-2.43181000	0.62885100
H	1.19035800	-1.67844800	0.80094200
H	0.76156300	-0.37685300	-1.38251100
O	1.32491600	0.18039600	-0.82599500
N	-0.77266300	0.77007700	0.19317900
C	-1.01468700	1.93960000	-0.64245900
H	-0.42733600	2.77541200	-0.26983600
H	-0.76058900	1.78195700	-1.69391300
H	-2.06245300	2.22616700	-0.57623600
H	-1.56166500	-1.31739100	1.90238800
O	-1.21768200	-0.88652200	-1.41085200
H	-1.71037700	-1.69014000	-1.60372900
C	1.42085400	1.41656700	1.18302700
H	2.41341000	1.02058700	1.39430800
H	1.54408700	2.32553400	0.59681100
H	0.92888000	1.66089400	2.12295700
O	3.98484100	-0.80484200	-0.57305700
H	4.57650300	-0.31336500	-1.14779000
H	3.10121500	-0.42777400	-0.72852200

34-cis_gas

1 1			
C	0.81742000	-0.89570200	-0.18742600
C	-0.27472800	-1.89128000	-0.55523500
C	-1.53656200	-1.05257800	-0.82297600
C	-1.33109200	0.34374400	-0.18928800
H	-2.42305800	-1.52919100	-0.41133400

C	2.01117200	-1.45983400	0.55845200
H	2.71035700	-0.67548600	0.85151600
H	1.72660800	-2.02760000	1.44068900
H	2.53067900	-2.13455100	-0.11992400
H	-0.43004000	-2.58700000	0.26807300
H	-1.71743400	-0.91885000	-1.88737500
H	0.04088800	-2.47266100	-1.41771500
O	1.20583700	-0.24213800	-1.36499700
H	1.91337300	0.39275100	-1.17617100
O	2.04529500	2.23993000	-0.02841800
H	1.70628700	2.98744600	-0.53522500
H	2.82481900	2.57456400	0.42928600
H	0.52384400	1.04736200	0.56288900
C	-2.47588500	0.82613600	0.67601900
H	-2.25735100	1.79637200	1.11995400
H	-3.33829300	0.94954800	0.02318800
H	-2.74209800	0.11371800	1.45247900
O	-1.07080000	1.35023500	-1.11170500
H	-0.48848600	1.00722000	-1.80290700
C	-0.14295300	-0.15911400	2.08917700
H	-0.65539500	-1.10831200	2.21279900
H	0.83685900	-0.20901800	2.55245300
H	-0.71712900	0.62883600	2.56407200
N	0.01552500	0.15891500	0.64312500

34-cis_sol

1 1			
C	0.79769100	-0.86766100	-0.19144400
C	-0.28659000	-1.86426900	-0.58202600
C	-1.57678000	-1.04783400	-0.77566900
C	-1.34406500	0.36105300	-0.18596500
H	-2.41834800	-1.52695100	-0.28178700
C	1.97751600	-1.44548800	0.56590900
H	2.67850900	-0.67019300	0.87270500
H	1.67183100	-2.01625100	1.43845900
H	2.49447300	-2.12065900	-0.11376900
H	-0.40558800	-2.60335300	0.20729500
H	-1.84106200	-0.93509100	-1.82428400
H	0.02262100	-2.39194100	-1.48028500
O	1.21308100	-0.20184900	-1.35789700
H	1.86558800	0.48120800	-1.12002900
O	2.17622300	2.07944800	-0.02292000
H	2.03035400	2.91296500	-0.48462700
H	2.94401100	2.22567400	0.54094200
H	0.50364500	1.06986300	0.57536200
C	-2.48129700	0.88947200	0.66202900
H	-2.23989500	1.86515100	1.08089200
H	-3.34206600	1.00460600	0.00542800
H	-2.75673300	0.20417900	1.45825300
O	-1.08062200	1.33382100	-1.15351500
H	-0.42124600	0.98829600	-1.77311300
C	-0.17775000	-0.15441700	2.07939400
H	-0.69301800	-1.10329600	2.18504200
H	0.80138500	-0.20831100	2.54110000
H	-0.74891500	0.63233200	2.55756400
N	-0.00962100	0.18218300	0.63659000

35_gas

1 1			
C	-1.06211300	-0.17984500	0.03244000
C	-0.59251900	-1.60302300	-0.30595900
C	0.90909200	-1.61387600	-0.01201600
C	1.29781900	-0.17164600	-0.04281400
H	1.49724600	-2.19605000	-0.72093100
C	-2.10689800	0.38254300	-0.91194700
H	-2.42499800	1.38336500	-0.61801700

H	-1.74014000	0.42039400	-1.93635500
H	-2.97910500	-0.27000700	-0.89076900
H	-0.77144700	-1.80993700	-1.35930800
H	1.14841700	-2.00359600	0.98202900
H	-1.15166700	-2.32211300	0.28440400
O	-1.44594900	-0.11088400	1.37399700
H	-2.21973900	0.44929900	1.49430000
C	2.71527200	0.25564800	-0.03549100
H	3.17347900	-0.04595100	-0.98131200
H	2.86587100	1.32098800	0.09872700
H	3.24735700	-0.28627400	0.74807100
N	0.26304800	0.59924900	-0.06273700
C	0.24003600	2.05952300	-0.00626900
H	1.22337700	2.45354600	0.21920700
H	-0.09866900	2.45931000	-0.95990500
H	-0.44785400	2.36340400	0.77938200

35_sol

1 1			
C	-1.05925100	-0.17543800	0.03187200
C	-0.59712200	-1.60913400	-0.26748400
C	0.91100100	-1.61953300	-0.01101700
C	1.29700800	-0.17982300	-0.02411700
H	1.48131900	-2.17699700	-0.75272100
C	-2.06072000	0.38127600	-0.96192600
H	-2.37726000	1.38962300	-0.69642000
H	-1.64544400	0.39725400	-1.96763600
H	-2.93829300	-0.26312200	-0.96049500
H	-0.80340100	-1.84751500	-1.30789600
H	1.18333300	-2.03110600	0.96427800
H	-1.14333900	-2.30721500	0.35870900
O	-1.52176100	-0.10074900	1.35436700
H	-2.14732700	0.62523100	1.45660400
C	2.71066200	0.25298500	-0.03726100
H	3.08378600	0.15229200	-1.06019400
H	2.86343100	1.27706300	0.28490500
H	3.29992300	-0.42053300	0.58259500
N	0.26365400	0.59190700	-0.02836000
C	0.25427900	2.05216300	0.00539000
H	1.23296600	2.43297700	0.26801700
H	-0.03264800	2.43713900	-0.97043200
H	-0.46367700	2.38256600	0.75152400

36_gas

0 1			
C	1.77682500	-0.27698800	-0.18994900
C	0.90195100	-0.51052000	1.03543600
C	-0.46922900	-1.07389500	0.70105200
C	-1.46543900	-0.12412300	0.07990400
H	0.82257400	0.41356400	1.60781200
H	-0.36000900	-1.92868300	0.02832500
C	2.93526200	0.67433900	-0.01489500
H	3.59664200	0.62662200	-0.87582600
H	2.54426400	1.68933500	0.08741000
H	3.48972200	0.45237900	0.89903000
O	1.56441400	-0.84437200	-1.23736300
H	1.44450700	-1.22222000	1.66790300
H	-0.93996800	-1.47183700	1.60751100
C	-2.70210700	-0.79632500	-0.43990400
H	-3.45697300	-0.07566100	-0.73867400
H	-2.43643700	-1.41100500	-1.30541000
H	-3.11720200	-1.47723100	0.30834200
S	-1.24787600	1.48779900	-0.02608600

36_sol

O	1			
C		-1.78708700	-0.24504800	0.21393800
C		-0.90750000	-0.58244800	-0.97502100
C		0.47167800	-1.11062200	-0.62052700
C		1.48210100	-0.13452900	-0.07869900
H		-0.84814800	0.28632000	-1.63088100
H		0.38871500	-1.93228100	0.09587000
C		-3.01737100	0.57260200	-0.08058000
H		-3.68082900	0.59199600	0.78001500
H		-2.71358800	1.59318900	-0.32514500
H		-3.54277400	0.18130900	-0.95264200
O		-1.52775400	-0.63244500	1.33707200
H		-1.44935800	-1.34627900	-1.54288100
H		0.92810500	-1.55881100	-1.51004700
C		2.74710800	-0.77291600	0.40674200
H		3.50355200	-0.03782200	0.66281400
H		2.52593800	-1.37858300	1.29058600
H		3.14027500	-1.46085600	-0.34583100
S		1.25228600	1.48494600	-0.02584700

37_gas

O	1			
C		-2.70641200	-0.26055600	0.00008300
C		-1.26118600	0.12361200	0.00000900
C		-0.71274000	1.37089000	-0.00006800
C		0.71276700	1.37089000	-0.00003800
C		1.26120600	0.12361500	-0.00000600
H		-2.97287300	-0.84971300	-0.87969100
H		-2.97277800	-0.84978000	0.87984100
H		-1.31188200	2.27082000	0.00005500
H		-3.32470200	0.63662400	0.00016100
H		1.31192200	2.27081100	0.00000700
C		2.70640500	-0.26058200	0.00008500
H		2.97275900	-0.84960800	0.87997700
H		2.97282100	-0.84992700	-0.87957600
H		3.32474100	0.63657400	-0.00006500
S		-0.00001500	-1.07643800	-0.00006800

37_sol

O	1			
C		-2.70969600	-0.26024200	0.00001300
C		-1.26415900	0.12391500	-0.00000300
C		-0.71370700	1.37098900	-0.00005000
C		0.71370700	1.37098900	-0.00005100
C		1.26415900	0.12391500	-0.00000600
H		-2.97497300	-0.85046200	-0.87907600
H		-2.97497000	-0.85040300	0.87914200
H		-1.31271200	2.27120500	-0.00008200
H		-3.32688500	0.63743700	-0.00001600
H		1.31271200	2.27120500	-0.00008500
C		2.70969600	-0.26024200	0.00000700
H		2.97497300	-0.85039700	0.87913900
H		2.97497000	-0.85046800	-0.87907800
H		3.32688600	0.63743600	-0.00003000
S		0.00000000	-1.07696900	0.00003900

38_gas

O	1			
C		1.34554300	-0.48801000	0.02329200
C		0.23186400	-1.07290400	0.47902000
C		-0.95937600	-0.38153400	1.09377800

C	-1.87644900	0.19865700	0.02021100
O	-1.79637100	1.36496000	-0.30079800
H	-1.51458400	-1.09779300	1.70148800
C	2.51257200	-1.27970600	-0.49875100
H	3.42926700	-1.02030500	0.03599100
H	2.33923600	-2.34774800	-0.37656500
H	2.68814700	-1.07024400	-1.55538000
H	0.18471600	-2.15386300	0.41159000
H	-0.63957900	0.44091900	1.73486500
C	-2.85937200	-0.74233400	-0.63275900
H	-3.32817400	-0.26573800	-1.48935800
H	-2.36425200	-1.66488800	-0.93968100
H	-3.62861500	-1.01886400	0.09296600
S	1.65342200	1.26126800	-0.01166300
H	0.38134900	1.69354500	0.06833200

39_gas

O 1			
C	1.47128100	0.13849800	-0.06140700
C	0.93945100	1.35507100	-0.16115300
C	-0.54542800	1.41230500	-0.36723500
C	-1.14205400	0.05990000	0.05719300
H	-0.77716200	1.61090900	-1.41847900
C	2.90920600	-0.22817000	0.10257000
H	3.07352200	-0.76997600	1.03624400
H	3.24856000	-0.87519800	-0.70939900
H	3.53111500	0.66630900	0.10806300
H	1.54170300	2.25364600	-0.12926400
O	-1.46208400	0.18895700	1.43461800
H	-1.60505600	-0.68665100	1.80894100
H	-1.02529000	2.19440500	0.22412800
C	-2.36451600	-0.37983700	-0.73795000
H	-2.72690300	-1.34890800	-0.39112100
H	-3.16424300	0.34805300	-0.59406800
H	-2.14183400	-0.45987100	-1.80023400
S	0.25841400	-1.16193600	-0.16274200

39_sol

O 1			
C	1.47860300	0.13747400	-0.05611000
C	0.94403100	1.35394400	-0.15485600
C	-0.53998900	1.40985200	-0.36843900
C	-1.14628700	0.06198400	0.05640600
H	-0.76487000	1.59982300	-1.42212400
C	2.91753500	-0.22803700	0.10631000
H	3.08363300	-0.77904100	1.03424100
H	3.25898100	-0.86675000	-0.71113400
H	3.53635400	0.66828500	0.12060100
H	1.54520900	2.25340800	-0.12535100
O	-1.46788000	0.18482000	1.43412300
H	-1.83295500	-0.64984000	1.74987900
H	-1.02264000	2.20157800	0.20715800
C	-2.36295500	-0.37590800	-0.74520200
H	-2.73408100	-1.34102200	-0.39746900
H	-3.15838600	0.35965600	-0.61747500
H	-2.12933000	-0.45989600	-1.80436700
S	0.26346800	-1.16378800	-0.15847500

