

Supporting Information

Testing Semiempirical QM Methods on a Data Set of Interaction Energies Mapping Repulsive Contacts in Organic Molecules

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Table S1: Heat Map of RMSE in kcal/mol for different SQM methods tested over R160x6 benchmark dataset. The colour scheme is green for minimum value, yellow for middle range and red for maximum value.

Method	N-N	N-C	N-O	N-H	C-C	C-O	C-H	O-O	O-H	H-H
DFT-D3	1.551	1.196	0.719	0.614	1.667	0.809	0.734	0.573	0.388	0.835
PBE-D3	1.631	1.235	0.698	0.675	1.573	0.795	0.511	0.537	0.555	1.173
MNDO	4.961	3.634	3.399	6.626	7.041	4.227	7.063	2.795	7.804	4.027
AM1	2.802	2.053	1.612	2.197	2.961	1.583	2.191	1.903	0.953	1.135
RM1	2.083	1.691	1.106	2.117	2.25	1.442	2.056	1.875	1.567	2.462
PM6	2.207	1.504	0.977	1.25	1.982	1.604	1.826	1.595	1.704	3.755
PM6-D3H4	1.365	1.413	1.161	0.977	1.655	1.78	1.69	1.806	1.786	4.062
PM6-D3H4'	1.357	1.412	1.163	0.979	1.656	1.774	1.683	1.812	1.778	1.56
PM7	1.079	1.281	1.152	1.023	1.667	2.002	1.778	1.506	0.971	3.387
OM2	2.152	2.057	1.135	1.245	2.108	1.759	1.903	1.626	1.646	2.291
OM2-D3 (Grimme)	1.305	1.962	1.353	1.508	2.014	1.871	2.395	1.921	1.993	2.702
OM3	1.971	1.872	1.014	1.723	2.077	1.354	1.648	1.516	1.21	1.913
OM3-D3 (Grimme)	1.074	1.842	1.379	2.13	1.838	1.509	2.048	1.885	1.581	2.464
OM3-D3H4	1.128	1.751	1.252	1.906	1.596	1.338	1.814	1.813	1.393	2.397
DFTB	2.415	1.59	1.83	2.275	1.977	1.803	1.592	1.303	1.663	2.035
DFTB-D	2.329	1.793	1.949	2.471	1.662	1.912	1.698	1.373	1.766	2.186
DFTB3	2.523	1.426	1.622	1.247	2.118	1.613	1.826	1.176	0.881	1.767
DFTB3-D3H4	2.195	1.535	1.925	1.445	1.491	1.942	1.636	1.551	1.006	2.774
GFN-xTB	2.145	2.086	1.925	1.37	1.711	2.721	1.365	1.654	0.944	2.085
PM6-D3H4R	1.36	1.372	0.86	0.98	1.625	1.604	1.777	1.194	0.968	1.589
DFTB3-D3H4R	1.879	1.14	1.213	0.557	1.364	1.37	1.64	0.986	0.477	1.442

Table S2: Element pairwise parameters optimized over R160x6 benchmark dataset for SCC-DFTB and PM6 Methods.

Element Pair	SCC-DFTB (c_1)	SCC-DFTB (c_2)	PM6 (c_1)	PM6 (c_2)
N-N	1.37E-01	1.40E+00	3.89E-02	2.38
N-C	1.38E-03	1.57E+00	1.46E-03	1.18
N-O	7.23E-04	3.20E+00	1.18E+00	1.83
N-H	0.00601	2.70E-01	3.69E-03	1.15
C-C	6.68E-03	3.91E+00	4.93E-03	1.77
C-O	1.68E-01	1.11E+00	1.04E-01	2.41
C-H	1.73E-03	2.62E-02	8.19E-02	0.79
O-O	3.10E-03	1.22E-01	1.32E-02	0.48
O-H	1.78E-02	4.47E+00	9.99E-02	1.83
H-H	2.07E-02	7.99E-01	2.36E-02	0.76

Table S3: Element pairwise parameters optimized over S66x8 benchmark dataset for SCC-DFTB and PM6 methods.

Element Pair	SCC-DFTB (c_1)	SCC-DFTB (c_2)	PM6 (c_1)	PM6 (c_2)
H-H	8.38E-03	3.3	1.10E-02	0.93
C-C	7.56E-03	2.7	1.36E-03	1.5
C-H	9.72E-04	1.84	1.75E-04	0.14
N-N	9.86E-04	1.09	1.87E-02	1.58
N-C	9.47E-04	1.36	1.66E-03	2.35
N-H	8.54E-04	1.77	0.47	1.2
O-O	9.47E-04	1.29	1.17E-02	0.25
O-N	9.33E-04	1.37	4.80E-02	0.53
O-C	9.36E-04	1.44	3.67E-02	2.17
O-H	9.42E-04	2.26	1.05E-01	0.84

Table S4: List of Benchmark energies for the 960 complexes corresponding to different element pair contacts calculated at CCSD(T)/CBS.

No.	System name	Dist. scaling	ΔE (kcal/mol)	element pair
1	acetylene(a)...acetylene(a)	1.00	5.346	H-H
1	acetylene(a)...acetylene(a)	1.05	4.320	H-H
1	acetylene(a)...acetylene(a)	1.10	3.520	H-H
1	acetylene(a)...acetylene(a)	1.15	2.896	H-H
1	acetylene(a)...acetylene(a)	1.25	2.020	H-H
1	acetylene(a)...acetylene(a)	1.65	0.719	H-H
2	acetylene(a)...ammonia(l)	1.00	5.863	H-H
2	acetylene(a)...ammonia(l)	1.05	4.716	H-H
2	acetylene(a)...ammonia(l)	1.10	3.818	H-H
2	acetylene(a)...ammonia(l)	1.15	3.112	H-H
2	acetylene(a)...ammonia(l)	1.25	2.119	H-H
2	acetylene(a)...ammonia(l)	1.65	0.665	H-H
3	acetylene(a)...benzene(p)	1.00	1.750	C-H
3	acetylene(a)...benzene(p)	1.05	-0.025	C-H
3	acetylene(a)...benzene(p)	1.10	-1.222	C-H
3	acetylene(a)...benzene(p)	1.15	-1.995	C-H
3	acetylene(a)...benzene(p)	1.25	-2.705	C-H
3	acetylene(a)...benzene(p)	1.65	-1.930	C-H
4	acetylene(a)...ethylene(a)	1.00	5.479	H-H
4	acetylene(a)...ethylene(a)	1.05	4.235	H-H
4	acetylene(a)...ethylene(a)	1.10	3.269	H-H
4	acetylene(a)...ethylene(a)	1.15	2.519	H-H
4	acetylene(a)...ethylene(a)	1.25	1.489	H-H
4	acetylene(a)...ethylene(a)	1.65	0.183	H-H
5	acetylene(a)...ethylene(p)	1.00	3.514	C-H
5	acetylene(a)...ethylene(p)	1.05	1.590	C-H
5	acetylene(a)...ethylene(p)	1.10	0.259	C-H
5	acetylene(a)...ethylene(p)	1.15	-0.638	C-H
5	acetylene(a)...ethylene(p)	1.25	-1.565	C-H
5	acetylene(a)...ethylene(p)	1.65	-1.350	C-H
6	acetylene(a)...formaldehyde_c(p)	1.00	4.237	C-H
6	acetylene(a)...formaldehyde_c(p)	1.05	2.904	C-H
6	acetylene(a)...formaldehyde_c(p)	1.10	1.964	C-H
6	acetylene(a)...formaldehyde_c(p)	1.15	1.309	C-H
6	acetylene(a)...formaldehyde_c(p)	1.25	0.550	C-H
6	acetylene(a)...formaldehyde_c(p)	1.65	0.004	C-H
7	acetylene(a)...methane(l)	1.00	5.370	H-H
7	acetylene(a)...methane(l)	1.05	4.102	H-H
7	acetylene(a)...methane(l)	1.10	3.117	H-H
7	acetylene(a)...methane(l)	1.15	2.354	H-H
7	acetylene(a)...methane(l)	1.25	1.311	H-H
7	acetylene(a)...methane(l)	1.65	0.034	H-H
8	acetylene(a)...water(l)	1.00	6.203	H-H
8	acetylene(a)...water(l)	1.05	5.176	H-H
8	acetylene(a)...water(l)	1.10	4.361	H-H
8	acetylene(a)...water(l)	1.15	3.711	H-H
8	acetylene(a)...water(l)	1.25	2.766	H-H
8	acetylene(a)...water(l)	1.65	1.168	H-H
9	acetylene(p)...acetylene(a)	1.00	3.606	C-H
9	acetylene(p)...acetylene(a)	1.05	1.626	C-H

