

Description	No. of Fluorines	Index	Shape	Conformer	Total Energy		Relative Energy		Boltzmann Ratios	DF-MP2 Overall Relative Energy
					cc-pVTZ DF-MP2	DZP MP2	DF-MP2 rel.	MP2 rel.		
fluorocyclohexane	1	2	chair	equatorial	-334.4619	-334.1489	0.000	0.000	1.00	0.000
	1	1	chair	axial	-334.4619	-334.1488	0.029	0.111	0.95	0.029
	1	3	boat		-334.4529	-334.1394	5.673	6.015		5.673
	1	5	boat		-334.4524	-334.1390	6.000	6.222		6.000
	1	4	boat		-334.4513	-334.1381	6.648	6.789		6.648
trans-1,2-difluoro	2	7	chair	diaxial	-433.5919	-433.1910	0.000	0.000	1.00	2.431
	2	9	chair	diequatorial	-433.5914	-433.1906	0.326	0.263	0.58	2.757
	2	10	boat		-433.5831	-433.1821	5.541	5.594		7.972
	2	11	boat		-433.5826	-433.1819	5.852	5.743		8.283
	2	18	boat		-433.5827	-433.1828	5.750	5.192		8.181
	2	20	boat		-433.5797	-433.1789	7.649	7.631		10.080
cis-1,2-difluoro	2	8	chair	ax, eq	-433.5912	-433.1904	0.000	0.000		2.861
	2	19	boat		-433.5821	-433.1812	5.695	5.785		8.555
cis-1,3-difluoro	2	4	chair	diaxial	-433.5912	-433.1904	1.174	1.202	0.14	2.872
	2	6	chair	diequatorial	-433.5931	-433.1923	0.000	0.000	1.00	1.698
	2	12	boat		-433.5845	-433.1837	5.364	5.426		7.062
	2	21	boat		-433.5837	-433.1828	5.896	5.986		7.594
	2	24	boat		-433.5832	-433.1823	6.189	6.293		7.888
trans-1,3-difluoro	2	5	chair	axial, equatorial	-433.5941	-433.1935	0.000	0.000		1.028
	2	13	boat		-433.5869	-433.1858	4.547	4.832		5.574
	2	14	boat		-433.5827	-433.1819	7.186	7.285		8.214
	2	22	boat		-433.5857	-433.1849	5.274	5.422		6.302
	2	23	boat		-433.5836	-433.1829	6.631	6.629		7.659
trans-1,4-difluoro	2	1	chair	diaxial	-433.5958	-433.1951	0.000	0.000	1.00	0.000
	2	3	chair	diequatorial	-433.5938	-433.1932	1.202	1.193	0.13	1.202
	2	15	boat		-433.5857	-433.1848	6.344	6.469		6.344
	2	25	boat		-433.5856	-433.1848	6.358	6.460		6.358
	2	2	chair	axial, equatorial	-433.5945	-433.1938	0.000	0.000		0.785

cis-1,4-difluoro	2	16	boat		-433.5833	-433.1821	7.036	7.344		7.821
	2	17	boat		-433.5831	-433.1822	7.141	7.295		7.927
	2	26	boat		-433.5851	-433.1842	5.890	6.018		6.676
r-1, t-2, c-3-trifluoro	3	13	chair	triaxial	-532.7172	-532.2285	0.948	0.899	0.20	4.253
	3	18	chair	triequatorial	-532.7187	-532.2299	0.000	0.000	1.00	3.305
	3	19	boat		-532.7121	-532.2236	4.143	3.946		7.448
	3	36	boat		-532.7104	-532.2217	5.237	5.117		8.542
r-1, t-2, t-3-trifluoro	3	14	chair	1ax, 2ax, 3eq	-532.7198	-532.2312	0.000	0.000	1.00	2.629
	3	16	chair	1eq, 2eq, 3ax	-532.7195	-532.2307	0.212	0.291	0.70	2.841
	3	20	boat		-532.7103	-532.2215	5.950	6.040		8.579
	3	37	boat		-532.7106	-532.2221	5.774	5.721		8.403
r-1, c-2, c-3-trifluoro	3	15	chair	1ax, 2eq, 3ax	-532.7156	-532.2268	1.899	1.855	0.04	5.284
	3	17	chair	1eq, 2ax, 3eq	-532.7186	-532.2297	0.000	0.000	1.00	3.386
			no boats considered							
r-1, t-2, t-4-trifluoro	3	5	chair	triaxial	-532.7215	-532.2329	0.000	0.000	1.00	1.574
	3	12	chair	triequatorial	-532.7213	-532.2325	0.099	0.220	0.85	1.674
	3	21	boat		-532.7136	-532.2248	4.952	5.043		6.526
	3	27	boat		-532.7139	-532.2254	4.768	4.685		6.342
	3	28	boat		-532.7133	-532.2246	5.156	5.174		6.731
	3	35	boat		-532.7140	-532.2255	4.701	4.636		6.275
	3	40	boat		-532.7129	-532.2243	5.363	5.395		6.937
r-1, t-2, c-4-trifluoro	3	6	chair	ax, ax, eq	-532.7232	-532.2347	0.000	0.000	1.00	0.470
	3	11	chair	eq, eq, ax	-532.7228	-532.2342	0.289	0.300	0.61	0.758
	3	22	boat		-532.7125	-532.2238	6.761	6.817		7.230
	3	26	boat		-532.7129	-532.2244	6.482	6.475		6.952
	3	29	boat		-532.7149	-532.2263	5.249	5.253		5.719
	3	34	boat		-532.7138	-532.2255	5.894	5.756		6.364
	3	43	boat		-532.7128	-532.2239	6.525	6.732		6.995
	3	7	chair	ax, eq, ax	-532.7239	-532.2353	0.000	0.000	1.00	0.082