40_gas

O 1			
C	1.61983800	-0.54412600	0.08498900
C	0.53186500	-1.14269000	0.58347300
C	-0.76077400	-0.50306300	1.01169700

C	-1.86998300	-0.62702300	-0.02858800
O	-2.43063300	0.35188500	-0.48199700
H	-1.11923100	-1.00670300	1.91620300
C	2.85617100	-1.33052300	-0.26466700
H	3.72124200	-0.96545500	0.29291700
H	2.72019500	-2.38553100	-0.03287400
H	3.09412700	-1.23474600	-1.32577600
H	0.59174900	-2.21905800	0.70230900
H	-0.63674400	0.54904200	1.25644400
C	-2.25676300	-2.01377000	-0.47711600
H	-3.12885800	-1.96738800	-1.12323600
H	-1.42525600	-2.46690800	-1.01993600
H	-2.46045700	-2.65296600	0.38392200
S	1.86047200	1.18372500	-0.23271600
H	0.62763000	1.67304500	0.01249900
O	-1.22635800	2.78757300	0.19308400
H	-1.42459200	3.53397700	-0.37786400
H	-1.79355300	2.05461300	-0.10857100

40_sol

O 1			
C	1.60613400	-0.61855400	0.04773600
C	0.49343500	-1.20903800	0.49494600
C	-0.76553400	-0.56291500	1.00992300
C	-1.87898500	-0.57950200	-0.02903000
O	-2.26540200	0.44995600	-0.55890100
H	-1.11447400	-1.12424500	1.88087400
C	2.80479700	-1.41489400	-0.39489000
H	3.69305900	-1.13726600	0.17671500
H	2.62804100	-2.47972300	-0.25646500
H	3.02994200	-1.23278900	-1.44741000
H	0.49912500	-2.29306000	0.49748700
H	-0.59767700	0.46564600	1.32062300
C	-2.49496100	-1.90603100	-0.36943500
H	-3.16580100	-1.81069500	-1.21860500
H	-1.72715700	-2.65083600	-0.57864400
H	-3.05501100	-2.26508800	0.49756100
S	1.91964500	1.12915700	-0.08777200
H	0.69132500	1.63492000	0.13583000
O	-1.16604800	2.92128100	0.13875500
H	-1.12036700	3.49460100	-0.63259200
H	-1.61303700	2.10771800	-0.16534500

41_gas

O 1			
C	1.70818400	0.26451700	-0.02574100
C	1.71630500	-0.93110600	-0.61114200
C	0.49568100	-1.77957300	-0.40881700
C	-0.67026200	-0.86455500	0.00310900
H	0.67881400	-2.52734600	0.36959100
C	2.79025900	1.29322200	-0.01588300
H	2.45701300	2.22241200	-0.48310100
H	3.09649600	1.53747600	1.00374100
H	3.66411500	0.93051900	-0.55614000
H	2.56738800	-1.28965800	-1.17561200
O	-1.28423500	-0.43801200	-1.18390900
H	-1.90387200	0.28669600	-0.99600700
H	0.19935800	-2.31490500	-1.31248100
C	-1.67851600	-1.49496400	0.95503400
H	-2.46688200	-0.78556200	1.20848000
H	-2.14343600	-2.34930400	0.46047200
H	-1.20505100	-1.83062600	1.87580500
S	0.19755600	0.58815700	0.86238900
O	-2.47679900	2.04696600	-0.38020800
H	-1.57618200	2.16093200	-0.03910100
H	-2.61029300	2.75199600	-1.02030800

41_sol

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0 1
C      -1.87193000   -0.33032100   -0.09624200
C      -1.81752700    0.85895200   -0.69562600
C      -0.58780500    1.67698500   -0.43323200
C       0.53022600    0.74490900    0.06690300
H      -0.79666900    2.44142100    0.32152900
C      -2.98322900   -1.32811100   -0.12954800
H      -2.65158900   -2.27631400   -0.55766300
H      -3.35289200   -1.54299600    0.87548600
H      -3.81396100   -0.95122400   -0.72504800
H      -2.62964000    1.23626800   -1.30372800
O       1.23310000    0.29293300   -1.06600000
H       1.96896000   -0.28887900   -0.79562600
H      -0.22691000    2.19777100   -1.32188800
C       1.47205000    1.37471500    1.08434500
H       2.22842800    0.66025900    1.40946100
H       1.98199700    2.22040700    0.61983600
H       0.93142600    1.72956000    1.95920800
S      -0.41192100   -0.69607900    0.85722700
O       3.38093100   -1.40525500   -0.38409600
H       3.33164300   -2.29234900   -0.75653400
H       4.25699400   -1.08085500   -0.61949300

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42_gas

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1 1
C      -1.45731500   -0.80444700   -0.10430800
C      -0.21632400   -1.22214800    0.16543500
C       0.83233100   -0.48301400    0.97805000
C       2.01553100   -0.25094500    0.09140000
O       2.13805800    0.79684500   -0.59177500
H       0.45826500    0.46654600    1.35780500
C      -2.43295500   -1.63593200   -0.88324700
H      -2.78211000   -1.09864000   -1.76720700
H      -1.97372300   -2.56697700   -1.20925900
H      -3.30805700   -1.87478800   -0.27721800
H       0.07085300   -2.20109200   -0.19711200
H      -0.51101100    2.30366100   -0.29327200
H       1.14219400   -1.09214000    1.82976400
H       1.39340500    1.53580800   -0.49833400
O       0.41917100    2.58563800   -0.37809100
H       0.46058300    3.38623100   -0.91288200
H      -3.17128400    0.81121900   -0.22717200
C       3.07882000   -1.26579700   -0.03061800
H       3.72702200   -1.07218400   -0.87972800
H       3.67153600   -1.23023700    0.89161700
H       2.65342100   -2.26883000   -0.07554500
S      -2.07559100    0.73845300    0.54482500

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42_sol

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1 1
C      -1.45923500   -0.80413800   -0.11872000
C      -0.21462600   -1.22717100    0.11202800
C       0.83413600   -0.52544200    0.95104200
C       2.03207600   -0.23492300    0.09904900
O       2.13963500    0.83574200   -0.54651200
H       0.45695800    0.40139800    1.37865500
C      -2.43560800   -1.58403900   -0.94800900
H      -2.78502000   -0.98912800   -1.79404100
H      -1.97103800   -2.49000300   -1.33275000
H      -3.31195300   -1.86094500   -0.36035900
H       0.07952100   -2.17546000   -0.31970400

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H	-0.51375400	2.22847200	-0.23663600
H	1.14586200	-1.17287500	1.77173000
H	1.35587900	1.55444600	-0.46896400
O	0.37875700	2.58219600	-0.42100700
H	0.31715200	3.09755900	-1.23503600
H	-3.11197200	0.87750400	-0.21000600
C	3.12481800	-1.21529000	-0.01508100
H	3.80522800	-0.96837200	-0.82317600
H	3.66532100	-1.20854100	0.93776400
H	2.72281200	-2.22252900	-0.12542000
S	-2.08071900	0.69568700	0.62976500

43_gas

1 1			
C	-1.38944800	-0.74404700	0.12779200
C	-0.71817900	-1.12085200	1.21081500
C	0.70365900	-0.69707400	1.38534600
C	1.31950600	-0.30419300	0.03637900
H	1.31162000	-1.48630600	1.83210200
C	-2.80685400	-0.98936800	-0.26221700
H	-3.35730800	-0.05374000	-0.37663200
H	-2.87485000	-1.52750700	-1.20880200
H	-3.30052200	-1.58075500	0.50712500
H	-1.20650600	-1.70034700	1.98463100
O	2.10612600	0.80599200	0.16758700
H	2.77504300	0.85003500	-0.52726300
H	0.76087900	0.16248400	2.05838200
O	-0.61762700	3.03809200	0.30408800
H	-1.29320400	3.70652500	0.14628800
H	-0.47466700	1.45031700	-0.48882900
H	0.15617700	3.50839400	0.63267400
C	1.96064900	-1.43787000	-0.73533900
H	2.28759100	-1.11480100	-1.72394800
H	2.82961500	-1.78412700	-0.17329000
H	1.27725300	-2.27694200	-0.85508500
S	-0.32594400	0.17840700	-1.00983800

43_sol

1 1			
C	-1.31478800	-0.84378100	0.11654500
C	-0.61583600	-1.22181900	1.18083800
C	0.77585400	-0.71246200	1.36525200
C	1.34163200	-0.20514200	0.03276700
H	1.44006000	-1.48329400	1.75900900
C	-2.71351500	-1.17116700	-0.27839000
H	-3.32254700	-0.26955400	-0.36105600
H	-2.74414900	-1.67766800	-1.24405900
H	-3.16078900	-1.82172800	0.47116700
H	-1.05745500	-1.86687800	1.92964800
O	2.05242400	0.95016500	0.22009000
H	2.64818000	1.11526600	-0.52218300
H	0.78116500	0.11053400	2.08414800
O	-0.94403000	2.96511500	0.37930200
H	-1.43677500	3.57784200	-0.17918900
H	-0.58785300	1.43730500	-0.42283500
H	-0.14008400	3.43582700	0.62918300
C	2.06070900	-1.25102700	-0.79263500
H	2.35251700	-0.85616900	-1.76480900
H	2.95649200	-1.55294900	-0.24896300
H	1.43738600	-2.13013500	-0.94487100
S	-0.32735200	0.19323400	-0.98291200

44_gas

0	1			
C		1.87857800	-0.47923500	0.02650600
C		1.06723700	-1.28325500	0.71032700
C		-0.26972100	-0.71233200	1.08038200
C		-0.54043300	0.49459300	0.16848400
H		-0.27065700	-0.39269200	2.12712400
C		3.27317100	-0.74409100	-0.43485600
H		3.34524000	-0.69349000	-1.52320500
H		3.97086000	-0.00690500	-0.03123200
H		3.59873200	-1.73256800	-0.11284700
H		1.36265800	-2.27834900	1.01590300
O		-1.20828300	-0.02493900	-0.99162400
H		-1.09035000	0.59216800	-1.72193300
H		-1.08800500	-1.42516400	0.96486000
O		-3.85920500	-0.99874000	-0.37043500
H		-2.98677000	-0.72556700	-0.69457100
H		-4.08337300	-1.78879600	-0.86828600
C		-1.37157800	1.60314800	0.79715200
H		-1.51900300	2.42557300	0.09592100
H		-2.35234600	1.20789900	1.06391200
H		-0.89065600	1.99707800	1.69032800
S		1.14500300	1.10858000	-0.32484200

45_gas

1	1			
C		-2.67280300	-0.33688800	0.00002200
C		-1.24035000	0.02575500	-0.00000600
C		-0.71545100	1.41279100	0.00000100
C		0.76936800	1.36216300	0.00001600
C		1.30254300	0.13725900	0.00000300
H		-3.16269600	0.09899200	0.87545200
H		-3.16287200	0.09943800	-0.87508100
H		-1.11890300	1.95657600	-0.86575400
H		-2.83745400	-1.41082200	-0.00021800
H		1.36662500	2.26306200	0.00002900
C		2.71985300	-0.32056900	0.00000200
H		2.94489600	-0.92306800	0.88121600
H		2.94490300	-0.92304500	-0.88122700
H		3.38167000	0.54319200	0.00001600
H		-1.11893700	1.95660000	0.86572400
S		-0.01351200	-1.08400000	-0.00002400

45_sol

1	1			
C		-2.66781000	-0.33467400	0.00002200
C		-1.23748100	0.02642200	-0.00000500
C		-0.71525200	1.41064400	0.00001000
C		0.76754700	1.36011100	0.00002200
C		1.29780700	0.13505400	0.00000200
H		-3.15111800	0.10498600	0.87575500
H		-3.15126800	0.10535200	-0.87543900
H		-1.11968400	1.95149000	-0.86559600
H		-2.82954400	-1.40821100	-0.00017400
H		1.36445200	2.26027800	0.00003900
C		2.71704000	-0.31613700	-0.00000100
H		2.94139800	-0.91886900	0.88075900
H		2.94140600	-0.91883200	-0.88078500
H		3.37239700	0.55238700	0.00002000
H		-1.11971000	1.95149700	0.86559800
S		-0.01371400	-1.08553800	-0.00003000

