E-mail:

CNC2H1Naph	XX	YY	ZZ	XY	XZ	YZ
0	-10.1286	-3.5294	13.658	-7.1542	0.0	0.0
1	-23.707	10.4827	13.2242	-0.6477	0.0	0.0
2	-9.6367	-2.4346	12.0713	-1.8607	0.0	0.0
3	3.3193	-21.6415	18.3222	-0.1459	0.0	0.0
4	-3.4307	-17.4343	20.865	22.7588	0.0	0.0
5	-20.5671	4.4581	16.109	17.3789	0.0	0.0
6	3.3525	-29.075	25.7225	24.5493	0.0	0.0
7	-14.0206	-0.6958	14.7164	-2.4312	0.0	0.0
8	-11.7867	-2.9504	14.7371	-15.0755	0.0	0.0
9	-6.25	-9.2132	15.4632	-9.9367	0.0	0.0
10	-0.1373	-21.2453	21.3826	5.0554	0.0	0.0
11	-22.4675	0.4085	22.0591	13.9112	0.0	0.0
12	-25.4347	8.5159	16.9188	-4.4086	0.0	0.0
13	18.1469	-49.6679	31.5209	-1.5318	0.0	0.0
14	5.2251	-21.618	16.3929	-2.1892	0.0	0.0
15	-5.9402	-10.6064	16.5466	7.1575	0.0	0.0
16	-1.4929	-13.502	14.9949	-14.1726	0.0	0.0
17	-15.5154	-3.6569	19.1723	-1.6298	0.0	0.0
18	2.5972	-21.6426	19.0454	9.1975	0.0	0.0
19	-9.2871	-5.5068	14.7939	-19.3361	0.0	0.0
20	19.0798	-46.2556	27.1758	29.4304	0.0	0.0
21	-17.2663	3.6179	13.6484	-4.9349	0.0	0.0
22	-9.8332	-7.1017	16.9349	8.6215	0.0	0.0
23	7.5788	-22.3197	14.7409	-0.9882	0.0	0.0
24	-7.0352	-7.0932	14.1284	9.5139	0.0	0.0
25	-0.2972	-16.8439	17.1411	23.3632	0.0	0.0
26	12.424	-27.2785	14.8545	11.5365	0.0	0.0
27	-1.7456	-17.6642	19.4099	-20.2294	0.0	0.0
28	1.5557	-19.2282	17.6725	-11.3112	0.0	0.0
29	11.2039	-31.8481	20.6442	-1.6929	0.0	0.0
30	-20.6498	3.838	16.8118	2.7088	0.0	0.0
31	-8.1493	-3.982	12.1313	-6.9705	0.0	0.0
32	-5.5681	-10.9537	16.5219	20.4767	0.0	0.0
33	-21.0369	6.0042	15.0327	-15.401	0.0	0.0
34	4.9327	-34.9491	30.0165	21.8645	0.0	0.0
35	9.8164	-30.2077	20.3913	-7.5357	0.0	0.0
36	-2.5575	-20.4279	22.9855	-25.046	0.0	0.0
37	-2.6218	-14.698	17.3198	11.4769	0.0	0.0
38	7.1861	-21.5731	14.387	5.0449	0.0	0.0
39	-1.834	-15.1094	16.9434	-4.1626	0.0	0.0
40	13.9779	-30.1317	16.1538	8.1528	0.0	0.0
41	22.6025	-57.9005	35.298	-31.314	0.0	0.0
42	-7.9478	-10.0616	18.0094	-19.7104	0.0	0.0
43	-7.0764	-10.9651	18.0415	-2.2568	0.0	0.0
44	10.3479	-25.2921	14.9441	-4.5	0.0	0.0
45	10.5688	-25.8954	15.3266	-5.6173	0.0	0.0
46	-6.159	-12.2095	18.3685	1.7216	0.0	0.0
47 48	-2.2779	-16.1236	18.4015	-19.3614	0.0	0.0
48	24.8192	-53.1195	28.3003	31.5184	0.0	0.0

CNC2H1Naph	X	Y	Z	Tot
0	-0.6157	5.971	0.0	6.0027
1	1.4919	2.0865	0.0	2.565
2	-6.6767	-4.1399	0.0	7.856
3	-4.6549	-8.6373	0.0	9.8118
4	0.4677	-8.3828	0.0	8.3958
5	2.1526	-4.3207	0.0	4.8272
6	-9.2852	11.7368	0.0	14.9656
7	-8.6358	1.3746	0.0	8.7446
8	-0.8999	2.924	0.0	3.0593
9	-4.8335	-7.0948	0.0	8.5848
10	-0.9204	-9.6576	0.0	9.7013
11	3.7069	-7.17	0.0	8.0716
12	2.9193	-2.5104	0.0	3.8503
13	-4.9564	12.735	0.0	13.6655
14	3.2614	8.6575	0.0	9.2515
15	5.7366	3.8898	0.0	6.9311
16	6.6453	5.726	0.0	8.772
17	9.8539	2.1559	0.0	10.087
18	7.3283	-2.5459	0.0	7.7579
19	2.9865	-1.3555	0.0	3.2797
20	0.1988	7.9697	0.0	7.9722
21	8.9785	2.5958	0.0	9.3462
22	8.438	-0.884	0.0	8.4842
23	-4.2389	-1.9946	0.0	4.6847
24	7.5264	1.9568	0.0	7.7766
25	6.1208	-1.5832	0.0	6.3223
26	1.7993	-2.229	0.0	2.8646
27	8.425	11.001	0.0	13.8565
28	-5.2783	-8.2676	0.0	9.8088
29	-2.0754	-9.7072	0.0	9.9265
30	1.3355	-4.1972	0.0	4.4045
31	-7.6313	1.1498	0.0	7.7174
32	-0.6601	6.2525	0.0	6.2872
33	1.5387	2.3225	0.0	2.786
34	-10.8057	10.9636	0.0	15.3936
35	-1.5639	-9.8918	0.0	10.0147
36	-5.4383	-8.5382	0.0	10.123
37	-3.4616	-2.0696	0.0	4.0331
38	5.8853	-5.4245	0.0	8.0039
39	8.3687	-1.4552	0.0	8.4943
40	1.4644	2.6529	0.0	3.0303
41	8.9301	10.1853	0.0	13.5458
42	8.0059	6.3853	0.0	10.2404
43	7.991	1.1479	0.0	8.073
44	-3.5765	-0.1025	0.0	3.5779
45	-2.5376	7.5881	0.0	8.0011
46	6.8624	5.761	0.0	8.96
47	-6.6661	0.2143	0.0	6.6695
48	-3.8563	7.9694	0.0	8.8534