9	acetylene(p)...acetylene(a)	1.10	0.266	C-H
9	acetylene(p)...acetylene(a)	1.15	-0.640	C-H
9	acetylene(p)...acetylene(a)	1.25	-1.561	C-H
9	acetylene(p)...acetylene(a)	1.65	-1.308	C-H
10	acetylene(p)...acetylene(p)	1.00	2.136	C-C
10	acetylene(p)...acetylene(p)	1.05	1.033	C-C
10	acetylene(p)...acetylene(p)	1.10	0.415	C-C
10	acetylene(p)...acetylene(p)	1.15	0.088	C-C
10	acetylene(p)...acetylene(p)	1.25	-0.129	C-C
10	acetylene(p)...acetylene(p)	1.65	0.008	C-C
11	acetylene(p)...ammonia(l)	1.00	3.444	C-H
11	acetylene(p)...ammonia(l)	1.05	1.704	C-H
11	acetylene(p)...ammonia(l)	1.10	0.517	C-H
11	acetylene(p)...ammonia(l)	1.15	-0.272	C-H
11	acetylene(p)...ammonia(l)	1.25	-1.074	C-H
11	acetylene(p)...ammonia(l)	1.65	-0.937	C-H
12	acetylene(p)...benzene(p)	1.00	0.480	C-C
12	acetylene(p)...benzene(p)	1.05	-0.951	C-C
12	acetylene(p)...benzene(p)	1.10	-1.670	C-C
12	acetylene(p)...benzene(p)	1.15	-1.952	C-C
12	acetylene(p)...benzene(p)	1.25	-1.860	C-C
12	acetylene(p)...benzene(p)	1.65	-0.495	C-C
13	acetylene(p)...ethylene(a)	1.00	2.957	C-H
13	acetylene(p)...ethylene(a)	1.05	1.451	C-H
13	acetylene(p)...ethylene(a)	1.10	0.435	C-H
13	acetylene(p)...ethylene(a)	1.15	-0.228	C-H
13	acetylene(p)...ethylene(a)	1.25	-0.886	C-H
13	acetylene(p)...ethylene(a)	1.65	-0.728	C-H
14	acetylene(p)...ethylene(p)	1.00	2.608	C-C
14	acetylene(p)...ethylene(p)	1.05	1.253	C-C
14	acetylene(p)...ethylene(p)	1.10	0.466	C-C
14	acetylene(p)...ethylene(p)	1.15	0.030	C-C
14	acetylene(p)...ethylene(p)	1.25	-0.286	C-C
14	acetylene(p)...ethylene(p)	1.65	-0.090	C-C
15	acetylene(p)...formaldehyde_c(p)	1.00	3.132	C-C
15	acetylene(p)...formaldehyde_c(p)	1.05	1.203	C-C
15	acetylene(p)...formaldehyde_c(p)	1.10	0.007	C-C
15	acetylene(p)...formaldehyde_c(p)	1.15	-0.693	C-C
15	acetylene(p)...formaldehyde_c(p)	1.25	-1.222	C-C
15	acetylene(p)...formaldehyde_c(p)	1.65	-0.585	C-C
16	acetylene(p)...methane(l)	1.00	3.303	C-H
16	acetylene(p)...methane(l)	1.05	1.889	C-H
16	acetylene(p)...methane(l)	1.10	0.928	C-H
16	acetylene(p)...methane(l)	1.15	0.291	C-H
16	acetylene(p)...methane(l)	1.25	-0.369	C-H
16	acetylene(p)...methane(l)	1.65	-0.431	C-H
17	acetylene(p)...water(l)	1.00	2.491	C-H
17	acetylene(p)...water(l)	1.05	0.474	C-H
17	acetylene(p)...water(l)	1.10	-0.905	C-H
17	acetylene(p)...water(l)	1.15	-1.812	C-H
17	acetylene(p)...water(l)	1.25	-2.690	C-H
17	acetylene(p)...water(l)	1.65	-2.016	C-H
18	ammonia(a)...ammonia(a)	1.00	5.187	N-N
18	ammonia(a)...ammonia(a)	1.05	4.192	N-N

18	ammonia(a)...ammonia(a)	1.10	3.467	N-N
18	ammonia(a)...ammonia(a)	1.15	2.924	N-N
18	ammonia(a)...ammonia(a)	1.25	2.175	N-N
18	ammonia(a)...ammonia(a)	1.65	0.889	N-N
19	ammonia(a)...benzene(p)	1.00	3.567	N-C
19	ammonia(a)...benzene(p)	1.05	2.088	N-C
19	ammonia(a)...benzene(p)	1.10	1.172	N-C
19	ammonia(a)...benzene(p)	1.15	0.628	N-C
19	ammonia(a)...benzene(p)	1.25	0.172	N-C
19	ammonia(a)...benzene(p)	1.65	0.248	N-C
20	ammonia(a)...formaldehyde(l)	1.00	4.566	N-O
20	ammonia(a)...formaldehyde(l)	1.05	3.577	N-O
20	ammonia(a)...formaldehyde(l)	1.10	2.912	N-O
20	ammonia(a)...formaldehyde(l)	1.15	2.450	N-O
20	ammonia(a)...formaldehyde(l)	1.25	1.867	N-O
20	ammonia(a)...formaldehyde(l)	1.65	0.923	N-O
21	ammonia(a)...formaldehyde(p)	1.00	4.208	N-O
21	ammonia(a)...formaldehyde(p)	1.05	2.695	N-O
21	ammonia(a)...formaldehyde(p)	1.10	1.723	N-O
21	ammonia(a)...formaldehyde(p)	1.15	1.104	N-O
21	ammonia(a)...formaldehyde(p)	1.25	0.472	N-O
21	ammonia(a)...formaldehyde(p)	1.65	0.101	N-O
22	ammonia(a)...methane(l)	1.00	4.771	N-H
22	ammonia(a)...methane(l)	1.05	3.024	N-H
22	ammonia(a)...methane(l)	1.10	1.779	N-H
22	ammonia(a)...methane(l)	1.15	0.905	N-H
22	ammonia(a)...methane(l)	1.25	-0.102	N-H
22	ammonia(a)...methane(l)	1.65	-0.574	N-H
23	ammonia(a)...methanol(a)	1.00	5.096	N-O
23	ammonia(a)...methanol(a)	1.05	4.053	N-O
23	ammonia(a)...methanol(a)	1.10	3.323	N-O
23	ammonia(a)...methanol(a)	1.15	2.795	N-O
23	ammonia(a)...methanol(a)	1.25	2.097	N-O
23	ammonia(a)...methanol(a)	1.65	0.933	N-O
24	ammonia(a)...methanol(p)	1.00	5.201	N-O
24	ammonia(a)...methanol(p)	1.05	3.754	N-O
24	ammonia(a)...methanol(p)	1.10	2.754	N-O
24	ammonia(a)...methanol(p)	1.15	2.060	N-O
24	ammonia(a)...methanol(p)	1.25	1.234	N-O
24	ammonia(a)...methanol(p)	1.65	0.361	N-O
25	ammonia(a)...pyridine(a)	1.00	5.106	N-N
25	ammonia(a)...pyridine(a)	1.05	4.071	N-N
25	ammonia(a)...pyridine(a)	1.10	3.339	N-N
25	ammonia(a)...pyridine(a)	1.15	2.805	N-N
25	ammonia(a)...pyridine(a)	1.25	2.092	N-N
25	ammonia(a)...pyridine(a)	1.65	0.908	N-N
26	ammonia(a)...pyridine(p)	1.00	3.286	N-N
26	ammonia(a)...pyridine(p)	1.05	1.924	N-N
26	ammonia(a)...pyridine(p)	1.10	1.109	N-N
26	ammonia(a)...pyridine(p)	1.15	0.643	N-N
26	ammonia(a)...pyridine(p)	1.25	0.278	N-N
26	ammonia(a)...pyridine(p)	1.65	0.341	N-N
27	ammonia(a)...water(a)	1.00	4.993	N-O
27	ammonia(a)...water(a)	1.05	3.990	N-O