46-cis_gas

O 1			
C	-1.26344400	-0.40493000	0.05856700
C	-0.18266000	-0.81000800	-0.97446300
C	1.25686200	-1.01856400	-0.49924800
C	2.06395200	0.20200900	-0.09861600
O	1.61166300	1.32555500	-0.11898400
H	1.31030400	-1.73552700	0.32519100
H	-0.52334600	-1.76364500	-1.38075900
H	1.81493500	-1.50061100	-1.30935000
H	-0.52303100	1.90614300	0.10374900
H	-0.19740500	-0.09815600	-1.79703700
C	3.49083700	-0.05941100	0.33472200
H	3.49743200	-0.65036300	1.25359300
H	4.02650900	-0.63978300	-0.41835600
H	4.00350900	0.88238600	0.50968300
S	-1.75117900	1.39882500	-0.09508100
C	-0.90885500	-0.73518600	1.50529500
H	-0.67991200	-1.79907100	1.60137500
H	-0.05916300	-0.15272300	1.85791600
H	-1.75308000	-0.50510400	2.15445400
O	-2.42230900	-1.13437000	-0.32964700
H	-3.15287300	-0.89768800	0.25234500

47-cis_gas

O 1			
C	1.36024800	0.03698400	0.01569600
C	0.68162100	1.08747900	0.90844800
C	-0.68096500	1.38040100	0.29656900
C	-1.38768300	0.04787400	-0.02443900
H	-1.31040600	1.98796200	0.94842100
C	2.54892400	-0.65558000	0.66920800
H	2.96095400	-1.41666200	0.00776400
H	3.33508400	0.07644700	0.87773600
H	2.26559800	-1.12533900	1.60894800
H	1.30462700	1.98348200	0.96986000
H	-0.54807200	1.92868800	-0.63622800
H	-1.69198000	0.31785100	-1.92874500
O	-2.23372200	0.14575500	-1.15078000
H	0.57675100	0.69061000	1.92002200
O	1.75620100	0.62438200	-1.23128100
H	2.58197100	1.10341900	-1.09566300
C	-2.26444600	-0.46036000	1.11003000
H	-3.11781700	0.20873300	1.23247300
H	-2.63890800	-1.45791900	0.88646400
H	-1.70647100	-0.50136300	2.04364800
S	0.01641500	-1.16111200	-0.35195500

48-cis_gas

O 1			
C	-1.54745100	-0.25489500	-0.18418400
C	-0.43616700	-0.49098100	-1.21769100
C	0.73077600	-1.36989200	-0.76799100
C	1.93520900	-0.64553200	-0.18975800
O	2.22126700	0.49315600	-0.49738700
H	0.41654800	-2.14819400	-0.07237300
H	-0.92155200	-0.94160300	-2.08608800
H	1.13347500	-1.90732200	-1.63540300
H	-0.34597300	1.58517000	0.83706200
H	-0.06225900	0.47892800	-1.54227800
O	0.91725600	3.01017600	-0.27239600
H	1.49044600	2.25370600	-0.47013200
H	1.49574100	3.68682300	0.08833300
C	2.80926700	-1.44420800	0.74372600
H	3.75174200	-0.93127400	0.91469000

H	2.28372700	-1.56199200	1.69453700
H	2.98926200	-2.44652200	0.35113600
S	-0.91187300	0.49550900	1.39878500
C	-2.27722200	-1.53962600	0.21517500
H	-3.09924400	-1.31209100	0.89396700
H	-2.69086500	-2.00506800	-0.67978100
H	-1.62287300	-2.25330200	0.71397300
O	-2.44442400	0.63115100	-0.83082700
H	-3.06746700	0.96954300	-0.17898300

48-cis_sol

0 1			
C	-1.55326500	-0.27271800	-0.19998500
C	-0.40016800	-0.44198500	-1.19858700
C	0.77064400	-1.31675400	-0.75435300
C	1.97048500	-0.60583400	-0.16308200
O	2.18556100	0.58228900	-0.33155700
H	0.46408600	-2.10708400	-0.06897500
H	-0.84580000	-0.86842600	-2.09921000
H	1.17639400	-1.84796700	-1.62305900
H	-0.40315400	1.51496000	0.96676500
H	-0.03642400	0.54760200	-1.47217200
O	0.87504100	3.08501900	-0.32278400
H	1.37488400	2.25402200	-0.39272700
H	1.43446100	3.67428500	0.19249200
C	2.93146900	-1.46551000	0.61083900
H	3.86241400	-0.93538300	0.79202700
H	2.47214800	-1.72607100	1.56762400
H	3.12399700	-2.40249900	0.08730000
S	-0.97888200	0.39844700	1.45158700
C	-2.28281100	-1.58001400	0.10298700
H	-3.13504600	-1.39957700	0.75851000
H	-2.64922200	-2.00618000	-0.83098100
H	-1.63624400	-2.30898200	0.58801300
O	-2.43020100	0.65181900	-0.82303700
H	-3.20171300	0.78003200	-0.25889300

49-cis_gas

0 1			
C	-0.86870800	-0.88315900	0.01684000
C	0.22825900	-1.87819400	0.42218000
C	1.60860400	-1.18435800	0.43681300
C	1.48179000	0.30868800	0.05958300
H	2.27089600	-1.66962000	-0.27897200
C	-2.05785700	-1.51763600	-0.68853900
H	-2.80914700	-0.76739400	-0.93562600
H	-1.75127300	-2.01623800	-1.60667300
H	-2.51808600	-2.24967200	-0.02321500
H	0.23287900	-2.69961200	-0.29229400
H	2.08848500	-1.24215500	1.41397800
H	-0.03569700	-2.29236800	1.39546000
O	-1.28179600	-0.22741500	1.21190200
H	-1.90506400	0.48647500	0.98926200
S	0.01386900	0.31367700	-1.11306000
O	-2.35398700	2.18116400	0.21241400
H	-3.06320100	2.57881600	-0.29966700
H	-1.59414700	2.09637900	-0.38613400
C	2.71115500	0.87532200	-0.62613000
H	2.55801400	1.92482700	-0.87207300
H	3.55973400	0.81069500	0.05663200
H	2.94535100	0.32497200	-1.53516400
O	1.23244800	1.11603800	1.18408900
H	0.40657900	0.81378900	1.59170000

50-cis_gas

1	1			
C		-1.59846000	0.35951600	-0.16093200
C		-0.37451700	0.74100500	-1.01869100
C		0.57982000	-0.41905600	-1.36093800
C		1.37951100	-0.99305200	-0.23376500
O		2.22702500	-0.29451500	0.40610900
H		0.04038700	-1.22667400	-1.84883000
H		-0.75389500	1.15295300	-1.95408900
H		1.31703000	-0.05215400	-2.08549400
H		0.17318600	1.54824500	-0.52907800
O		2.59337900	2.24635200	0.08791800
H		2.30313600	0.69566800	0.19980900
H		2.70059900	2.73486600	0.91295600
C		1.43500600	-2.44788500	0.01383500
H		1.88132400	-2.66971800	0.97863700
H		0.45717700	-2.90919500	-0.08727600
H		2.07746100	-2.87378300	-0.76916700
H		3.25230200	2.59786200	-0.52220800
S		-0.88840600	-0.25669200	1.46524200
H		-1.90067800	-1.06765000	1.81520600
O		-2.40945700	1.48697100	0.02898400
H		-1.96438900	2.15121500	0.56670900
C		-2.49620100	-0.68723800	-0.80590000
H		-3.36828600	-0.85752000	-0.17805700
H		-2.84806500	-0.30964400	-1.76669500
H		-1.99133400	-1.63760400	-0.96203400

50-cis_sol

1	1			
C		-1.60452400	0.31369500	-0.17954200
C		-0.33846700	0.73375900	-0.95057200
C		0.64738400	-0.38997300	-1.31963600
C		1.51420500	-0.93063000	-0.23058600
O		2.26143500	-0.18887700	0.46527200
H		0.13558200	-1.21960300	-1.79886600
H		-0.67912700	1.18633100	-1.88180600
H		1.34766900	0.00986600	-2.06227800
H		0.17429000	1.52205700	-0.39994700
O		2.44323500	2.30651300	0.13049600
H		2.27778400	0.83400000	0.28246500
H		2.58913400	2.78247400	0.95733800
C		1.65443600	-2.38394900	-0.02657100
H		2.25454200	-2.60902100	0.84885400
H		0.67677200	-2.85803600	0.02780800
H		2.14588600	-2.78596000	-0.92012700
H		3.14634900	2.58161200	-0.47061600
S		-1.04193600	-0.37364100	1.47253800
H		-2.08342700	-1.19527300	1.67795200
O		-2.42525800	1.45114800	0.00397100
H		-1.94159500	2.12889000	0.49059000
C		-2.46361500	-0.69800200	-0.92278900
H		-3.38027600	-0.88339400	-0.36579500
H		-2.73164500	-0.28980400	-1.89817200
H		-1.95277900	-1.64555500	-1.06773800

51-cis_gas

1	1			
C		1.26204900	-0.75856800	0.12071800
C		0.48149200	-0.54145000	1.40060800
C		-0.98245100	-0.83918100	1.19662800
C		-1.54120500	0.06493500	0.11455800
O		-1.55694300	1.36017300	0.56959400
H		-1.13559600	-1.88174900	0.90410400
H		0.92288600	-1.19104300	2.16243800

H	-1.56419200	-0.67066800	2.10582400
H	0.25485200	1.18876700	-1.13132100
H	0.61173500	0.48879200	1.74193200
O	1.46588400	2.59296200	0.00625000
H	0.98453200	3.08460500	0.67751900
H	2.05280000	3.22813700	-0.41478100
C	-2.84994800	-0.39120600	-0.46471500
H	-3.20247800	0.28598500	-1.24544500
H	-2.76975500	-1.38987600	-0.89403600
H	-3.59305400	-0.41918100	0.33611800
S	-0.17324600	-0.08943900	-1.26515400
H	-2.22280300	1.87765700	0.10472300
C	1.50975800	-2.17819800	-0.28053500
H	0.59998400	-2.77728300	-0.27237400
H	1.96440700	-2.22556300	-1.26860000
H	2.21324700	-2.60621300	0.43794700
O	2.35957300	-0.02711900	-0.04807300
H	2.22909600	0.89254400	0.25268100

51-cis_sol

1 1			
C	1.23757600	-0.72933200	0.10059900
C	0.48978800	-0.50264200	1.40121100
C	-0.97381500	-0.81610600	1.21756100
C	-1.54356800	0.05502300	0.11692000
O	-1.60460700	1.34827700	0.55404500
H	-1.12292000	-1.86602500	0.95493500
H	0.94853200	-1.13677300	2.16415800
H	-1.55225200	-0.62427600	2.12366400
H	0.26860300	1.20815700	-1.09937700
H	0.62091600	0.53521900	1.71756100
O	1.40828500	2.55483000	0.01059800
H	0.93699900	3.01678500	0.70976400
H	1.92299900	3.22603600	-0.44648500
C	-2.81499700	-0.44714900	-0.50146600
H	-3.16123800	0.21510400	-1.29616800
H	-2.68463000	-1.44709900	-0.91373500
H	-3.57871500	-0.48737200	0.27843800
S	-0.12617200	-0.08218300	-1.24112000
H	-2.17318700	1.87963200	-0.01497400
C	1.48412700	-2.16405100	-0.26057500
H	0.56914400	-2.75460600	-0.24689900
H	1.93900300	-2.23726400	-1.24725400
H	2.17568400	-2.57955300	0.47541700
O	2.37200200	-0.01841500	-0.05752500
H	2.22970800	0.91496300	0.19642900

52-cis_gas

0 1			
C	-1.76231100	-0.41295400	-0.02103800
C	-0.64879500	-1.31380100	0.54902100
C	0.47224600	-0.44597500	1.10572700
C	0.79196500	0.61491800	0.05200200
H	1.37008100	-1.02250900	1.33319600
H	-0.25999200	-1.93414100	-0.25899500
H	0.15774900	0.05525700	2.02165000
H	-1.06595200	-1.98421000	1.30168600
O	1.52066800	-0.06148300	-0.99223800
H	1.50739200	0.48959100	-1.78157200
C	1.60437100	1.79445300	0.56700800
H	2.57618900	1.43948000	0.91241700
H	1.77238700	2.52889500	-0.22213300
H	1.09245600	2.29191500	1.38863300
O	3.98626800	-1.13675100	0.06033700
H	4.30622900	-1.90662100	-0.41627200
H	3.20306100	-0.83397500	-0.42521800

S	-0.86244500	1.15995900	-0.56044600
O	-2.43872800	-1.00524300	-1.10611700
H	-1.80717500	-1.17466500	-1.81316400
C	-2.83684600	-0.06039400	0.99626300
H	-3.52846600	0.67296000	0.58516500
H	-3.39885400	-0.96083200	1.24949700
H	-2.39544000	0.34984600	1.90250000

52-cis_sol

O 1			
C	-1.73675500	-0.47025400	-0.01662800
C	-0.61978500	-1.21749100	0.73330600
C	0.40844700	-0.21119000	1.23320500
C	0.76072700	0.71062600	0.06523600
H	1.31116900	-0.69782500	1.60489300
H	-0.14318600	-1.91249700	0.04120700
H	-0.00023200	0.38987300	2.04528200
H	-1.04872100	-1.80454500	1.54598000
O	1.61180800	-0.04728000	-0.80913800
H	1.73860700	0.44312500	-1.62950800
C	1.44515200	2.00935700	0.46486000
H	2.39918600	1.78084200	0.94194800
H	1.64200800	2.63294500	-0.40809100
H	0.83016900	2.57622900	1.16086500
O	4.08245500	-1.26593600	-0.01668100
H	3.95803900	-2.21521100	-0.10978800
H	3.22979000	-0.87246400	-0.27156900
S	-0.87620300	1.04877200	-0.74095900
O	-2.32178900	-1.25182800	-1.03870200
H	-1.63039000	-1.55499600	-1.63844500
C	-2.88149400	-0.02898800	0.88211000
H	-3.58676500	0.59210600	0.33158100
H	-3.40817100	-0.90987900	1.25290000
H	-2.50980000	0.53992900	1.73172300

53_gas

1 1			
C	1.22412100	0.08919100	0.04672300
C	0.56250500	1.32906800	-0.54612100
C	-0.88993500	1.39539700	-0.07798600
C	-1.43977100	0.00921500	-0.03522600
H	-1.51658500	2.03809100	-0.69864600
C	2.39545600	-0.49250800	-0.70975800
H	2.75909300	-1.40799700	-0.24118000
H	2.13765900	-0.71300300	-1.74352900
H	3.20715100	0.23705900	-0.70451100
H	0.59689000	1.26781800	-1.63313400
H	-0.96821900	1.79486100	0.94163700
H	1.13090400	2.20502400	-0.23626400
O	1.45103000	0.29337000	1.38484200
H	2.10422300	-0.32243700	1.73956700
C	-2.89147400	-0.25451600	0.04622800
H	-3.37445500	0.13846700	-0.85426200
H	-3.13505000	-1.30691200	0.15567100
H	-3.31337700	0.31105300	0.88247600
S	-0.31261800	-1.19025400	-0.06435800

53_sol

1 1			
C	1.21037700	0.08404000	0.04344300
C	0.55425100	1.34329600	-0.51371700
C	-0.90261300	1.39709400	-0.06123900
C	-1.43923400	0.00915000	-0.03191200

H	-1.52697800	2.03259300	-0.68991900
C	2.37093200	-0.47581800	-0.74750300
H	2.75085600	-1.39333900	-0.29806300
H	2.08504800	-0.68274600	-1.77616400
H	3.17247200	0.26372800	-0.74923800
H	0.59570100	1.31075000	-1.60075800
H	-1.00403300	1.79027900	0.95786300
H	1.12124400	2.20877100	-0.17587600
O	1.48399900	0.26657500	1.38599600
H	2.08408400	-0.41575100	1.71205100
C	-2.88616300	-0.27009000	0.03329400
H	-3.34994400	0.09123100	-0.88933800
H	-3.11584200	-1.32222300	0.16624200
H	-3.32572700	0.31629500	0.84364300
S	-0.30026100	-1.17863900	-0.05766200

TS(1-11)_gas

O 1			
C	-1.17716400	-0.62473900	0.05907700
C	0.09383100	-1.47918200	-0.08474900
C	1.32770500	-0.91367200	0.62047800
C	2.11244300	0.13262700	-0.12905800
O	1.63807900	0.77273700	-1.05340700
H	1.00010000	-0.44412800	1.55651400
C	-2.42079400	-1.34370600	-0.44808100
H	-2.66350000	-2.14701100	0.24765200
H	-3.26248200	-0.65317100	-0.47379600
H	-2.27632600	-1.76035600	-1.44418200
O	-1.29620900	-0.04570600	1.23872400
H	-0.14456700	-2.43760400	0.37978500
H	2.01278500	-1.71365000	0.90909400
H	-0.05567500	0.72363800	-1.17976200
H	0.29190600	-1.68141400	-1.13846000
C	3.52940900	0.37628900	0.31954300
H	3.57908200	0.46718300	1.40563500
H	4.14653700	-0.48284000	0.04491600
H	3.92769800	1.27011900	-0.15220700
H	-1.49639300	1.42845700	-0.52031100
O	-1.96588200	2.10833700	0.48935800
H	-1.76733600	1.10458900	1.05700300
H	-2.90398000	2.31171100	0.44842000
O	-1.02354300	0.55573000	-1.07012200

TS(1-21)_gas

O 1			
C	-1.25385100	-0.57209000	0.24761800
C	-0.08579000	-1.57385400	0.03612900
C	1.30020500	-1.13294500	0.50084900
C	2.07613900	-0.25192300	-0.45643300
O	1.67986500	-0.00299300	-1.58132700
H	1.24713800	-0.62153600	1.46338100
C	-2.55723700	-1.21738700	-0.22134800
H	-2.72263000	-2.10842300	0.38179300
H	-3.40032200	-0.55092700	-0.05431600
H	-2.52762100	-1.51514500	-1.27136900
O	-1.36125200	-0.10238200	1.50622400
H	-0.37251800	-2.44992400	0.61835800
H	1.92627600	-2.01615300	0.67005700
H	-0.34185700	0.40194600	-1.46988000
H	-0.04481800	-1.88743800	-1.00980300
C	3.36699800	0.32036400	0.06357400
H	3.10635100	1.10351300	0.78012500
H	3.95133500	-0.42873100	0.59906300
H	3.94945500	0.74778200	-0.74834600
N	-0.92937800	0.68797600	-0.68647300
C	-2.06882700	1.52348400	-1.11147600

H	-1.68736100	2.43550800	-1.56698300
H	-2.69234900	0.99706700	-1.82849500
H	-2.65555800	1.78294200	-0.23435300
H	-0.32306500	1.27699000	-0.02483200
O	0.29375400	1.63431400	1.40594800
H	-0.55885700	0.75493800	1.64500500
H	0.08729000	2.45635500	1.85567200

TS(3-4)_gas

O 1			
C	1.42101800	-0.02626200	-0.12009600
C	0.88539300	1.17131800	0.23710900
C	-0.59100300	1.28973300	0.07052200
C	-1.35438000	0.01728900	0.12715500
H	-1.03814300	1.87057800	0.89488900
C	2.90433700	-0.28452000	-0.16430800
H	3.19454300	-0.56547800	-1.17820000
H	3.47852400	0.58846400	0.14217300
H	3.15823800	-1.12344300	0.48597300
H	1.47388500	2.03089500	0.51573000
H	-0.87939100	1.82055500	-0.84399100
H	-0.25156400	-1.13212800	1.00262500
O	-1.21240600	-0.86113100	1.08445100
O	0.62844600	-1.00915500	-0.45049100
C	-2.57650200	-0.14969000	-0.70049100
H	-3.30640400	-0.76678300	-0.18093900
H	-3.00431000	0.80773500	-0.99420300
H	-2.28688600	-0.67532400	-1.61507200

TS(4-2)_gas

O 1			
C	-1.38683700	0.01546000	-0.07350400
C	-0.95259000	-1.03453800	-0.77140100
C	0.51611800	-0.93301900	-0.89643900
C	0.80395800	0.34521100	-0.27695800
O	-0.30716500	0.88759800	0.19027600
H	1.03312400	-1.20502300	-1.81038100
C	-2.69037300	0.44755300	0.47657100
H	-2.66078700	0.49399400	1.56686400
H	-2.96491800	1.43876400	0.11025600
H	-3.46551000	-0.25722600	0.18293400
H	-1.55964400	-1.86105300	-1.09924800
O	1.59375500	-0.96527300	1.27162600
H	1.72954600	-1.09777200	2.21825600
H	1.01808800	-1.51761600	0.04584200
C	1.99493300	1.21329600	-0.39410200
H	2.88923800	0.60399400	-0.46914000
H	1.90018800	1.83046700	-1.29425500
H	2.07670300	1.86909700	0.46864800

TS(5-6)_gas

O 1			
C	1.45595500	-0.17188700	0.11489500
C	1.17497900	-1.33244400	-0.48425800
C	-0.27719200	-1.73784400	-0.48787800
C	-1.12363900	-0.54445400	-0.07739800
O	-1.53118300	0.22137200	-1.01762200
H	-0.60241800	-2.03923200	-1.48621900
C	2.80770800	0.45313800	0.25790800
H	3.57794300	-0.16376200	-0.20107000
H	2.82898000	1.44009600	-0.21129800
H	3.04967600	0.59479900	1.31311300
O	0.42287100	0.49569700	0.67691600

H	1.92883400	-1.96170900	-0.93219900
H	-0.01276600	1.61738200	0.20595000
H	-0.45970600	-2.57799400	0.18887600
H	-1.34144000	1.38830800	-0.72415500
O	-0.76440800	2.33438200	-0.26491100
H	-0.35683100	2.85210900	-0.96593800
C	-1.91222600	-0.60925700	1.20097200
H	-2.26621800	0.37920900	1.48570100
H	-2.78540400	-1.24229400	1.01540900
H	-1.33240900	-1.04203400	2.01132100

TS(7-8)_gas

1 1			
C	1.56762300	0.05533000	0.10030200
C	1.46831500	-1.15950500	-0.41912400
C	0.13214000	-1.86689700	-0.39358900
C	-0.97662400	-0.91093000	-0.07831500
H	-0.07822000	-2.30505700	-1.37250300
C	2.75416000	0.94787600	0.18361400
H	2.99594900	1.16805800	1.22451800
H	3.61616300	0.48200100	-0.28707200
H	2.56503200	1.89922900	-0.32005400
H	2.31696700	-1.67412600	-0.84116200
H	0.13115300	-2.67307300	0.34235000
H	0.12615200	1.41121500	0.39367500
O	-1.42148000	-0.25644600	-1.10105700
O	0.39437400	0.52339600	0.69957400
O	-1.39148000	2.50130100	-0.24970100
H	-1.80375700	3.09586900	0.38846100
H	-2.09094600	0.41073200	-0.86556700
H	-1.25910600	3.03688200	-1.04127100
C	-1.79802200	-1.02430900	1.14871500
H	-2.40014500	-0.13498600	1.32598600
H	-2.47476200	-1.87329200	0.99642500
H	-1.18134000	-1.23884900	2.01607200

TS(7-8)_sol

1 1			
C	1.51880600	-0.22247300	0.14351600
C	1.17808600	-1.39652200	-0.37636100
C	-0.25468700	-1.87363100	-0.28629000
C	-1.19659100	-0.72863900	-0.11737800
H	-0.53336900	-2.38399000	-1.21203500
C	2.86108900	0.42402100	0.12967200
H	3.21458400	0.59165300	1.14851700
H	3.58219800	-0.19497200	-0.39869600
H	2.81272500	1.39769000	-0.36357200
H	1.90362200	-2.03925900	-0.84934600
H	-0.39492700	-2.57725500	0.53441200
H	0.37361000	1.36899400	0.48461700
O	-1.34467500	0.00361200	-1.16095300
O	0.51354500	0.45491100	0.81429400
O	-0.71957900	2.65337300	-0.24417000
H	-1.09614900	3.29889500	0.36484400
H	-1.89337800	0.79498300	-1.00538800
H	-0.36866000	3.16836100	-0.97982700
C	-2.11996200	-0.61333200	1.02496800
H	-2.56308100	0.37645400	1.10355400
H	-2.92241800	-1.33776500	0.83976800
H	-1.62952700	-0.89550700	1.95102600

TS(8-10)_gas

1 1

C	1.49664600	-0.10975900	0.03556700
C	1.39013600	-1.28328900	-0.56185800
C	-0.03092400	-1.76357300	-0.55254100
C	-0.79119300	-0.58748600	0.08734100
O	0.22916400	0.35601900	0.49534700
H	-0.15263500	-2.67147700	0.04023800
C	2.63213400	0.78269600	0.35641000
H	2.52702600	1.76188100	-0.11796900
H	2.71153300	0.94027700	1.43344000
H	3.55963700	0.33929300	0.00283100
H	2.21568300	-1.83792900	-0.97545100
O	-1.54214000	0.15605800	-0.92872100
H	-2.36570300	-0.29918500	-1.14258400
H	-0.41731200	-1.97247100	-1.55118900
O	-0.96244700	2.41940200	-0.18105700
H	-0.60799600	3.11035400	-0.76147400
H	-0.23337000	1.80832300	0.22802100
H	-1.45062800	1.66185400	-0.69274600
C	-1.67865300	-0.91663400	1.26377600
H	-2.13509700	-0.01796500	1.67674000
H	-2.46653400	-1.60772700	0.96137900
H	-1.09009500	-1.39879100	2.04204800