27	ammonia(a)...water(a)	1.10	3.286	N-O
27	ammonia(a)...water(a)	1.15	2.775	N-O
27	ammonia(a)...water(a)	1.25	2.094	N-O
27	ammonia(a)...water(a)	1.65	0.941	N-O
28	ammonia(a)...water(p)	1.00	5.511	N-O
28	ammonia(a)...water(p)	1.05	4.045	N-O
28	ammonia(a)...water(p)	1.10	3.044	N-O
28	ammonia(a)...water(p)	1.15	2.348	N-O
28	ammonia(a)...water(p)	1.25	1.501	N-O
28	ammonia(a)...water(p)	1.65	0.460	N-O
29	ammonia(l)...ammonia(l)	1.00	5.918	H-H
29	ammonia(l)...ammonia(l)	1.05	4.711	H-H
29	ammonia(l)...ammonia(l)	1.10	3.765	H-H
29	ammonia(l)...ammonia(l)	1.15	3.023	H-H
29	ammonia(l)...ammonia(l)	1.25	1.978	H-H
29	ammonia(l)...ammonia(l)	1.65	0.485	H-H
30	ammonia(l)...benzene(p)	1.00	2.569	C-H
30	ammonia(l)...benzene(p)	1.05	0.880	C-H
30	ammonia(l)...benzene(p)	1.10	-0.276	C-H
30	ammonia(l)...benzene(p)	1.15	-1.041	C-H
30	ammonia(l)...benzene(p)	1.25	-1.795	C-H
30	ammonia(l)...benzene(p)	1.65	-1.387	C-H
31	ammonia(l)...ethylene(a)	1.00	5.634	H-H
31	ammonia(l)...ethylene(a)	1.05	4.362	H-H
31	ammonia(l)...ethylene(a)	1.10	3.371	H-H
31	ammonia(l)...ethylene(a)	1.15	2.598	H-H
31	ammonia(l)...ethylene(a)	1.25	1.531	H-H
31	ammonia(l)...ethylene(a)	1.65	0.157	H-H
32	ammonia(l)...ethylene(p)	1.00	3.706	C-H
32	ammonia(l)...ethylene(p)	1.05	1.864	C-H
32	ammonia(l)...ethylene(p)	1.10	0.584	C-H
32	ammonia(l)...ethylene(p)	1.15	-0.282	C-H
32	ammonia(l)...ethylene(p)	1.25	-1.196	C-H
32	ammonia(l)...ethylene(p)	1.65	-1.123	C-H
33	ammonia(l)...formaldehyde_c(p)	1.00	4.918	C-H
33	ammonia(l)...formaldehyde_c(p)	1.05	3.550	C-H
33	ammonia(l)...formaldehyde_c(p)	1.10	2.569	C-H
33	ammonia(l)...formaldehyde_c(p)	1.15	1.870	C-H
33	ammonia(l)...formaldehyde_c(p)	1.25	1.030	C-H
33	ammonia(l)...formaldehyde_c(p)	1.65	0.295	C-H
34	ammonia(l)...methane(l)	1.00	5.528	H-H
34	ammonia(l)...methane(l)	1.05	4.250	H-H
34	ammonia(l)...methane(l)	1.10	3.254	H-H
34	ammonia(l)...methane(l)	1.15	2.480	H-H
34	ammonia(l)...methane(l)	1.25	1.412	H-H
34	ammonia(l)...methane(l)	1.65	0.067	H-H
35	ammonia(l)...water(l)	1.00	6.337	H-H
35	ammonia(l)...water(l)	1.05	5.182	H-H
35	ammonia(l)...water(l)	1.10	4.270	H-H
35	ammonia(l)...water(l)	1.15	3.548	H-H
35	ammonia(l)...water(l)	1.25	2.511	H-H
35	ammonia(l)...water(l)	1.65	0.879	H-H
36	benzene(p)...benzene(p)	1.00	-2.230	C-C
36	benzene(p)...benzene(p)	1.05	-4.191	C-C

36	benzene(p)...benzene(p)	1.10	-5.165	C-C
36	benzene(p)...benzene(p)	1.15	-5.501	C-C
36	benzene(p)...benzene(p)	1.25	-5.142	C-C
36	benzene(p)...benzene(p)	1.65	-1.857	C-C
37	benzene(p)...ethylene(a)	1.00	2.455	C-H
37	benzene(p)...ethylene(a)	1.05	0.805	C-H
37	benzene(p)...ethylene(a)	1.10	-0.322	C-H
37	benzene(p)...ethylene(a)	1.15	-1.062	C-H
37	benzene(p)...ethylene(a)	1.25	-1.781	C-H
37	benzene(p)...ethylene(a)	1.65	-1.330	C-H
38	benzene(p)...formaldehyde(l)	1.00	2.396	C-O
38	benzene(p)...formaldehyde(l)	1.05	1.005	C-O
38	benzene(p)...formaldehyde(l)	1.10	0.210	C-O
38	benzene(p)...formaldehyde(l)	1.15	-0.208	C-O
38	benzene(p)...formaldehyde(l)	1.25	-0.443	C-O
38	benzene(p)...formaldehyde(l)	1.65	0.054	C-O
39	benzene(p)...formaldehyde(p)	1.00	2.525	C-O
39	benzene(p)...formaldehyde(p)	1.05	1.037	C-O
39	benzene(p)...formaldehyde(p)	1.10	0.154	C-O
39	benzene(p)...formaldehyde(p)	1.15	-0.336	C-O
39	benzene(p)...formaldehyde(p)	1.25	-0.662	C-O
39	benzene(p)...formaldehyde(p)	1.65	-0.178	C-O
40	benzene(p)...methane(l)	1.00	3.217	C-H
40	benzene(p)...methane(l)	1.05	1.557	C-H
40	benzene(p)...methane(l)	1.10	0.411	C-H
40	benzene(p)...methane(l)	1.15	-0.357	C-H
40	benzene(p)...methane(l)	1.25	-1.144	C-H
40	benzene(p)...methane(l)	1.65	-0.969	C-H
41	benzene(p)...methanol(a)	1.00	3.186	C-O
41	benzene(p)...methanol(a)	1.05	1.644	C-O
41	benzene(p)...methanol(a)	1.10	0.713	C-O
41	benzene(p)...methanol(a)	1.15	0.181	C-O
41	benzene(p)...methanol(a)	1.25	-0.217	C-O
41	benzene(p)...methanol(a)	1.65	0.090	C-O
42	benzene(p)...methanol(p)	1.00	3.456	C-O
42	benzene(p)...methanol(p)	1.05	1.941	C-O
42	benzene(p)...methanol(p)	1.10	0.888	C-O
42	benzene(p)...methanol(p)	1.15	0.176	C-O
42	benzene(p)...methanol(p)	1.25	-0.572	C-O
42	benzene(p)...methanol(p)	1.65	-0.544	C-O
43	benzene(p)...pyridine(a)	1.00	1.452	N-C
43	benzene(p)...pyridine(a)	1.05	-0.118	N-C
43	benzene(p)...pyridine(a)	1.10	-1.004	N-C
43	benzene(p)...pyridine(a)	1.15	-1.441	N-C
43	benzene(p)...pyridine(a)	1.25	-1.574	N-C
43	benzene(p)...pyridine(a)	1.65	-0.374	N-C
44	benzene(p)...water(a)	1.00	3.358	C-O
44	benzene(p)...water(a)	1.05	1.886	C-O
44	benzene(p)...water(a)	1.10	0.994	C-O
44	benzene(p)...water(a)	1.15	0.478	C-O
44	benzene(p)...water(a)	1.25	0.066	C-O
44	benzene(p)...water(a)	1.65	0.205	C-O
45	benzene(p)...water(l)	1.00	3.564	C-H
45	benzene(p)...water(l)	1.05	1.355	C-H

45	benzene(p)...water(l)	1.10	-0.195	C-H
45	benzene(p)...water(l)	1.15	-1.255	C-H
45	benzene(p)...water(l)	1.25	-2.379	C-H
45	benzene(p)...water(l)	1.65	-2.124	C-H
46	benzene(p)...water(p)	1.00	4.283	C-O
46	benzene(p)...water(p)	1.05	2.687	C-O
46	benzene(p)...water(p)	1.10	1.675	C-O
46	benzene(p)...water(p)	1.15	1.048	C-O
46	benzene(p)...water(p)	1.25	0.449	C-O
46	benzene(p)...water(p)	1.65	0.229	C-O
47	CO(a)...acetylene(a)	1.00	3.763	C-H
47	CO(a)...acetylene(a)	1.05	1.956	C-H
47	CO(a)...acetylene(a)	1.10	0.709	C-H
47	CO(a)...acetylene(a)	1.15	-0.130	C-H
47	CO(a)...acetylene(a)	1.25	-1.009	C-H
47	CO(a)...acetylene(a)	1.65	-0.991	C-H
48	CO(a)...acetylene(p)	1.00	4.305	C-C
48	CO(a)...acetylene(p)	1.05	2.677	C-C
48	CO(a)...acetylene(p)	1.10	1.651	C-C
48	CO(a)...acetylene(p)	1.15	1.013	C-C
48	CO(a)...acetylene(p)	1.25	0.387	C-C
48	CO(a)...acetylene(p)	1.65	0.071	C-C
49	CO(a)...ammonia(a)	1.00	5.428	N-C
49	CO(a)...ammonia(a)	1.05	3.865	N-C
49	CO(a)...ammonia(a)	1.10	2.815	N-C
49	CO(a)...ammonia(a)	1.15	2.105	N-C
49	CO(a)...ammonia(a)	1.25	1.283	N-C
49	CO(a)...ammonia(a)	1.65	0.407	N-C
50	CO(a)...ammonia(l)	1.00	4.184	C-H
50	CO(a)...ammonia(l)	1.05	2.440	C-H
50	CO(a)...ammonia(l)	1.10	1.219	C-H
50	CO(a)...ammonia(l)	1.15	0.381	C-H
50	CO(a)...ammonia(l)	1.25	-0.539	C-H
50	CO(a)...ammonia(l)	1.65	-0.761	C-H
51	CO(a)...benzene(p)	1.00	3.829	C-C
51	CO(a)...benzene(p)	1.05	1.979	C-C
51	CO(a)...benzene(p)	1.10	0.839	C-C
51	CO(a)...benzene(p)	1.15	0.167	C-C
51	CO(a)...benzene(p)	1.25	-0.381	C-C
51	CO(a)...benzene(p)	1.65	-0.141	C-C
52	CO(a)...CO(a)	1.00	4.954	C-C
52	CO(a)...CO(a)	1.05	3.150	C-C
52	CO(a)...CO(a)	1.10	1.994	C-C
52	CO(a)...CO(a)	1.15	1.259	C-C
52	CO(a)...CO(a)	1.25	0.504	C-C
52	CO(a)...CO(a)	1.65	0.031	C-C
53	CO(a)...ethylene(a)	1.00	4.581	C-H
53	CO(a)...ethylene(a)	1.05	2.893	C-H
53	CO(a)...ethylene(a)	1.10	1.710	C-H
53	CO(a)...ethylene(a)	1.15	0.893	C-H
53	CO(a)...ethylene(a)	1.25	-0.024	C-H
53	CO(a)...ethylene(a)	1.65	-0.430	C-H
54	CO(a)...ethylene(p)	1.00	4.696	C-C
54	CO(a)...ethylene(p)	1.05	2.982	C-C