TS(8-10)_sol

1 1			
C	1.47006700	-0.18142500	0.04979300
C	1.32719600	-1.35878400	-0.53709300
C	-0.11140500	-1.78279200	-0.53155300
C	-0.83483200	-0.55990200	0.06833000
O	0.23341400	0.33350100	0.50117600
H	-0.27577100	-2.67017600	0.08146100
C	2.64322700	0.67075200	0.34893700
H	2.56936200	1.64039500	-0.14800200
H	2.72474400	0.85400000	1.42175800
H	3.55083900	0.17866100	0.00827100
H	2.13659300	-1.94223200	-0.94289500
O	-1.51050500	0.19908000	-0.95332400
H	-2.38447600	-0.17489200	-1.11866700
H	-0.50231600	-1.99602500	-1.52664200
O	-0.79047200	2.50977000	-0.16779700
H	-0.31555000	3.15845800	-0.71327500
H	-0.15474100	1.79694300	0.22861800
H	-1.35007400	1.89923600	-0.73413300
C	-1.74941900	-0.84173400	1.23833900
H	-2.17680600	0.08053200	1.62868400
H	-2.55839500	-1.50147700	0.92424100
H	-1.19189900	-1.33892100	2.02963700

TS(9-2)_gas

0 1			
C	-1.65088400	-0.26702800	-0.05652900
C	-0.96885900	-1.02221800	-0.91628100
C	0.35722500	-0.39953700	-1.14571500
C	0.28078100	0.79847800	-0.32887400
O	-0.90585300	0.89494600	0.24682900
H	0.68480000	-0.22407500	-2.17069000
C	-2.95456000	-0.37024300	0.63431500
H	-2.81995700	-0.42289700	1.71628900
H	-3.58289800	0.49669000	0.42060700
H	-3.47678700	-1.26631300	0.30575800
H	-1.29633400	-1.96802600	-1.31347400
O	1.34673700	0.09728600	1.41999600
H	1.97373300	0.73875400	1.76612100
H	1.25729400	-1.08663100	-0.70037000
O	2.38941400	-1.60112400	0.09504400
H	1.93245000	-0.75831500	0.91702800

H	2.23627600	-2.50238200	0.39272200
C	1.05677500	2.05230200	-0.48729300
H	0.97326500	2.67490500	0.39982100
H	2.10055500	1.82835300	-0.68928900
H	0.65235200	2.61055100	-1.33721000

TS(11-12)-cis_gas

O 1			
C	-1.21085800	0.01045500	-0.08820600
C	-0.66461100	-0.28556600	1.32012900
C	0.75606200	0.27457200	1.35307400
C	1.41992900	-0.09573500	0.03548700
O	1.57504100	-1.36938900	-0.24094900
H	0.75682700	1.35672900	1.48812200
H	-1.29952700	0.13848000	2.09622100
H	1.34484900	-0.16366700	2.16082700
O	-0.09827500	-0.10514400	-0.98048100
H	0.51377300	-1.17663400	-0.83647400
H	-0.64837500	-1.36637200	1.45006000
C	2.38190100	0.87724300	-0.58013500
H	3.31231600	0.82368200	-0.00736300
H	2.60002400	0.58677600	-1.60459900
H	2.01600200	1.90129700	-0.54568000
O	-2.16244900	-0.98329500	-0.38695700
H	-2.52051200	-0.81324100	-1.26507000
C	-1.80467800	1.40533700	-0.24190600
H	-2.11100700	1.56495700	-1.27665500
H	-2.67154000	1.51903200	0.40806200
H	-1.07383800	2.17375100	0.00898600

TS(12-4)-cis_gas

O 1			
C	1.25887800	0.06464000	-0.06057600
C	0.76215100	0.36077200	1.36208800
C	-0.74958100	0.16462800	1.27026300
C	-0.96211900	-0.56305900	0.05116900
H	-1.28046700	-0.19168000	2.14695000
H	1.04736100	1.37442000	1.63393600
H	-1.32164800	1.13547000	0.82497500
H	1.22095200	-0.32701300	2.07297000
C	-2.12869100	-1.38580600	-0.33884200
H	-1.96558400	-2.40876700	0.01994700
H	-3.03076100	-0.98293400	0.10794200
H	-2.23672700	-1.41095900	-1.41945200
O	-2.04490200	1.41773100	-0.40634500
H	-2.20520200	2.12868200	-1.03649000
O	0.11113500	-0.65899300	-0.69111100
C	2.45165800	-0.86240200	-0.18624900
H	2.67584000	-1.05659800	-1.23608700
H	3.31935600	-0.39199300	0.27438800
H	2.26139200	-1.81420500	0.30680800
O	1.44139900	1.26376000	-0.73116600
H	1.66065800	1.09296000	-1.65402200

TS(13-14)-cis_gas

O 1			
C	-1.32992200	0.02775600	0.04474900
C	-0.94108400	-0.84522200	-1.16451300
C	0.31441300	-1.60761400	-0.75487000
C	1.21825600	-0.57692200	-0.09104000
O	1.76367900	0.28443400	-0.90502700
H	0.07870500	-2.41515700	-0.06093100
H	-1.76204200	-1.49802600	-1.45656900

H	0.83651300	-2.03271000	-1.61153500
H	0.31305500	1.36360600	0.57905500
H	-0.71317900	-0.19638200	-2.01085400
O	0.98989500	2.29668600	0.06638500
H	1.58750000	1.41492800	-0.47378000
H	1.52758800	2.80518300	0.67870900
C	2.05710000	-1.03162800	1.08218300
H	2.86056700	-1.66049800	0.69308200
H	2.51438700	-0.17470200	1.57426200
H	1.47910000	-1.60073400	1.80667700
C	-2.28197000	-0.65028100	1.01313800
H	-2.42915300	-0.01360900	1.88342900
H	-3.24396900	-0.81877600	0.53121600
H	-1.87662100	-1.60584200	1.34210800
O	-1.92971500	1.24119700	-0.31972200
H	-1.35285200	1.72110400	-0.92594000
O	-0.07890400	0.27956900	0.74251300

TS(15-16)-cis_gas

1 1			
C	0.84805800	-0.98346200	-0.08062200
C	-0.37382700	-1.69202000	-0.60230600
C	-1.35590400	-0.62298900	-1.08369600
C	-1.47498000	0.43535300	0.01598000
O	-0.12008900	0.37586100	0.70758900
H	-2.33136200	-1.04651700	-1.31238600
C	1.59145800	-1.51235600	1.10277700
H	2.34651800	-0.81018700	1.45197800
H	0.91928900	-1.75816400	1.91903600
H	2.09991900	-2.42554600	0.78280600
H	-0.80108400	-2.30990900	0.18548800
H	-0.98166400	-0.13935600	-1.98395500
H	-0.06968200	-2.34876000	-1.41755100
O	1.53318000	-0.38659000	-1.03206500
H	2.27571300	0.14770000	-0.67982600
O	2.68188800	1.79854700	0.08162800
H	2.78961900	2.49131400	-0.58116200
H	3.34433500	1.98628300	0.75646600
H	0.35830200	1.19770600	0.50188700
C	-2.50567300	0.15368300	1.08708700
H	-2.44757000	0.89855700	1.88122000
H	-3.50057500	0.17750500	0.64442100
H	-2.35186400	-0.82616400	1.53485200
O	-1.58972100	1.68793400	-0.55102700
H	-2.06674700	2.29026900	0.03239300

TS(15-16)-cis_sol

1 1			
C	1.03174600	-0.97095300	-0.09290000
C	-0.16426300	-1.75510100	-0.53469500
C	-1.22795800	-0.77810900	-1.04148500
C	-1.44089900	0.31008900	0.02006400
O	-0.13953500	0.44647500	0.70335600
H	-2.16078000	-1.29407500	-1.25567400
C	1.80111100	-1.31729800	1.12845900
H	2.48759900	-0.52257600	1.41192700
H	1.14189800	-1.55949400	1.95496000
H	2.39095500	-2.20555000	0.88217800
H	-0.52832400	-2.35978500	0.29225800
H	-0.89070600	-0.29988200	-1.95929700
H	0.15133500	-2.43036500	-1.33150300
O	1.62263400	-0.32939100	-1.05934300
H	2.30077000	0.29721300	-0.73095600
O	2.13068500	2.06957300	0.06609400
H	2.16330600	2.77189900	-0.59382500
H	2.65133800	2.39042600	0.81141800

H	0.30750100	1.26949700	0.42597200
C	-2.45697300	-0.04379700	1.08885300
H	-2.50684400	0.74821800	1.83629100
H	-3.43735400	-0.17082700	0.63329500
H	-2.18308800	-0.96880900	1.59277900
O	-1.73780400	1.50619900	-0.63079800
H	-2.15202000	2.12227900	-0.01408100

TS(16-18)-cis_gas

1 1			
C	0.96170500	-0.66255700	0.06197600
C	0.14631400	-1.63127100	-0.79242800
C	-1.06031900	-0.79820100	-1.21520000
C	-1.35212600	0.08301800	-0.00345500
O	0.01349500	0.22588400	0.63546700
H	-1.92422600	-1.40131500	-1.48309300
C	1.84021100	-1.27184000	1.13119400
H	2.36250600	-0.49992200	1.69509600
H	1.23299300	-1.85293800	1.82213100
H	2.57849200	-1.93955100	0.68532900
H	-0.15028700	-2.48293700	-0.18013300
H	-0.82099500	-0.15325500	-2.05896400
H	0.72557700	-2.01355800	-1.63003900
O	1.78143500	0.19800200	-0.81969300
H	2.56900800	-0.26662400	-1.12518100
O	1.16983400	2.38421500	0.07974000
H	1.69065200	2.87496200	0.73293500
H	1.71353100	1.64483600	-0.40999200
H	0.49124800	1.74105300	0.51040800
C	-2.27561200	-0.50741600	1.04088600
H	-2.29631200	0.12179300	1.93152100
H	-3.28389700	-0.58605900	0.63537600
H	-1.94913900	-1.50138500	1.34011300
O	-1.73145700	1.35577000	-0.39843400
H	-2.36664500	1.73354100	0.22001700

TS(16-18)-cis_sol

1 1			
C	0.95698900	-0.67057200	0.04833900
C	0.10015300	-1.69080500	-0.69935200
C	-1.10716000	-0.87477600	-1.14983400
C	-1.34551800	0.10319600	-0.00243900
O	0.01750100	0.25813600	0.60073500
H	-1.98785200	-1.48246100	-1.34084100
C	1.84907300	-1.22030800	1.14022500
H	2.40056200	-0.41979200	1.63090500
H	1.24607100	-1.74002400	1.88171200
H	2.56181500	-1.92929200	0.71844600
H	-0.19342800	-2.48495300	-0.01390000
H	-0.88052400	-0.30293200	-2.04822700
H	0.65167400	-2.14115600	-1.52059800
O	1.73767100	0.11613600	-0.89813700
H	2.55597500	-0.34455800	-1.11859100
O	1.23203700	2.37503700	0.06628400
H	1.77631000	2.81060000	0.74222100
H	1.77511000	1.69728300	-0.45650300
H	0.56965100	1.69786800	0.48612200
C	-2.26462600	-0.38542900	1.09872000
H	-2.25537600	0.31358300	1.93540700
H	-3.28042700	-0.47037500	0.71554100
H	-1.94667800	-1.35927100	1.46567000
O	-1.73106900	1.34226800	-0.50313500
H	-2.17546600	1.85502400	0.18271100

TS(17-9)-cis_gas

O	1			
C		-1.17435000	-0.80022400	0.10358300
C		-0.40493000	-0.33287800	1.34531800
C		0.37429700	0.93813600	1.01094400
C		-0.22308700	1.53278100	-0.13808500
H		0.59790200	1.61213000	1.83402600
C		-2.67281500	-0.88251000	0.18941800
H		-3.09186800	-1.02208600	-0.80393100
H		-2.92935100	-1.75315900	0.79788300
H		-3.10050200	0.00346500	0.65150600
H		0.26056200	-1.13630900	1.66022800
H		1.54884800	0.58313500	0.65563400
H		3.34778500	0.46872500	-0.08269300
O		2.74646100	-0.06809100	0.44112000
H		-1.11854900	-0.15663900	2.15108900
O		-0.64929000	-1.66829300	-0.68731800
H		0.43846500	-1.78798000	-0.67378100
C		0.14864200	2.88872600	-0.65367000
H		0.51907600	2.79787300	-1.67536600
H		-0.74106900	3.51888300	-0.68808200
H		0.90385900	3.36380300	-0.03266300
O		1.77941900	-1.94041100	-0.74540200
H		2.11026100	-2.78683800	-0.43683800
H		2.31684300	-1.10015800	-0.21923000
O		-1.04519000	0.84316700	-0.79375400

TS(20-21)_gas

O	1			
C		0.85273600	-0.75339800	-0.26080600
C		-0.13795100	-0.35970100	-1.31517000
C		-1.31874600	0.50582500	-0.89720000
C		-2.34656800	-0.20540400	-0.03665300
O		-2.25510600	-1.38373700	0.23237500
H		-0.98174300	1.42335400	-0.40578500
C		1.72800600	-1.91863500	-0.57234700
H		1.91892500	-1.94934500	-1.64085400
H		2.67716800	-1.87651500	-0.04795600
H		1.20510200	-2.83817600	-0.29023500
H		0.45549500	0.15484700	-2.07267000
H		-1.83762800	0.85028400	-1.79749600
H		-0.50109300	-1.29093000	-1.75627200
C		-3.49579000	0.63717100	0.46823600
H		-3.11838100	1.39259500	1.16139000
H		-3.97238100	1.17523300	-0.35311100
H		-4.22498300	0.01129000	0.97559700
N		0.80108300	-0.25419100	0.93580100
C		1.75740700	-0.54467000	1.99398500
H		1.41020200	-0.06753100	2.90562000
H		1.83432300	-1.61539300	2.16387800
H		2.73564000	-0.13671500	1.73236700
H		0.39213000	0.68510300	1.00889400
O		0.97072400	2.31593200	0.44584500
H		1.66479500	1.83082600	-0.29776700
H		1.11632300	3.26212200	0.48070000
O		2.30085000	1.00286200	-1.12040500
H		3.25221500	1.12070900	-1.05969700

TS(21-30)_gas

O	1			
C		-1.20524100	-0.15757500	-0.01546100
C		-0.68339900	-1.60207300	-0.09604900
C		0.72408800	-1.53768600	0.49538700
C		1.32855200	-0.23471400	-0.07412000
O		1.69561600	-0.31066600	-1.37844700

H	0.69024200	-1.51874900	1.58748400
H	-1.34405600	-2.29616700	0.42306600
H	1.34840900	-2.37449600	0.18885700
H	0.50840400	0.34069200	-1.42126600
H	-0.63589600	-1.88725800	-1.14614100
N	-0.00338100	0.63693800	-0.35915000
C	-0.02376800	2.07160800	-0.07744900
H	0.83957900	2.52852400	-0.55588900
H	-0.92675300	2.50701600	-0.50210800
H	0.01114700	2.28318300	0.99166600
C	2.33082300	0.44182000	0.84592100
H	1.92380100	0.66341000	1.83493100
H	3.17395500	-0.23849200	0.97193200
H	2.71281000	1.35452200	0.39251400
C	-1.77202700	0.17954700	1.36452200
H	-2.12836900	1.20706200	1.40353400
H	-2.61466300	-0.47955800	1.57952600
H	-1.03140400	0.03321400	2.15040400
O	-2.15963500	0.15441400	-1.02350000
H	-2.98555400	-0.29701000	-0.82538000

TS(22-23)_gas

0 1			
C	-1.29863800	-0.33525100	-0.05793900
C	-0.79522600	-1.52667000	-0.37088100
C	0.69922400	-1.56479500	-0.39771400
C	1.15497300	-0.19195200	0.15742000
H	1.10140500	-2.33256900	0.26635100
C	-2.72947600	0.05154900	0.11735000
H	-3.03663500	0.82885100	-0.58580600
H	-3.37102300	-0.81298900	-0.04088600
H	-2.91350400	0.43300700	1.12494800
H	-1.41416200	-2.39590300	-0.54404800
H	1.08238800	-1.76295300	-1.40283300
H	0.18202000	0.52870200	1.34909400
O	1.37425600	-0.14696400	1.48869600
N	-0.26090200	0.62452100	0.23522300
C	-0.39001000	1.96646000	-0.33792000
H	0.43967200	2.57815500	0.00757700
H	-0.38375600	1.93129900	-1.42862200
H	-1.31781500	2.42827100	-0.00432500
C	2.19670100	0.50205600	-0.70562800
H	2.47618500	1.46234600	-0.27631200
H	3.08794000	-0.12691800	-0.70903500
H	1.87424800	0.63637700	-1.74036500

TS(23-20)_gas

0 1			
C	-1.35141100	-0.35465000	-0.12559800
C	-0.82798500	-1.55871100	-0.39136200
C	0.63547200	-1.41819100	-0.55580800
C	0.85852000	0.02678600	-0.46882300
H	1.14488200	-1.95533700	-1.35201900
C	-2.74070300	0.03651400	0.23786400
H	-2.79200100	0.47641500	1.23644000
H	-3.16686600	0.75660700	-0.46486000
H	-3.37364900	-0.84820200	0.23213900
H	-1.37140000	-2.48848700	-0.39086600
O	1.65911500	-0.61074500	1.58809000
H	1.99393100	-0.41020500	2.46906900
H	1.14865300	-1.65716000	0.46083300
C	2.10477500	0.74841200	-0.82660200
H	2.94958900	0.08154300	-0.69016600
H	2.06323800	1.06378800	-1.87628400
H	2.26724900	1.62280700	-0.20333200
N	-0.30790000	0.61783700	-0.22203800

C	-0.43954600	1.99820600	0.20888200
H	-0.10641100	2.08914000	1.24547800
H	0.16560000	2.64720900	-0.41844200
H	-1.47517400	2.31278800	0.13023100

TS(24-25)_gas

0 1			
C	1.41567400	-0.23164300	-0.29596700
C	0.97102800	-1.12300500	-1.17420100
C	-0.52210500	-1.20693300	-1.22057100
C	-1.02367000	-0.52671900	0.08583300
H	-0.92078400	-0.65444300	-2.07485900
C	2.81576500	0.19823800	-0.01809800
H	3.09640600	0.04567300	1.02609600
H	3.50585500	-0.37030500	-0.63826500
H	2.95420400	1.25935000	-0.24090700
H	1.62525500	-1.68788200	-1.82258100
H	-0.02594600	1.31390100	-0.22442300
H	-0.89375500	-2.23038100	-1.28972000
H	-1.73346100	1.21598600	-0.61259200
O	-0.95916800	2.07803500	-1.08919500
H	-1.23237800	2.97209100	-0.87240700
O	-2.08853800	0.26617900	-0.01344700
N	0.30595600	0.43574700	0.36804600
C	0.48943100	0.86955800	1.76096800
H	0.81210000	0.04515400	2.39275500
H	1.22681300	1.66924600	1.80827600
H	-0.46360700	1.25281900	2.11861800
C	-1.15613600	-1.52724400	1.22563800
H	-1.42345200	-1.02732800	2.15414600
H	-1.97399600	-2.19971100	0.96931700
H	-0.25322200	-2.12162400	1.36974700

TS(27-29)_gas

1 1			
C	1.44307600	-0.28332200	-0.26066400
C	1.07231300	-1.14069900	-1.20614500
C	-0.41524700	-1.31390800	-1.22551900
C	-0.87382600	-0.54956100	0.03381700
H	-0.73500800	-2.35538900	-1.18531000
C	2.80955100	0.20136500	0.07982400
H	2.88568600	1.28926200	0.00643900
H	3.10215500	-0.07599100	1.09376700
H	3.53220300	-0.23398000	-0.60577200
H	1.74166200	-1.61683400	-1.90384600
O	-1.97988900	0.39365600	-0.38152400
H	-2.69555500	0.41437600	0.26764000
H	-0.87450300	-0.88505200	-2.11965400
O	-0.75281700	2.39218600	-0.75575100
H	-0.54805300	2.73368900	-1.63718500
H	0.00465300	1.84141900	-0.37555900
H	-1.51696000	1.50545400	-0.68264500
C	-1.45341600	-1.44843000	1.10714000
H	-1.79212300	-0.89779800	1.98449800
H	-2.29006100	-2.01283000	0.69712700
H	-0.69727700	-2.16394200	1.42776300
N	0.29381100	0.26535900	0.43577400
C	0.45168700	0.57971100	1.86789400
H	-0.44853500	1.06405300	2.24101000

H	0.66005200	-0.30357200	2.47428700
H	1.27180600	1.28194300	1.98713000

TS(27-29)_sol

1	1		
C	1.41007000	-0.39443700	-0.19632200
C	1.04895300	-1.46911600	-0.89120500
C	-0.41198300	-1.75282800	-0.72492900
C	-0.92573100	-0.50683900	0.02182700
H	-0.58910800	-2.65815600	-0.13935100
C	2.76568300	0.21011100	-0.05944600
H	2.76308600	1.26636500	-0.33763300
H	3.13922300	0.14547200	0.96382700
H	3.46762100	-0.31374900	-0.70429700
H	1.71587700	-2.06196300	-1.49672300
O	-1.57685700	0.37691400	-1.00105000
H	-2.52597600	0.20848200	-1.05669200
H	-0.94899400	-1.87106700	-1.66566700
O	-0.54970500	2.51277100	-0.71870400
H	-0.13010700	2.91436900	-1.49474400
H	0.12436300	1.97042700	-0.21113900
H	-1.17961700	1.61915700	-0.97428500
C	-1.94993600	-0.79534900	1.09878200
H	-2.34855200	0.11692700	1.53800600
H	-2.77333300	-1.36180900	0.66411100
H	-1.51338100	-1.40653200	1.88575300
N	0.28254900	0.23783400	0.45174900
C	0.45085900	0.51502100	1.89297800
H	-0.40491000	1.06678600	2.26984000
H	0.58126900	-0.39642900	2.48093600
H	1.32969900	1.14002500	2.02374100

TS(28-20)_gas

0	1		
C	1.49207300	-0.68994300	0.09858100
C	0.71821600	-1.58292000	0.72487200
C	-0.52363900	-0.90895500	1.17692400
C	-0.30431400	0.49473800	0.80351900
H	-0.83119600	-1.05507600	2.21351300
C	2.77882100	-0.86156700	-0.62742700
H	2.67871000	-0.61474100	-1.68622500
H	3.57361000	-0.23827900	-0.21180900
H	3.09458300	-1.89987200	-0.55421900
H	0.92204000	-2.63655100	0.81245800
O	-1.39275100	0.55342900	-1.50071300
H	-1.98335300	1.20133900	-1.89480800
H	-1.40822100	-1.25248100	0.54354600
O	-2.70822900	-1.32352000	-0.62884400
H	-2.17390100	-0.49515900	-1.11328900
H	-2.74107300	-2.05067300	-1.25501400
N	0.85981800	0.59398400	0.19531300
C	1.28203100	1.77344400	-0.54830200
H	2.30700200	1.65047000	-0.87988400
H	0.60422300	1.86514600	-1.39998100
H	1.22350700	2.65744400	0.08178800
C	-1.16224600	1.63170600	1.21005000
H	-0.88221100	1.95322100	2.22041800
H	-1.08161400	2.47293900	0.53107200
H	-2.19864700	1.30608400	1.23239200

TS(30-23)_gas

0	1		
C	1.26211300	-0.23031300	0.01380500

C	0.69254000	-1.53368400	-0.58895600
C	-0.80277100	-1.28087500	-0.77379200
C	-0.98135400	0.14231000	-0.58757300
H	-1.27424200	-1.70612600	-1.65587200
H	0.89837000	-2.35232900	0.09642500
H	-1.42043600	-1.56616600	0.19024900
H	1.18700000	-1.75152300	-1.53564800
C	-2.22214500	0.88595900	-0.92699900
H	-2.11626200	1.32141300	-1.92784800
H	-3.05944000	0.19665600	-0.91994100
H	-2.43490000	1.68085900	-0.21919500
O	-2.10873900	-0.83347200	1.35321200
H	-2.41401200	-0.94538900	2.25849400
C	2.49363100	0.29716000	-0.71585300
H	2.86040200	1.22686000	-0.27482600
H	3.28942200	-0.44402700	-0.65053900
H	2.27479800	0.48276900	-1.76633500
O	1.54732800	-0.44645900	1.37691400
H	2.12574300	0.24615300	1.71076900
N	0.11566700	0.72431900	-0.14118500
C	0.12175800	2.01196500	0.53321400
H	-0.36684200	2.76814600	-0.07648200
H	-0.39692800	1.92494500	1.49066000
H	1.14631600	2.33184900	0.70430500