54	CO(a)...ethylene(p)	1.10	1.881	C-C
54	CO(a)...ethylene(p)	1.15	1.183	C-C
54	CO(a)...ethylene(p)	1.25	0.473	C-C
54	CO(a)...ethylene(p)	1.65	0.070	C-C
55	CO(a)...formaldehyde_c(p)	1.00	3.672	C-C
55	CO(a)...formaldehyde_c(p)	1.05	1.860	C-C
55	CO(a)...formaldehyde_c(p)	1.10	0.710	C-C
55	CO(a)...formaldehyde_c(p)	1.15	0.011	C-C
55	CO(a)...formaldehyde_c(p)	1.25	-0.594	C-C
55	CO(a)...formaldehyde_c(p)	1.65	-0.377	C-C
56	CO(a)...formaldehyde(l)	1.00	4.899	C-O
56	CO(a)...formaldehyde(l)	1.05	3.311	C-O
56	CO(a)...formaldehyde(l)	1.10	2.299	C-O
56	CO(a)...formaldehyde(l)	1.15	1.655	C-O
56	CO(a)...formaldehyde(l)	1.25	0.981	C-O
56	CO(a)...formaldehyde(l)	1.65	0.412	C-O
57	CO(a)...formaldehyde(p)	1.00	4.379	C-O
57	CO(a)...formaldehyde(p)	1.05	2.661	C-O
57	CO(a)...formaldehyde(p)	1.10	1.574	C-O
57	CO(a)...formaldehyde(p)	1.15	0.898	C-O
57	CO(a)...formaldehyde(p)	1.25	0.244	C-O
57	CO(a)...formaldehyde(p)	1.65	-0.007	C-O
58	CO(a)...H2(a)	1.00	4.792	C-H
58	CO(a)...H2(a)	1.05	3.186	C-H
58	CO(a)...H2(a)	1.10	2.049	C-H
58	CO(a)...H2(a)	1.15	1.254	C-H
58	CO(a)...H2(a)	1.25	0.337	C-H
58	CO(a)...H2(a)	1.65	-0.224	C-H
59	CO(a)...methane(l)	1.00	4.816	C-H
59	CO(a)...methane(l)	1.05	3.178	C-H
59	CO(a)...methane(l)	1.10	2.022	C-H
59	CO(a)...methane(l)	1.15	1.217	C-H
59	CO(a)...methane(l)	1.25	0.295	C-H
59	CO(a)...methane(l)	1.65	-0.245	C-H
60	CO(a)...methanol(a)	1.00	5.229	C-O
60	CO(a)...methanol(a)	1.05	3.617	C-O
60	CO(a)...methanol(a)	1.10	2.561	C-O
60	CO(a)...methanol(a)	1.15	1.868	C-O
60	CO(a)...methanol(a)	1.25	1.104	C-O
60	CO(a)...methanol(a)	1.65	0.387	C-O
61	CO(a)...methanol(p)	1.00	5.322	C-O
61	CO(a)...methanol(p)	1.05	3.527	C-O
61	CO(a)...methanol(p)	1.10	2.320	C-O
61	CO(a)...methanol(p)	1.15	1.514	C-O
61	CO(a)...methanol(p)	1.25	0.632	C-O
61	CO(a)...methanol(p)	1.65	0.045	C-O
62	CO(a)...N2(a)	1.00	4.668	N-C
62	CO(a)...N2(a)	1.05	2.855	N-C
62	CO(a)...N2(a)	1.10	1.715	N-C
62	CO(a)...N2(a)	1.15	1.008	N-C
62	CO(a)...N2(a)	1.25	0.316	N-C
62	CO(a)...N2(a)	1.65	-0.010	N-C
63	CO(a)...pyridine(a)	1.00	5.157	N-C
63	CO(a)...pyridine(a)	1.05	3.558	N-C

63	CO(a)...pyridine(a)	1.10	2.504	N-C
63	CO(a)...pyridine(a)	1.15	1.807	N-C
63	CO(a)...pyridine(a)	1.25	1.034	N-C
63	CO(a)...pyridine(a)	1.65	0.323	N-C
64	CO(a)...pyridine(p)	1.00	3.404	N-C
64	CO(a)...pyridine(p)	1.05	1.638	N-C
64	CO(a)...pyridine(p)	1.10	0.581	N-C
64	CO(a)...pyridine(p)	1.15	-0.018	N-C
64	CO(a)...pyridine(p)	1.25	-0.462	N-C
64	CO(a)...pyridine(p)	1.65	-0.122	N-C
65	CO(a)...water(a)	1.00	5.186	C-O
65	CO(a)...water(a)	1.05	3.607	C-O
65	CO(a)...water(a)	1.10	2.573	C-O
65	CO(a)...water(a)	1.15	1.894	C-O
65	CO(a)...water(a)	1.25	1.143	C-O
65	CO(a)...water(a)	1.65	0.411	C-O
66	CO(a)...water(l)	1.00	4.074	C-H
66	CO(a)...water(l)	1.05	1.965	C-H
66	CO(a)...water(l)	1.10	0.485	C-H
66	CO(a)...water(l)	1.15	-0.529	C-H
66	CO(a)...water(l)	1.25	-1.623	C-H
66	CO(a)...water(l)	1.65	-1.590	C-H
67	CO(a)...water(p)	1.00	5.614	C-O
67	CO(a)...water(p)	1.05	3.809	C-O
67	CO(a)...water(p)	1.10	2.610	C-O
67	CO(a)...water(p)	1.15	1.812	C-O
67	CO(a)...water(p)	1.25	0.924	C-O
67	CO(a)...water(p)	1.65	0.171	C-O
68	ethylene(a)...ethylene(a)	1.00	5.485	H-H
68	ethylene(a)...ethylene(a)	1.05	4.181	H-H
68	ethylene(a)...ethylene(a)	1.10	3.165	H-H
68	ethylene(a)...ethylene(a)	1.15	2.377	H-H
68	ethylene(a)...ethylene(a)	1.25	1.296	H-H
68	ethylene(a)...ethylene(a)	1.65	-0.020	H-H
69	ethylene(a)...formaldehyde_c(p)	1.00	4.372	C-H
69	ethylene(a)...formaldehyde_c(p)	1.05	2.908	C-H
69	ethylene(a)...formaldehyde_c(p)	1.10	1.863	C-H
69	ethylene(a)...formaldehyde_c(p)	1.15	1.129	C-H
69	ethylene(a)...formaldehyde_c(p)	1.25	0.276	C-H
69	ethylene(a)...formaldehyde_c(p)	1.65	-0.231	C-H
70	ethylene(a)...methane(l)	1.00	5.461	H-H
70	ethylene(a)...methane(l)	1.05	4.152	H-H
70	ethylene(a)...methane(l)	1.10	3.133	H-H
70	ethylene(a)...methane(l)	1.15	2.341	H-H
70	ethylene(a)...methane(l)	1.25	1.255	H-H
70	ethylene(a)...methane(l)	1.65	-0.060	H-H
71	ethylene(a)...water(l)	1.00	6.078	H-H
71	ethylene(a)...water(l)	1.05	4.816	H-H
71	ethylene(a)...water(l)	1.10	3.830	H-H
71	ethylene(a)...water(l)	1.15	3.057	H-H
71	ethylene(a)...water(l)	1.25	1.975	H-H
71	ethylene(a)...water(l)	1.65	0.469	H-H
72	ethylene(p)...benzene(p)	1.00	0.851	C-C
72	ethylene(p)...benzene(p)	1.05	-0.823	C-C