TS(31-32)_gas

O 1			
C	1.27313200	-0.18115500	0.22127300
C	0.67150600	0.18289800	1.59059000
C	-0.70535100	-0.46231000	1.61794100
C	-1.33288400	-0.14377900	0.24639900
O	-1.81747100	1.10569000	0.13936500
H	-0.62855700	-1.54207700	1.76836700
H	1.32734600	-0.15370200	2.39167900
H	-1.35139200	-0.05855300	2.39477100
H	0.01275800	0.77519900	-1.06441200
H	0.58361000	1.26590400	1.65614500
O	0.06659100	2.44947800	-0.52218300
H	-0.98084700	1.88435700	-0.11153200
H	-0.12025900	3.25393700	-1.00868700
C	-2.35977300	-1.17518500	-0.19757300
H	-3.17925200	-1.13566100	0.51967500
H	-2.76844500	-0.92040600	-1.17376300
H	-1.97187900	-2.19390200	-0.21125000
N	0.01035100	-0.20028200	-0.70136700
C	0.04089600	-1.10897400	-1.86020300
H	0.95314200	-0.93066500	-2.42655000
H	0.00388600	-2.14813700	-1.54819400
H	-0.81345200	-0.89543800	-2.49715500
C	1.98903600	-1.52104400	0.23970100
H	2.38818800	-1.77429200	-0.74001200
H	2.82841800	-1.43648000	0.92705900
H	1.34218800	-2.32647100	0.58522300
O	2.14964000	0.76677100	-0.28787100
H	1.65264100	1.62014700	-0.33505800

TS(33-26)_gas

O 1			
C	-1.11646800	-0.69113200	0.33465900
C	-0.17475400	-0.65201700	1.57175400
C	0.72847000	0.56965400	1.38376700
C	0.13297500	1.32480700	0.30506800
H	0.94398000	1.16019700	2.27278700
C	-2.59124700	-0.79138900	0.69839300
H	-3.21290300	-0.77629500	-0.19605200

H	-2.75660100	-1.74300300	1.20176200
H	-2.89363700	0.01501800	1.36629700
H	0.39683600	-1.57603000	1.61489400
H	1.78746600	0.21616700	0.97194200
H	3.73735700	-0.06827900	0.12260200
O	2.96750800	-0.58441800	0.37484700
N	-0.83445300	0.68751700	-0.28875600
C	-1.47368400	1.05255700	-1.54387500
H	-0.80710300	1.65541900	-2.15388400
H	-1.69676400	0.13340800	-2.08010700
H	-2.39792200	1.60274400	-1.36333800
H	-0.76502800	-0.57801500	2.48479400
O	-0.84113500	-1.66064500	-0.59659700
H	0.13137800	-1.62963900	-0.89824000
C	0.66286300	2.62986700	-0.17659500
H	-0.12923200	3.31352100	-0.47823300
H	1.26955000	3.09694400	0.59447200
H	1.30591300	2.45197300	-1.04293400
O	1.58296000	-1.43421300	-1.44575700
H	1.95557700	-2.23427400	-1.82288300
H	2.28870800	-1.07234200	-0.67155100

TS(34-35)_gas

1 1			
C	1.06411200	-0.57881500	-0.12040900
C	0.48086200	-1.02758100	-1.47142500
C	-0.81279900	-0.23287700	-1.62753300
C	-1.31571700	-0.06753600	-0.18432900
H	-1.54173900	-0.73055000	-2.26265400
C	1.77648900	-1.68515000	0.63704100
H	2.24804500	-1.31743000	1.54527800
H	1.07846200	-2.47936200	0.89793600
H	2.54818100	-2.12500700	0.00441900
H	0.27645700	-2.09693500	-1.42424000
H	-0.62819700	0.75605900	-2.04615600
H	1.18718500	-0.87581600	-2.28573800
O	2.08061600	0.50904300	-0.32777600
H	2.84056800	0.19779500	-0.83225600
O	0.75810400	2.51123000	-0.14420600
H	0.95896800	3.22378700	0.47996500
H	1.55328400	1.82005600	-0.30290100
H	0.10654700	1.82094800	0.24760300
C	-2.20133300	-1.21942300	0.28083300
H	-2.49722000	-1.10058200	1.32111600
H	-3.10611900	-1.25501100	-0.32689100
H	-1.69823600	-2.17981000	0.16965900
O	-1.96600600	1.18180300	0.02687600
H	-2.90616900	1.12170000	-0.17022800
N	-0.04021500	0.08091700	0.57074000
C	-0.11211200	-0.00920400	2.03607700
H	-0.25775200	-1.02794600	2.39736300
H	0.80300500	0.38407100	2.47500200
H	-0.94249000	0.60451600	2.37686400

TS(34-35)_sol

1 1			
C	1.04307900	-0.60530300	-0.11650000
C	0.44620400	-1.02794100	-1.47085900
C	-0.82217000	-0.19604500	-1.62487500
C	-1.32419200	-0.02257200	-0.18962500
H	-1.56886000	-0.66788800	-2.25832600
C	1.69093500	-1.75078300	0.64302000
H	2.17896700	-1.40313900	1.55049900
H	0.94838600	-2.50332400	0.90434200
H	2.43976400	-2.22661300	0.01028500
H	0.20886400	-2.09019300	-1.43110700
H	-0.60637300	0.78872000	-2.03888900

H	1.15789300	-0.88891500	-2.28179100
O	2.10859300	0.42169600	-0.31349600
H	2.78148000	0.11593900	-0.93313400
O	0.89143300	2.49930900	-0.13731300
H	1.17354100	3.15036500	0.52397800
H	1.63324800	1.74888400	-0.30809600
H	0.20938400	1.85697300	0.26174100
C	-2.21630000	-1.16738100	0.27997100
H	-2.52209800	-1.03717400	1.31788800
H	-3.11141800	-1.20195100	-0.33883100
H	-1.70640300	-2.12629500	0.19736300
O	-2.01866500	1.21411900	-0.09720300
H	-2.64994000	1.18778100	0.62994100
N	-0.04011400	0.09931400	0.57080000
C	-0.10987200	0.01525100	2.03386000
H	-0.31094900	-0.99241500	2.40081300
H	0.82595000	0.36347900	2.46554300
H	-0.89763400	0.67822300	2.38632300

TS(36-46)_gas

O 1			
C	-0.97932200	-0.65087600	-0.28343400
C	0.32737600	-1.46261300	-0.34702100
C	1.51816300	-0.95017100	0.46884900
C	2.28154600	0.21356600	-0.09660700
O	1.78996700	0.98993800	-0.90460800
H	1.14100300	-0.62014200	1.44850600
C	-2.09461400	-1.40943900	-0.99263000
H	-2.33473200	-2.31467900	-0.43908800
H	-2.99662400	-0.80144700	-1.03859000
H	-1.79910600	-1.67496000	-2.01091700
H	0.08147500	-2.45506700	0.02986700
H	2.21969700	-1.76193300	0.67211900
H	0.18949300	0.81746600	-1.11209000
H	0.60866100	-1.58639200	-1.39731300
C	3.69017800	0.41850900	0.38959000
H	4.33065500	-0.36457800	-0.02385700
H	4.06267900	1.38984200	0.07650100
H	3.73840700	0.32609500	1.47556000
H	-1.44334300	1.49407100	-0.65285200
O	-2.05409300	2.20043200	0.08810500
H	-1.98149000	1.40075200	0.85873200
H	-2.97845100	2.28448000	-0.17379300
O	-0.78006900	0.58035000	-1.12715300
S	-1.43404500	-0.20332100	1.43774900

TS(38-39)_gas

O 1			
C	1.47684800	0.24308100	-0.04776700
C	0.69382000	1.33913400	0.00330300
C	-0.76742900	1.30533100	-0.28551600
C	-1.58376000	0.14930700	0.15575200
H	-1.26592400	2.14562500	0.23170500
C	2.96366300	0.34242700	0.16509500
H	3.27444100	-0.28472100	1.00182200
H	3.49469200	-0.02178600	-0.71565300
H	3.27253900	1.36956900	0.36435500
H	1.13167900	2.31384700	0.18107700
H	-0.97947200	1.47820200	-1.34663900
H	-0.38162300	-0.81294300	1.20620400
O	-1.35285900	-0.51240800	1.24611000
S	0.80166300	-1.33318000	-0.39111700
C	-2.91820200	-0.08552600	-0.45521700
H	-2.83296900	-0.92301200	-1.15269200
H	-3.63182300	-0.37749400	0.31407000
H	-3.27491900	0.78033600	-1.00915400

TS(39-37)_gas

0 1			
C	1.51742900	0.13042700	-0.10505500
C	0.91077200	1.17936900	-0.67601800
C	-0.55289300	1.07622200	-0.78162100
C	-0.99012500	-0.22854000	-0.30709400
H	-1.04699300	1.45959800	-1.67201100
C	2.95189600	-0.05840100	0.26325200
H	3.08229100	-0.13547500	1.34452800
H	3.36918000	-0.96380500	-0.18222500
H	3.53740100	0.79097800	-0.08629100
H	1.44708600	2.07244500	-0.96624600
O	-1.75766300	1.01979500	1.32700600
H	-2.08373000	1.07074000	2.23525600
H	-1.04924100	1.63154900	0.16085200
C	-2.29267600	-0.87004400	-0.63298500
H	-3.07464000	-0.11630700	-0.64103600
H	-2.23159100	-1.33407100	-1.62300900
H	-2.55774900	-1.63931000	0.08857600
S	0.33767900	-1.14805600	0.26016800

TS(40-41)_gas

0 1			
C	-1.55864200	-0.33654200	-0.00036800
C	-1.00841100	-1.39135500	-0.60797000
C	0.41886100	-1.78621400	-0.34784900
C	1.33154500	-0.58878300	-0.16416400
O	1.49660300	0.16865900	-1.16437800
H	0.48597700	-2.43646300	0.52864500
C	-2.99063900	0.07319800	-0.18500100
H	-3.52268400	0.05852400	0.76804900
H	-3.06184300	1.09396600	-0.56716000
H	-3.50363100	-0.59295600	-0.87964400
H	-1.59794900	-2.00323200	-1.28100400
H	0.09654500	1.87443800	0.08565400
H	0.81704700	-2.34813900	-1.19937900
H	1.27077800	1.43290100	-0.97412800
O	0.78417000	2.38439800	-0.63532000
H	0.26049500	2.74706900	-1.36037700
C	2.38656300	-0.62261400	0.90871900
H	3.20535100	-1.25034800	0.53731100
H	2.79005100	0.37188800	1.08518900
H	2.01701900	-1.04538700	1.83791100
S	-0.56118800	0.59919600	1.13727000

TS(41-43)_gas

1 1			
C	1.31291200	-0.07264300	-0.04297400
C	1.09843400	-1.49097600	-0.60871800
C	-0.36980200	-1.77076000	-0.70308500
C	-1.20774800	-1.01566800	-0.00325200
O	1.23721100	0.92226000	-1.03410800
H	1.59149700	-1.56076800	-1.58220100
S	-0.28263100	0.19310100	0.97546900
H	1.71887000	0.64194200	-1.82169000
H	1.58644400	-2.23114900	0.03049700
H	-0.69296100	1.39419100	0.38058300
H	-0.73488000	-2.59448200	-1.30332300
O	-1.23842400	2.75174500	-0.42459000
H	-1.63758900	3.53957400	-0.03840800
H	-0.62958900	3.05170400	-1.10905700
C	-2.68875300	-1.06858400	0.14303600

H	-3.08547400	-1.88320500	-0.46008700
H	-2.98314400	-1.23610200	1.18047200
H	-3.15379400	-0.13885900	-0.18935600
C	2.52614100	0.10187200	0.84920600
H	3.42085100	-0.10856400	0.26052500
H	2.59734100	1.12548200	1.21171900
H	2.50711100	-0.58086700	1.69712700

TS(41-43)_sol

1 1			
C	1.22727400	-0.33932400	-0.02606800
C	0.72412600	-1.67041300	-0.61629200
C	-0.76722600	-1.62766800	-0.72386800
C	-1.42622100	-0.72027300	-0.01420600
O	1.38317600	0.65664000	-1.01364500
H	1.20123200	-1.82901600	-1.58565700
S	-0.27541800	0.25292600	0.98176200
H	1.87671200	0.29478200	-1.76060000
H	1.03256400	-2.50373800	0.01888400
H	-0.40252600	1.52939900	0.38398900
H	-1.29568200	-2.34461600	-1.33843800
O	-0.43703500	2.91311300	-0.47406600
H	-0.29608000	3.71126800	0.04972500
H	0.35666300	2.80257200	-1.01479700
C	-2.88717500	-0.46937900	0.12825300
H	-3.43692600	-1.17331200	-0.49368100
H	-3.21157600	-0.59355400	1.16251700
H	-3.14885500	0.54383500	-0.18008200
C	2.44462800	-0.44357800	0.87120800
H	3.27340600	-0.83380300	0.27882700
H	2.72691100	0.53535100	1.25326500
H	2.26927400	-1.12019100	1.70537900