72	ethylene(p)...benzene(p)	1.10	-1.697	C-C
72	ethylene(p)...benzene(p)	1.15	-2.074	C-C
72	ethylene(p)...benzene(p)	1.25	-2.060	C-C
72	ethylene(p)...benzene(p)	1.65	-0.603	C-C
73	ethylene(p)...ethylene(a)	1.00	3.310	C-H
73	ethylene(p)...ethylene(a)	1.05	1.773	C-H
73	ethylene(p)...ethylene(a)	1.10	0.719	C-H
73	ethylene(p)...ethylene(a)	1.15	0.014	C-H
73	ethylene(p)...ethylene(a)	1.25	-0.719	C-H
73	ethylene(p)...ethylene(a)	1.65	-0.697	C-H
74	ethylene(p)...ethylene(p)	1.00	3.805	C-C
74	ethylene(p)...ethylene(p)	1.05	2.070	C-C
74	ethylene(p)...ethylene(p)	1.10	1.013	C-C
74	ethylene(p)...ethylene(p)	1.15	0.389	C-C
74	ethylene(p)...ethylene(p)	1.25	-0.147	C-C
74	ethylene(p)...ethylene(p)	1.65	-0.101	C-C
75	ethylene(p)...methane(l)	1.00	3.679	C-H
75	ethylene(p)...methane(l)	1.05	2.197	C-H
75	ethylene(p)...methane(l)	1.10	1.171	C-H
75	ethylene(p)...methane(l)	1.15	0.476	C-H
75	ethylene(p)...methane(l)	1.25	-0.275	C-H
75	ethylene(p)...methane(l)	1.65	-0.451	C-H
76	ethylene(p)...water(l)	1.00	3.960	C-H
76	ethylene(p)...water(l)	1.05	1.634	C-H
76	ethylene(p)...water(l)	1.10	-0.020	C-H
76	ethylene(p)...water(l)	1.15	-1.165	C-H
76	ethylene(p)...water(l)	1.25	-2.405	C-H
76	ethylene(p)...water(l)	1.65	-2.194	C-H
77	formaldehyde_c(p)...benzene(p)	1.00	1.892	C-C
77	formaldehyde_c(p)...benzene(p)	1.05	-0.658	C-C
77	formaldehyde_c(p)...benzene(p)	1.10	-2.180	C-C
77	formaldehyde_c(p)...benzene(p)	1.15	-3.008	C-C
77	formaldehyde_c(p)...benzene(p)	1.25	-3.460	C-C
77	formaldehyde_c(p)...benzene(p)	1.65	-1.679	C-C
78	formaldehyde_c(p)...ethylene(p)	1.00	3.639	C-C
78	formaldehyde_c(p)...ethylene(p)	1.05	1.512	C-C
78	formaldehyde_c(p)...ethylene(p)	1.10	0.163	C-C
78	formaldehyde_c(p)...ethylene(p)	1.15	-0.651	C-C
78	formaldehyde_c(p)...ethylene(p)	1.25	-1.318	C-C
78	formaldehyde_c(p)...ethylene(p)	1.65	-0.715	C-C
79	formaldehyde_c(p)...formaldehyde_c(p)	1.00	2.778	C-C
79	formaldehyde_c(p)...formaldehyde_c(p)	1.05	0.779	C-C
79	formaldehyde_c(p)...formaldehyde_c(p)	1.10	-0.454	C-C
79	formaldehyde_c(p)...formaldehyde_c(p)	1.15	-1.173	C-C
79	formaldehyde_c(p)...formaldehyde_c(p)	1.25	-1.719	C-C
79	formaldehyde_c(p)...formaldehyde_c(p)	1.65	-1.048	C-C
80	formaldehyde_c(p)...methane(l)	1.00	4.438	C-H
80	formaldehyde_c(p)...methane(l)	1.05	2.970	C-H
80	formaldehyde_c(p)...methane(l)	1.10	1.918	C-H
80	formaldehyde_c(p)...methane(l)	1.15	1.175	C-H
80	formaldehyde_c(p)...methane(l)	1.25	0.305	C-H
80	formaldehyde_c(p)...methane(l)	1.65	-0.232	C-H
81	formaldehyde_c(p)...water(l)	1.00	4.782	C-H
81	formaldehyde_c(p)...water(l)	1.05	3.553	C-H

81	formaldehyde_c(p)...water(l)	1.10	2.675	C-H
81	formaldehyde_c(p)...water(l)	1.15	2.049	C-H
81	formaldehyde_c(p)...water(l)	1.25	1.286	C-H
81	formaldehyde_c(p)...water(l)	1.65	0.504	C-H
82	formaldehyde(l)...formaldehyde(l)	1.00	3.703	O-O
82	formaldehyde(l)...formaldehyde(l)	1.05	2.715	O-O
82	formaldehyde(l)...formaldehyde(l)	1.10	2.113	O-O
82	formaldehyde(l)...formaldehyde(l)	1.15	1.740	O-O
82	formaldehyde(l)...formaldehyde(l)	1.25	1.347	O-O
82	formaldehyde(l)...formaldehyde(l)	1.65	0.828	O-O
83	formaldehyde(l)...formaldehyde(p)	1.00	3.426	O-O
83	formaldehyde(l)...formaldehyde(p)	1.05	1.809	O-O
83	formaldehyde(l)...formaldehyde(p)	1.10	0.840	O-O
83	formaldehyde(l)...formaldehyde(p)	1.15	0.280	O-O
83	formaldehyde(l)...formaldehyde(p)	1.25	-0.181	O-O
83	formaldehyde(l)...formaldehyde(p)	1.65	-0.085	O-O
84	formaldehyde(l)...methane(l)	1.00	3.975	O-H
84	formaldehyde(l)...methane(l)	1.05	2.398	O-H
84	formaldehyde(l)...methane(l)	1.10	1.307	O-H
84	formaldehyde(l)...methane(l)	1.15	0.566	O-H
84	formaldehyde(l)...methane(l)	1.25	-0.241	O-H
84	formaldehyde(l)...methane(l)	1.65	-0.494	O-H
85	formaldehyde(l)...methanol(a)	1.00	4.277	O-O
85	formaldehyde(l)...methanol(a)	1.05	3.196	O-O
85	formaldehyde(l)...methanol(a)	1.10	2.512	O-O
85	formaldehyde(l)...methanol(a)	1.15	2.070	O-O
85	formaldehyde(l)...methanol(a)	1.25	1.572	O-O
85	formaldehyde(l)...methanol(a)	1.65	0.878	O-O
86	formaldehyde(l)...methanol(p)	1.00	4.141	O-O
86	formaldehyde(l)...methanol(p)	1.05	2.664	O-O
86	formaldehyde(l)...methanol(p)	1.10	1.718	O-O
86	formaldehyde(l)...methanol(p)	1.15	1.118	O-O
86	formaldehyde(l)...methanol(p)	1.25	0.509	O-O
86	formaldehyde(l)...methanol(p)	1.65	0.164	O-O
87	formaldehyde(l)...pyridine(a)	1.00	4.348	N-C
87	formaldehyde(l)...pyridine(a)	1.05	3.322	N-C
87	formaldehyde(l)...pyridine(a)	1.10	2.654	N-C
87	formaldehyde(l)...pyridine(a)	1.15	2.208	N-C
87	formaldehyde(l)...pyridine(a)	1.25	1.680	N-C
87	formaldehyde(l)...pyridine(a)	1.65	0.899	N-C
88	formaldehyde(l)...pyridine(p)	1.00	2.179	N-C
88	formaldehyde(l)...pyridine(p)	1.05	0.903	N-C
88	formaldehyde(l)...pyridine(p)	1.10	0.202	N-C
88	formaldehyde(l)...pyridine(p)	1.15	-0.146	N-C
88	formaldehyde(l)...pyridine(p)	1.25	-0.306	N-C
88	formaldehyde(l)...pyridine(p)	1.65	0.160	N-C
89	formaldehyde(l)...water(a)	1.00	4.245	O-O
89	formaldehyde(l)...water(a)	1.05	3.214	O-O
89	formaldehyde(l)...water(a)	1.10	2.558	O-O
89	formaldehyde(l)...water(a)	1.15	2.131	O-O
89	formaldehyde(l)...water(a)	1.25	1.638	O-O
89	formaldehyde(l)...water(a)	1.65	0.911	O-O
90	formaldehyde(l)...water(p)	1.00	4.693	O-O
90	formaldehyde(l)...water(p)	1.05	3.223	O-O

90	formaldehyde(l)...water(p)	1.10	2.281	O-O
90	formaldehyde(l)...water(p)	1.15	1.673	O-O
90	formaldehyde(l)...water(p)	1.25	1.010	O-O
90	formaldehyde(l)...water(p)	1.65	0.365	O-O
91	formaldehyde(p)...formaldehyde(p)	1.00	2.208	O-O
91	formaldehyde(p)...formaldehyde(p)	1.05	0.179	O-O
91	formaldehyde(p)...formaldehyde(p)	1.10	-1.025	O-O
91	formaldehyde(p)...formaldehyde(p)	1.15	-1.695	O-O
91	formaldehyde(p)...formaldehyde(p)	1.25	-2.137	O-O
91	formaldehyde(p)...formaldehyde(p)	1.65	-1.230	O-O
92	formaldehyde(p)...methane(l)	1.00	4.000	O-H
92	formaldehyde(p)...methane(l)	1.05	2.497	O-H
92	formaldehyde(p)...methane(l)	1.10	1.448	O-H
92	formaldehyde(p)...methane(l)	1.15	0.729	O-H
92	formaldehyde(p)...methane(l)	1.25	-0.068	O-H
92	formaldehyde(p)...methane(l)	1.65	-0.380	O-H
93	formaldehyde(p)...methanol(a)	1.00	3.683	O-O
93	formaldehyde(p)...methanol(a)	1.05	2.157	O-O
93	formaldehyde(p)...methanol(a)	1.10	1.214	O-O
93	formaldehyde(p)...methanol(a)	1.15	0.642	O-O
93	formaldehyde(p)...methanol(a)	1.25	0.112	O-O
93	formaldehyde(p)...methanol(a)	1.65	-0.022	O-O
94	formaldehyde(p)...methanol(p)	1.00	3.370	O-O
94	formaldehyde(p)...methanol(p)	1.05	1.405	O-O
94	formaldehyde(p)...methanol(p)	1.10	0.165	O-O
94	formaldehyde(p)...methanol(p)	1.15	-0.589	O-O
94	formaldehyde(p)...methanol(p)	1.25	-1.241	O-O
94	formaldehyde(p)...methanol(p)	1.65	-0.865	O-O
95	formaldehyde(p)...pyridine(a)	1.00	3.826	N-O
95	formaldehyde(p)...pyridine(a)	1.05	2.147	N-O
95	formaldehyde(p)...pyridine(a)	1.10	1.100	N-O
95	formaldehyde(p)...pyridine(a)	1.15	0.465	N-O
95	formaldehyde(p)...pyridine(a)	1.25	-0.109	N-O
95	formaldehyde(p)...pyridine(a)	1.65	-0.126	N-O
96	formaldehyde(p)...pyridine(p)	1.00	1.559	N-O
96	formaldehyde(p)...pyridine(p)	1.05	-0.427	N-O
96	formaldehyde(p)...pyridine(p)	1.10	-1.585	N-O
96	formaldehyde(p)...pyridine(p)	1.15	-2.198	N-O
96	formaldehyde(p)...pyridine(p)	1.25	-2.508	N-O
96	formaldehyde(p)...pyridine(p)	1.65	-1.200	N-O
97	formaldehyde(p)...water(a)	1.00	3.781	O-O
97	formaldehyde(p)...water(a)	1.05	2.328	O-O
97	formaldehyde(p)...water(a)	1.10	1.427	O-O
97	formaldehyde(p)...water(a)	1.15	0.875	O-O
97	formaldehyde(p)...water(a)	1.25	0.346	O-O
97	formaldehyde(p)...water(a)	1.65	0.102	O-O
98	formaldehyde(p)...water(p)	1.00	4.346	O-O
98	formaldehyde(p)...water(p)	1.05	2.096	O-O
98	formaldehyde(p)...water(p)	1.10	0.684	O-O
98	formaldehyde(p)...water(p)	1.15	-0.180	O-O
98	formaldehyde(p)...water(p)	1.25	-0.962	O-O
98	formaldehyde(p)...water(p)	1.65	-0.816	O-O
99	H2(a)...acetylene(a)	1.00	5.434	H-H
99	H2(a)...acetylene(a)	1.05	4.225	H-H

99	H2(a)...acetylene(a)	1.10	3.283	H-H
99	H2(a)...acetylene(a)	1.15	2.550	H-H
99	H2(a)...acetylene(a)	1.25	1.537	H-H
99	H2(a)...acetylene(a)	1.65	0.228	H-H
100	H2(a)...acetylene(p)	1.00	3.733	C-H
100	H2(a)...acetylene(p)	1.05	2.304	C-H
100	H2(a)...acetylene(p)	1.10	1.317	C-H
100	H2(a)...acetylene(p)	1.15	0.646	C-H
100	H2(a)...acetylene(p)	1.25	-0.083	C-H
100	H2(a)...acetylene(p)	1.65	-0.330	C-H
101	H2(a)...ammonia(a)	1.00	5.217	N-H
101	H2(a)...ammonia(a)	1.05	3.426	N-H
101	H2(a)...ammonia(a)	1.10	2.121	N-H
101	H2(a)...ammonia(a)	1.15	1.184	N-H
101	H2(a)...ammonia(a)	1.25	0.063	N-H
101	H2(a)...ammonia(a)	1.65	-0.604	N-H
102	H2(a)...ammonia(l)	1.00	5.591	H-H
102	H2(a)...ammonia(l)	1.05	4.370	H-H
102	H2(a)...ammonia(l)	1.10	3.413	H-H
102	H2(a)...ammonia(l)	1.15	2.665	H-H
102	H2(a)...ammonia(l)	1.25	1.622	H-H
102	H2(a)...ammonia(l)	1.65	0.235	H-H
103	H2(a)...benzene(p)	1.00	3.966	C-H
103	H2(a)...benzene(p)	1.05	2.344	C-H
103	H2(a)...benzene(p)	1.10	1.203	C-H
103	H2(a)...benzene(p)	1.15	0.418	C-H
103	H2(a)...benzene(p)	1.25	-0.445	C-H
103	H2(a)...benzene(p)	1.65	-0.634	C-H
104	H2(a)...ethylene(a)	1.00	5.610	H-H
104	H2(a)...ethylene(a)	1.05	4.337	H-H
104	H2(a)...ethylene(a)	1.10	3.339	H-H
104	H2(a)...ethylene(a)	1.15	2.559	H-H
104	H2(a)...ethylene(a)	1.25	1.478	H-H
104	H2(a)...ethylene(a)	1.65	0.097	H-H
105	H2(a)...ethylene(p)	1.00	4.123	C-H
105	H2(a)...ethylene(p)	1.05	2.631	C-H
105	H2(a)...ethylene(p)	1.10	1.582	C-H
105	H2(a)...ethylene(p)	1.15	0.856	C-H
105	H2(a)...ethylene(p)	1.25	0.039	C-H
105	H2(a)...ethylene(p)	1.65	-0.335	C-H
106	H2(a)...formaldehyde_c(p)	1.00	4.597	C-H
106	H2(a)...formaldehyde_c(p)	1.05	3.182	C-H
106	H2(a)...formaldehyde_c(p)	1.10	2.163	C-H
106	H2(a)...formaldehyde_c(p)	1.15	1.437	C-H
106	H2(a)...formaldehyde_c(p)	1.25	0.572	C-H
106	H2(a)...formaldehyde_c(p)	1.65	-0.077	C-H
107	H2(a)...formaldehyde(l)	1.00	4.135	O-H
107	H2(a)...formaldehyde(l)	1.05	2.558	O-H
107	H2(a)...formaldehyde(l)	1.10	1.457	O-H
107	H2(a)...formaldehyde(l)	1.15	0.699	O-H
107	H2(a)...formaldehyde(l)	1.25	-0.143	O-H
107	H2(a)...formaldehyde(l)	1.65	-0.476	O-H
108	H2(a)...formaldehyde(p)	1.00	4.100	O-H
108	H2(a)...formaldehyde(p)	1.05	2.652	O-H

108	H2(a)...formaldehyde(p)	1.10	1.636	O-H
108	H2(a)...formaldehyde(p)	1.15	0.934	O-H
108	H2(a)...formaldehyde(p)	1.25	0.140	O-H
108	H2(a)...formaldehyde(p)	1.65	-0.264	O-H
109	H2(a)...H2(a)	1.00	5.886	H-H
109	H2(a)...H2(a)	1.05	4.597	H-H
109	H2(a)...H2(a)	1.10	3.579	H-H
109	H2(a)...H2(a)	1.15	2.778	H-H
109	H2(a)...H2(a)	1.25	1.655	H-H
109	H2(a)...H2(a)	1.65	0.168	H-H
110	H2(a)...methane(l)	1.00	5.745	H-H
110	H2(a)...methane(l)	1.05	4.447	H-H
110	H2(a)...methane(l)	1.10	3.427	H-H
110	H2(a)...methane(l)	1.15	2.628	H-H
110	H2(a)...methane(l)	1.25	1.515	H-H
110	H2(a)...methane(l)	1.65	0.085	H-H
111	H2(a)...methanol(a)	1.00	4.704	O-H
111	H2(a)...methanol(a)	1.05	2.968	O-H
111	H2(a)...methanol(a)	1.10	1.726	O-H
111	H2(a)...methanol(a)	1.15	0.851	O-H
111	H2(a)...methanol(a)	1.25	-0.158	O-H
111	H2(a)...methanol(a)	1.65	-0.624	O-H
112	H2(a)...methanol(p)	1.00	4.552	O-H
112	H2(a)...methanol(p)	1.05	2.965	O-H
112	H2(a)...methanol(p)	1.10	1.811	O-H
112	H2(a)...methanol(p)	1.15	0.983	O-H
112	H2(a)...methanol(p)	1.25	-0.003	O-H
112	H2(a)...methanol(p)	1.65	-0.547	O-H
113	H2(a)...N2(a)	1.00	4.487	N-H
113	H2(a)...N2(a)	1.05	2.938	N-H
113	H2(a)...N2(a)	1.10	1.854	N-H
113	H2(a)...N2(a)	1.15	1.107	N-H
113	H2(a)...N2(a)	1.25	0.261	N-H
113	H2(a)...N2(a)	1.65	-0.215	N-H
114	H2(a)...pyridine(a)	1.00	5.015	N-H
114	H2(a)...pyridine(a)	1.05	3.168	N-H
114	H2(a)...pyridine(a)	1.10	1.830	N-H
114	H2(a)...pyridine(a)	1.15	0.877	N-H
114	H2(a)...pyridine(a)	1.25	-0.242	N-H
114	H2(a)...pyridine(a)	1.65	-0.777	N-H
115	H2(a)...pyridine(p)	1.00	3.450	N-H
115	H2(a)...pyridine(p)	1.05	1.894	N-H
115	H2(a)...pyridine(p)	1.10	0.819	N-H
115	H2(a)...pyridine(p)	1.15	0.095	N-H
115	H2(a)...pyridine(p)	1.25	-0.666	N-H
115	H2(a)...pyridine(p)	1.65	-0.682	N-H
116	H2(a)...water(a)	1.00	4.902	O-H
116	H2(a)...water(a)	1.05	3.157	O-H
116	H2(a)...water(a)	1.10	1.909	O-H
116	H2(a)...water(a)	1.15	1.029	O-H
116	H2(a)...water(a)	1.25	0.006	O-H
116	H2(a)...water(a)	1.65	-0.532	O-H
117	H2(a)...water(l)	1.00	5.703	H-H
117	H2(a)...water(l)	1.05	4.511	H-H