TS(43-45)_gas

1 1			
C	-1.65293500	0.01235400	0.14636800
C	-1.21691800	-0.60674700	1.23488000
C	0.24960600	-0.82131100	1.35216600
C	0.86197200	-0.69092400	-0.03811100
H	0.50932500	-1.79609000	1.77446400
C	-3.02863200	0.41058000	-0.22492900
H	-3.10445200	1.48919700	-0.38208800
H	-3.34530900	-0.07248900	-1.15156200
H	-3.72450200	0.13287500	0.56632500
H	-1.89502500	-0.89971900	2.02771900
O	2.12937400	-0.01437900	0.07601500
H	2.75594200	-0.33562100	-0.58268300
H	0.69322500	-0.07209700	2.02086700
O	1.40717200	2.29057900	0.42334100
H	1.85922900	3.09328400	0.12718100
H	0.57766600	2.07673600	-0.11656000
H	1.94752500	1.38224500	0.31139400
C	1.05114500	-2.00406000	-0.74115200
H	1.41350100	-1.86823000	-1.76268600
H	1.75347700	-2.62755000	-0.18152800
H	0.09618700	-2.52816200	-0.79336100
S	-0.33841100	0.37604200	-1.01422900

TS(43-45)_sol

1 1			
C	-1.58660200	-0.32731400	0.09298300
C	-1.08202900	-1.03723500	1.09591000
C	0.40219300	-1.10201400	1.25412900

C	1.10251500	-0.56365300	-0.00975300
H	0.74529500	-2.11940500	1.44907200
C	-3.01163100	-0.06321100	-0.25739900
H	-3.22952500	1.00638200	-0.24620300
H	-3.24923000	-0.43335300	-1.25600100
H	-3.66563400	-0.55480300	0.46091800
H	-1.72658700	-1.53196500	1.81105400
O	2.08644300	0.36343900	0.36542400
H	2.76106000	0.42995700	-0.32205100
H	0.71670600	-0.49746400	2.10864600
O	0.45899000	2.69400500	0.48005600
H	0.58613300	3.50730900	-0.03272600
H	0.02177400	1.78615100	-0.20316200
H	1.33579100	2.36357400	0.75193200
C	1.64974800	-1.64409600	-0.92160300
H	2.07098800	-1.21854700	-1.83217100
H	2.42993200	-2.19042000	-0.38977700
H	0.86483100	-2.34476500	-1.20011500
S	-0.30438400	0.36018400	-0.96180400

TS(44-37)_gas

O 1			
C	-1.73705800	0.34898000	0.09038800
C	-0.94946900	1.07376400	0.89393300
C	0.40772000	0.53664300	1.10387000
C	0.54942000	-0.72273500	0.38912800
H	0.77152100	0.49360600	2.13245700
C	-3.11306300	0.63593300	-0.41217800
H	-3.12493200	0.76988900	-1.49565300
H	-3.80650300	-0.17371900	-0.17550900
H	-3.49103100	1.54914900	0.04559100
H	-1.25751900	2.02554600	1.30519800
O	1.72220400	-0.07383700	-1.36243900
H	2.48792800	-0.63700900	-1.51254100
H	1.21314100	1.29648100	0.61171100
O	2.30433300	1.92514700	-0.19354900
H	2.10076300	0.96946500	-0.89601900
H	2.00334700	2.72748600	-0.62996300
C	1.52773400	-1.78106600	0.77844000
H	1.65314500	-2.52904600	-0.00097100
H	2.49303200	-1.33353400	1.00525000
H	1.16743700	-2.28662500	1.67917000
S	-0.90839500	-1.13945600	-0.41764400

TS(46-47)-cis_gas

O 1			
C	-1.78303100	0.11944000	-0.12604000
C	-0.85035200	1.28828600	-0.20238500
C	0.49949000	1.04620300	-0.85732900
C	1.41233200	0.13280400	-0.02436700
H	0.99639600	2.00456900	-1.02725000
C	-3.01139100	0.22869000	0.70691400
H	-2.92136300	0.98147000	1.48482200
H	-3.84562400	0.49537800	0.04904600
H	-3.24695400	-0.74074800	1.14171300
H	-0.74793500	1.72246200	0.79179900
H	0.36850000	0.58301000	-1.83549600
H	-1.41761500	2.03204300	-0.78808700
O	-1.78067900	-0.82193800	-1.00688700
H	-0.78395600	-1.22060300	-0.90259900
S	0.44679700	-1.33917000	0.53077400
O	2.46010000	-0.24314400	-0.91776000
H	2.88202300	-1.03141300	-0.56106600
C	2.00703700	0.85545400	1.18514300
H	2.65293300	0.17925700	1.74332900
H	2.60098800	1.70816300	0.84883600

H	1.23397900	1.20852600	1.86812800
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TS(48-49)-cis_gas

O 1			
C	1.47796600	-0.17006200	0.06624400
C	0.68762100	-0.40637400	1.36909800
C	-0.58617100	-1.19557700	1.11431700
C	-1.54781900	-0.45473000	0.18912300
O	-2.05416100	0.65432100	0.59938600
H	-0.35595200	-2.17503900	0.69457000
H	1.33318300	-0.91373600	2.08910400
H	-1.12651200	-1.36069300	2.05203000
H	-0.15270600	1.60931600	-0.67705300
H	0.43084600	0.56139900	1.80389000
O	-0.55904100	2.44913300	0.13670400
H	-1.33809900	1.67593200	0.50272700
H	-1.00592000	3.17258700	-0.31664600
C	-2.44847900	-1.30376800	-0.67537600
H	-3.22206900	-1.72954900	-0.02789800
H	-2.94413000	-0.68872300	-1.42259500
H	-1.91359800	-2.11590200	-1.16066700
S	0.20354900	0.15131500	-1.28587000
O	2.36590200	0.91670400	0.20250100
H	1.87172200	1.69869800	0.47448800
C	2.33226000	-1.36220900	-0.33723400
H	2.84210700	-1.15678700	-1.27617900
H	3.08247800	-1.54442400	0.43390900
H	1.72800000	-2.25907100	-0.46152500

TS(49-37)-cis_gas

O 1			
C	-1.33172200	0.11887600	0.01102600
C	-0.76114300	0.47971200	1.38960800
C	0.75234800	0.51449300	1.22185100
C	1.16909200	-0.43980200	0.22433300
H	1.34097900	0.49401800	2.13886900
C	-2.68162000	-0.58540000	0.09574300
H	-3.05137000	-0.85851600	-0.89822000
H	-2.61933900	-1.49625600	0.69229200
H	-3.40835900	0.09076600	0.55443900
H	-1.03455400	-0.29336000	2.11538100
H	1.14068200	1.46101800	0.54361100
H	-1.18024000	1.42922900	1.73152600
O	-1.39730200	1.29304300	-0.74471600
H	-2.01965600	1.17945300	-1.47265400
S	-0.11786200	-1.08099900	-0.71687500
C	2.50845900	-1.08609100	0.14907200
H	2.73937300	-1.43547300	-0.85628300
H	3.27228000	-0.37522600	0.46048700
H	2.51780700	-1.94811600	0.83086000
O	1.92559400	1.56573700	-0.69053400
H	2.02937700	2.16746900	-1.43810600

TS(50-51)-cis_gas

1 1			
C	-1.07819600	0.77514700	-0.06667800
C	0.10028900	1.52280100	-0.62121800
C	1.16884400	0.60925900	-1.21786600
C	1.88299500	-0.22907800	-0.14405800
O	-1.70022700	0.04011700	-0.92753600
H	-0.30434100	2.17367800	-1.40413900
S	0.55692600	-0.89969200	1.01949000
H	-2.57105200	-0.35075600	-0.61542300

H	0.51314900	2.16904200	0.15049800
H	0.16181700	-1.89114500	0.20158300
H	0.70655700	-0.06181000	-1.94299100
O	2.52191300	-1.35043500	-0.69654200
H	2.76179100	-1.18694700	-1.61547900
H	1.91035500	1.20908000	-1.75016600
C	2.85558900	0.56705700	0.71846100
H	3.61410800	1.01376100	0.07468500
H	2.36862400	1.36528200	1.27895100
H	3.35171400	-0.09688300	1.42238600
C	-1.80108800	1.26760700	1.13949000
H	-2.38882000	2.13845300	0.82429300
H	-2.48864800	0.52465800	1.53636300
H	-1.11414100	1.59210100	1.91446900
O	-3.98254500	-1.02010500	-0.19637900
H	-4.81632800	-0.66105700	-0.52051600
H	-4.09932300	-1.97576100	-0.15148500

TS(50-51)-cis_sol

1 1			
C	-1.07819600	0.77514700	-0.06667800
C	0.10028900	1.52280100	-0.62121800
C	1.16884400	0.60925900	-1.21786600
C	1.88299500	-0.22907800	-0.14405800
O	-1.70022700	0.04011700	-0.92753600
H	-0.30434100	2.17367800	-1.40413900
S	0.55692600	-0.89969200	1.01949000
H	-2.57105200	-0.35075600	-0.61542300
H	0.51314900	2.16904200	0.15049800
H	0.16181700	-1.89114500	0.20158300
H	0.70655700	-0.06181000	-1.94299100
O	2.52191300	-1.35043500	-0.69654200
H	2.76179100	-1.18694700	-1.61547900
H	1.91035500	1.20908000	-1.75016600
C	2.85558900	0.56705700	0.71846100
H	3.61410800	1.01376100	0.07468500
H	2.36862400	1.36528200	1.27895100
H	3.35171400	-0.09688300	1.42238600
C	-1.80108800	1.26760700	1.13949000
H	-2.38882000	2.13845300	0.82429300
H	-2.48864800	0.52465800	1.53636300
H	-1.11414100	1.59210100	1.91446900
O	-3.98254500	-1.02010500	-0.19637900
H	-4.81632800	-0.66105700	-0.52051600
H	-4.09932300	-1.97576100	-0.15148500

TS(51-53)_gas

1 1			
C	1.48991200	-0.21467100	0.09012500
C	0.75824000	-0.43757500	1.39728800
C	-0.50192000	-1.22121300	1.12879400
C	-1.31165100	-0.50937700	0.05283300
O	-1.98280800	0.61737900	0.58514900
H	-0.26797100	-2.23341100	0.78719200
H	1.42797300	-0.94978700	2.09275600
H	-1.12619200	-1.32225300	2.01948700
H	-0.14448400	1.64872600	-0.57598800
H	0.52859500	0.54049000	1.82858300
O	-0.37743200	2.70768300	0.07035000
H	-1.28288100	2.46197400	0.49542600
H	-0.44812600	3.53990900	-0.41236900
C	-2.26547700	-1.40768100	-0.68749400
H	-2.82267900	-0.85735300	-1.44642700
H	-1.73647500	-2.22815000	-1.17210600
H	-2.97391100	-1.84358900	0.02442100
S	-0.00767700	0.16112000	-1.12238700

H	-2.89974400	0.38626700	0.76586700
O	2.27581400	0.90018400	0.17402300
H	3.01503000	0.85367600	-0.44092600
C	2.21481300	-1.41335100	-0.45900000
H	2.63615900	-1.20221600	-1.44411400
H	3.02862800	-1.67158400	0.22329900
H	1.56080100	-2.27936600	-0.55836000

TS(51-53)_sol

1 1			
C	1.46593800	-0.24575400	0.08111500
C	0.74382700	-0.45419900	1.39545100
C	-0.53364700	-1.21194600	1.13537000
C	-1.34487000	-0.48870100	0.07317300
O	-2.00623300	0.58565500	0.66018400
H	-0.31809200	-2.22433400	0.78604800
H	1.40610200	-0.98355400	2.08488500
H	-1.15380200	-1.30320200	2.02866300
H	-0.11617400	1.64071400	-0.56219000
H	0.53381300	0.52792500	1.82843200
O	-0.25185744	2.75285468	0.05928671
H	-1.11080956	2.60659432	0.60856729
H	-0.39742744	3.50949668	-0.52337529
C	-2.27844800	-1.37879600	-0.69962600
H	-2.82987300	-0.81774600	-1.45631500
H	-1.73053300	-2.17878300	-1.19687700
H	-2.99302800	-1.82377700	-0.00294100
S	0.00519700	0.17798500	-1.11728200
H	-2.79576900	0.80252000	0.15190000
O	2.30688800	0.83617900	0.18545100
H	2.97156600	0.81523300	-0.51116800
C	2.15524600	-1.46535800	-0.47051300
H	2.59202900	-1.25342000	-1.44836500
H	2.95279100	-1.75689700	0.21672600
H	1.46808900	-2.30334100	-0.58501900