117	H2(a)...water(l)	1.10	3.577	H-H
117	H2(a)...water(l)	1.15	2.846	H-H
117	H2(a)...water(l)	1.25	1.821	H-H
117	H2(a)...water(l)	1.65	0.400	H-H
118	H2(a)...water(p)	1.00	5.317	O-H
118	H2(a)...water(p)	1.05	3.595	O-H
118	H2(a)...water(p)	1.10	2.348	O-H
118	H2(a)...water(p)	1.15	1.455	O-H
118	H2(a)...water(p)	1.25	0.386	O-H
118	H2(a)...water(p)	1.65	-0.343	O-H
119	methane(l)...methane(l)	1.00	5.622	H-H
119	methane(l)...methane(l)	1.05	4.293	H-H
119	methane(l)...methane(l)	1.10	3.255	H-H
119	methane(l)...methane(l)	1.15	2.447	H-H
119	methane(l)...methane(l)	1.25	1.333	H-H
119	methane(l)...methane(l)	1.65	-0.036	H-H
120	methane(l)...methanol(a)	1.00	4.508	O-H
120	methane(l)...methanol(a)	1.05	2.761	O-H
120	methane(l)...methanol(a)	1.10	1.531	O-H
120	methane(l)...methanol(a)	1.15	0.678	O-H
120	methane(l)...methanol(a)	1.25	-0.279	O-H
120	methane(l)...methanol(a)	1.65	-0.630	O-H
121	methane(l)...methanol(p)	1.00	4.309	O-H
121	methane(l)...methanol(p)	1.05	2.674	O-H
121	methane(l)...methanol(p)	1.10	1.506	O-H
121	methane(l)...methanol(p)	1.15	0.686	O-H
121	methane(l)...methanol(p)	1.25	-0.255	O-H
121	methane(l)...methanol(p)	1.65	-0.636	O-H
122	methane(l)...pyridine(a)	1.00	4.443	N-H
122	methane(l)...pyridine(a)	1.05	2.620	N-H
122	methane(l)...pyridine(a)	1.10	1.332	N-H
122	methane(l)...pyridine(a)	1.15	0.439	N-H
122	methane(l)...pyridine(a)	1.25	-0.559	N-H
122	methane(l)...pyridine(a)	1.65	-0.835	N-H
123	methane(l)...pyridine(p)	1.00	2.894	N-H
123	methane(l)...pyridine(p)	1.05	1.254	N-H
123	methane(l)...pyridine(p)	1.10	0.139	N-H
123	methane(l)...pyridine(p)	1.15	-0.594	N-H
123	methane(l)...pyridine(p)	1.25	-1.315	N-H
123	methane(l)...pyridine(p)	1.65	-1.014	N-H
124	methane(l)...water(a)	1.00	4.560	O-H
124	methane(l)...water(a)	1.05	2.864	O-H
124	methane(l)...water(a)	1.10	1.669	O-H
124	methane(l)...water(a)	1.15	0.841	O-H
124	methane(l)...water(a)	1.25	-0.095	O-H
124	methane(l)...water(a)	1.65	-0.505	O-H
125	methane(l)...water(l)	1.00	5.903	H-H
125	methane(l)...water(l)	1.05	4.588	H-H
125	methane(l)...water(l)	1.10	3.562	H-H
125	methane(l)...water(l)	1.15	2.762	H-H
125	methane(l)...water(l)	1.25	1.652	H-H
125	methane(l)...water(l)	1.65	0.196	H-H
126	methane(l)...water(p)	1.00	5.135	O-H
126	methane(l)...water(p)	1.05	3.408	O-H

126	methane(l)...water(p)	1.10	2.176	O-H
126	methane(l)...water(p)	1.15	1.307	O-H
126	methane(l)...water(p)	1.25	0.289	O-H
126	methane(l)...water(p)	1.65	-0.345	O-H
127	methanol(a)...methanol(a)	1.00	4.839	O-O
127	methanol(a)...methanol(a)	1.05	3.761	O-O
127	methanol(a)...methanol(a)	1.10	3.038	O-O
127	methanol(a)...methanol(a)	1.15	2.538	O-O
127	methanol(a)...methanol(a)	1.25	1.910	O-O
127	methanol(a)...methanol(a)	1.65	0.915	O-O
128	methanol(a)...methanol(p)	1.00	4.703	O-O
128	methanol(a)...methanol(p)	1.05	3.134	O-O
128	methanol(a)...methanol(p)	1.10	2.110	O-O
128	methanol(a)...methanol(p)	1.15	1.444	O-O
128	methanol(a)...methanol(p)	1.25	0.730	O-O
128	methanol(a)...methanol(p)	1.65	0.194	O-O
129	methanol(a)...pyridine(a)	1.00	4.901	N-O
129	methanol(a)...pyridine(a)	1.05	3.749	N-O
129	methanol(a)...pyridine(a)	1.10	2.980	N-O
129	methanol(a)...pyridine(a)	1.15	2.453	N-O
129	methanol(a)...pyridine(a)	1.25	1.812	N-O
129	methanol(a)...pyridine(a)	1.65	0.875	N-O
130	methanol(a)...pyridine(p)	1.00	2.790	N-O
130	methanol(a)...pyridine(p)	1.05	1.274	N-O
130	methanol(a)...pyridine(p)	1.10	0.395	N-O
130	methanol(a)...pyridine(p)	1.15	-0.080	N-O
130	methanol(a)...pyridine(p)	1.25	-0.380	N-O
130	methanol(a)...pyridine(p)	1.65	0.065	N-O
131	methanol(a)...water(a)	1.00	4.713	O-O
131	methanol(a)...water(a)	1.05	3.695	O-O
131	methanol(a)...water(a)	1.10	3.009	O-O
131	methanol(a)...water(a)	1.15	2.532	O-O
131	methanol(a)...water(a)	1.25	1.926	O-O
131	methanol(a)...water(a)	1.65	0.932	O-O
132	methanol(a)...water(p)	1.00	5.254	O-O
132	methanol(a)...water(p)	1.05	3.649	O-O
132	methanol(a)...water(p)	1.10	2.599	O-O
132	methanol(a)...water(p)	1.15	1.906	O-O
132	methanol(a)...water(p)	1.25	1.127	O-O
132	methanol(a)...water(p)	1.65	0.343	O-O
133	methanol(p)...methanol(p)	1.00	4.814	O-O
133	methanol(p)...methanol(p)	1.05	3.017	O-O
133	methanol(p)...methanol(p)	1.10	1.841	O-O
133	methanol(p)...methanol(p)	1.15	1.078	O-O
133	methanol(p)...methanol(p)	1.25	0.285	O-O
133	methanol(p)...methanol(p)	1.65	-0.092	O-O
134	methanol(p)...pyridine(a)	1.00	4.805	N-O
134	methanol(p)...pyridine(a)	1.05	3.200	N-O
134	methanol(p)...pyridine(a)	1.10	2.140	N-O
134	methanol(p)...pyridine(a)	1.15	1.443	N-O
134	methanol(p)...pyridine(a)	1.25	0.689	N-O
134	methanol(p)...pyridine(a)	1.65	0.152	N-O
135	methanol(p)...pyridine(p)	1.00	2.543	N-O
135	methanol(p)...pyridine(p)	1.05	0.588	N-O

135	methanol(p)...pyridine(p)	1.10	-0.606	N-O
135	methanol(p)...pyridine(p)	1.15	-1.288	N-O
135	methanol(p)...pyridine(p)	1.25	-1.760	N-O
135	methanol(p)...pyridine(p)	1.65	-0.869	N-O
136	methanol(p)...water(a)	1.00	4.673	O-O
136	methanol(p)...water(a)	1.05	3.187	O-O
136	methanol(p)...water(a)	1.10	2.214	O-O
136	methanol(p)...water(a)	1.15	1.577	O-O
136	methanol(p)...water(a)	1.25	0.881	O-O
136	methanol(p)...water(a)	1.65	0.285	O-O
137	methanol(p)...water(p)	1.00	5.090	O-O
137	methanol(p)...water(p)	1.05	3.139	O-O
137	methanol(p)...water(p)	1.10	1.854	O-O
137	methanol(p)...water(p)	1.15	1.015	O-O
137	methanol(p)...water(p)	1.25	0.130	O-O
137	methanol(p)...water(p)	1.65	-0.307	O-O
138	N2(a)...ammonia(a)	1.00	4.635	N-N
138	N2(a)...ammonia(a)	1.05	3.064	N-N
138	N2(a)...ammonia(a)	1.10	2.049	N-N
138	N2(a)...ammonia(a)	1.15	1.393	N-N
138	N2(a)...ammonia(a)	1.25	0.694	N-N
138	N2(a)...ammonia(a)	1.65	0.158	N-N
139	N2(a)...benzene(p)	1.00	2.851	N-C
139	N2(a)...benzene(p)	1.05	1.095	N-C
139	N2(a)...benzene(p)	1.10	0.049	N-C
139	N2(a)...benzene(p)	1.15	-0.536	N-C
139	N2(a)...benzene(p)	1.25	-0.943	N-C
139	N2(a)...benzene(p)	1.65	-0.396	N-C
140	N2(a)...formaldehyde(l)	1.00	4.044	N-O
140	N2(a)...formaldehyde(l)	1.05	2.418	N-O
140	N2(a)...formaldehyde(l)	1.10	1.427	N-O
140	N2(a)...formaldehyde(l)	1.15	0.833	N-O
140	N2(a)...formaldehyde(l)	1.25	0.285	N-O
140	N2(a)...formaldehyde(l)	1.65	0.078	N-O
141	N2(a)...formaldehyde(p)	1.00	3.810	N-O
141	N2(a)...formaldehyde(p)	1.05	2.127	N-O
141	N2(a)...formaldehyde(p)	1.10	1.093	N-O
141	N2(a)...formaldehyde(p)	1.15	0.474	N-O
141	N2(a)...formaldehyde(p)	1.25	-0.079	N-O
141	N2(a)...formaldehyde(p)	1.65	-0.122	N-O
142	N2(a)...methane(l)	1.00	4.598	N-H
142	N2(a)...methane(l)	1.05	2.980	N-H
142	N2(a)...methane(l)	1.10	1.850	N-H
142	N2(a)...methane(l)	1.15	1.072	N-H
142	N2(a)...methane(l)	1.25	0.196	N-H
142	N2(a)...methane(l)	1.65	-0.270	N-H
143	N2(a)...methanol(a)	1.00	4.409	N-O
143	N2(a)...methanol(a)	1.05	2.764	N-O
143	N2(a)...methanol(a)	1.10	1.733	N-O
143	N2(a)...methanol(a)	1.15	1.093	N-O
143	N2(a)...methanol(a)	1.25	0.459	N-O
143	N2(a)...methanol(a)	1.65	0.102	N-O
144	N2(a)...methanol(p)	1.00	4.515	N-O
144	N2(a)...methanol(p)	1.05	2.746	N-O

144	N2(a)...methanol(p)	1.10	1.603	N-O
144	N2(a)...methanol(p)	1.15	0.876	N-O
144	N2(a)...methanol(p)	1.25	0.148	N-O
144	N2(a)...methanol(p)	1.65	-0.115	N-O
145	N2(a)...N2(a)	1.00	4.175	N-N
145	N2(a)...N2(a)	1.05	2.394	N-N
145	N2(a)...N2(a)	1.10	1.306	N-N
145	N2(a)...N2(a)	1.15	0.654	N-N
145	N2(a)...N2(a)	1.25	0.059	N-N
145	N2(a)...N2(a)	1.65	-0.085	N-N
146	N2(a)...pyridine(a)	1.00	4.450	N-N
146	N2(a)...pyridine(a)	1.05	2.787	N-N
146	N2(a)...pyridine(a)	1.10	1.732	N-N
146	N2(a)...pyridine(a)	1.15	1.069	N-N
146	N2(a)...pyridine(a)	1.25	0.401	N-N
146	N2(a)...pyridine(a)	1.65	0.042	N-N
147	N2(a)...pyridine(p)	1.00	2.488	N-N
147	N2(a)...pyridine(p)	1.05	0.778	N-N
147	N2(a)...pyridine(p)	1.10	-0.207	N-N
147	N2(a)...pyridine(p)	1.15	-0.733	N-N
147	N2(a)...pyridine(p)	1.25	-1.044	N-N
147	N2(a)...pyridine(p)	1.65	-0.392	N-N
148	N2(a)...water(a)	1.00	4.370	N-O
148	N2(a)...water(a)	1.05	2.772	N-O
148	N2(a)...water(a)	1.10	1.771	N-O
148	N2(a)...water(a)	1.15	1.149	N-O
148	N2(a)...water(a)	1.25	0.526	N-O
148	N2(a)...water(a)	1.65	0.138	N-O
149	N2(a)...water(p)	1.00	5.018	N-O
149	N2(a)...water(p)	1.05	3.224	N-O
149	N2(a)...water(p)	1.10	2.069	N-O
149	N2(a)...water(p)	1.15	1.329	N-O
149	N2(a)...water(p)	1.25	0.554	N-O
149	N2(a)...water(p)	1.65	0.048	N-O
150	pyridine(a)...pyridine(a)	1.00	4.634	N-N
150	pyridine(a)...pyridine(a)	1.05	3.608	N-N
150	pyridine(a)...pyridine(a)	1.10	2.911	N-N
150	pyridine(a)...pyridine(a)	1.15	2.423	N-N
150	pyridine(a)...pyridine(a)	1.25	1.808	N-N
150	pyridine(a)...pyridine(a)	1.65	0.851	N-N
151	pyridine(a)...pyridine(p)	1.00	1.435	N-N
151	pyridine(a)...pyridine(p)	1.05	0.022	N-N
151	pyridine(a)...pyridine(p)	1.10	-0.741	N-N
151	pyridine(a)...pyridine(p)	1.15	-1.093	N-N
151	pyridine(a)...pyridine(p)	1.25	-1.155	N-N
151	pyridine(a)...pyridine(p)	1.65	-0.146	N-N
152	pyridine(a)...water(a)	1.00	4.904	N-O
152	pyridine(a)...water(a)	1.05	3.807	N-O
152	pyridine(a)...water(a)	1.10	3.066	N-O
152	pyridine(a)...water(a)	1.15	2.553	N-O
152	pyridine(a)...water(a)	1.25	1.912	N-O
152	pyridine(a)...water(a)	1.65	0.922	N-O
153	pyridine(a)...water(p)	1.00	5.528	N-O
153	pyridine(a)...water(p)	1.05	3.981	N-O

153	pyridine(a)...water(p)	1.10	2.940	N-O
153	pyridine(a)...water(p)	1.15	2.229	N-O
153	pyridine(a)...water(p)	1.25	1.389	N-O
153	pyridine(a)...water(p)	1.65	0.427	N-O
154	pyridine(p)...pyridine(p)	1.00	-1.692	N-N
154	pyridine(p)...pyridine(p)	1.05	-3.448	N-N
154	pyridine(p)...pyridine(p)	1.10	-4.277	N-N
154	pyridine(p)...pyridine(p)	1.15	-4.528	N-N
154	pyridine(p)...pyridine(p)	1.25	-4.149	N-N
154	pyridine(p)...pyridine(p)	1.65	-1.428	N-N
155	pyridine(p)...water(a)	1.00	3.079	N-O
155	pyridine(p)...water(a)	1.05	1.666	N-O
155	pyridine(p)...water(a)	1.10	0.838	N-O
155	pyridine(p)...water(a)	1.15	0.381	N-O
155	pyridine(p)...water(a)	1.25	0.054	N-O
155	pyridine(p)...water(a)	1.65	0.257	N-O
156	pyridine(p)...water(p)	1.00	3.570	N-O
156	pyridine(p)...water(p)	1.05	1.727	N-O
156	pyridine(p)...water(p)	1.10	0.600	N-O
156	pyridine(p)...water(p)	1.15	-0.060	N-O
156	pyridine(p)...water(p)	1.25	-0.599	N-O
156	pyridine(p)...water(p)	1.65	-0.355	N-O
157	water(a)...water(a)	1.00	4.576	O-O
157	water(a)...water(a)	1.05	3.610	O-O
157	water(a)...water(a)	1.10	2.958	O-O
157	water(a)...water(a)	1.15	2.503	O-O
157	water(a)...water(a)	1.25	1.919	O-O
157	water(a)...water(a)	1.65	0.939	O-O
158	water(a)...water(p)	1.00	5.262	O-O
158	water(a)...water(p)	1.05	3.719	O-O
158	water(a)...water(p)	1.10	2.704	O-O
158	water(a)...water(p)	1.15	2.029	O-O
158	water(a)...water(p)	1.25	1.257	O-O
158	water(a)...water(p)	1.65	0.418	O-O
159	water(l)...water(l)	1.00	6.795	H-H
159	water(l)...water(l)	1.05	5.777	H-H
159	water(l)...water(l)	1.10	4.958	H-H
159	water(l)...water(l)	1.15	4.294	H-H
159	water(l)...water(l)	1.25	3.303	H-H
159	water(l)...water(l)	1.65	1.480	H-H
160	water(p)...water(p)	1.00	5.608	O-O
160	water(p)...water(p)	1.05	3.527	O-O
160	water(p)...water(p)	1.10	2.169	O-O
160	water(p)...water(p)	1.15	1.284	O-O
160	water(p)...water(p)	1.25	0.335	O-O
160	water(p)...water(p)	1.65	-0.269	O-O