r-1, c-2, t-4-trifluoro	3	10	chair	eq, ax, eq	-532.7219	-532.2332	1.251	1.305	0.12	1.333
	3	23	boat		-532.7108	-532.2222	8.189	8.241		8.271
	3	25	boat		-532.7159	-532.2272	4.964	5.076		5.046
	3	31	boat		-532.7115	-532.2227	7.784	7.892		7.866
	3	32	boat		-532.7103	-532.2217	8.535	8.537		8.617
	3	42	boat		-532.7159	-532.2272	4.964	5.076		5.046
	3	45	boat		-532.7136	-532.2248	6.466	6.583		6.548
r-1, c-2, c-4-trifluoro	3	8	chair	ax, eq, eq	-532.7215	-532.2327	0.000	0.000	1.00	1.562
	3	9	chair	eq, ax, ax	-532.7194	-532.2308	1.306	1.239	0.11	2.868
	3	24	boat		-532.7127	-532.2238	5.520	5.600		7.081
	3	30	boat		-532.7127	-532.2238	5.520	5.600		7.081
	3	33	boat		-532.7095	-532.2206	7.515	7.602		9.077
	3	41	boat		-532.7112	-532.2224	6.438	6.472		8.000
	3	46	boat		-532.7127	-532.2238	5.520	5.600		7.081
r-1, c-3, c-5-trifluoro	3	1	chair	triaxial	-532.7160	-532.2274	3.451	3.240	0.003	5.010
	3	4	chair	triequatorial	-532.7215	-532.2325	0.000	0.000	1.00	1.559
	3	48	boat		-532.7132	-532.2245	5.199	5.016		6.758
r-1, c-3, t-5-trifluoro	3	2	chair	ax, ax, eq	-532.7221	-532.2336	1.210	1.157	0.13	1.210
	3	3	chair	eq, eq, ax	-532.7240	-532.2354	0.000	0.000	1.00	0.000
	3	49	boat		-532.7158	-532.2275	5.132	4.999		5.132
	3	50	boat		-532.7167	-532.2280	4.594	4.628		4.594
	3	51	boat		-532.7131	-532.2245	6.864	6.879		6.864
r-1, t-2, c-3, t-4-tetrafluoro	4	20	chair	all axial	-631.8434	-631.2667	1.124	0.869	0.15	4.599
	4	29	chair	all equatorial	-631.8452	-631.2681	0.000	0.000	1.00	3.474
	4	30	boat		-631.8385	-631.2617	4.222	3.975		7.697
	4	37	boat		-631.8393	-631.2629	3.679	3.236		7.153
	4	63	boat		-631.8372	-631.2606	5.019	4.685		8.493
	4	66	boat		-631.8383	-631.2617	4.336	4.014		7.810
r-1, t-2, c-3, c-4-tetrafluoro	4	21	chair	ax, ax, ax, eq	-631.8440	-631.2673	1.283	1.083	0.11	4.202
	4	26	chair	eq, eq, eq, ax	-631.8461	-631.2691	0.000	0.000	1.00	2.919
	4	31	boat		-631.8376	-631.2611	5.303	5.024		8.222
	4	35	boat		-631.8387	-631.2620	4.610	4.413		7.529
	4	65	boat		-631.8376	-631.2611	5.303	5.024		8.222

r-1, t-2, t-3, t-4-tetrafluoro	4	22	chair	eq, eq, ax, eq	-631.8446	-631.2679	0.636	0.414	0.34	3.848
	4	28	chair	ax, ax, eq, ax	-631.8456	-631.2685	0.000	0.000	1.00	3.212
	4	32	boat		-631.8375	-631.2606	5.117	4.980		8.329
r-1, c-2, t-3, t-4-tetrafluoro	4	25	chair	ax, eq, eq, ax	-631.8479	-631.2710	0.000	0.000	1.00	1.762
	4	27	chair	eq, ax, ax, eq	-631.8461	-631.2693	1.151	1.069	0.14	2.913
	4	34	boat		-631.8378	-631.2611	6.350	6.271		8.112
	4	36	boat		-631.8368	-631.2602	6.981	6.833		8.743
r-1, c-2, c-3, c-4-tetrafluoro	4	24	chair	ring flip -> enantiomer	-631.8419	-631.2649	0.000	0.000		5.533
			no boats considered							
r-1, t-2, t-3, c-4-tetrafluoro	4	23	chair	ring flip -> enantiomer	-631.8472	-631.2704	0.000	0.000		2.212
	4	33	boat		-631.8399	-631.2635	4.614	4.331		6.826
	4	64	boat		-631.8399	-631.2635	4.614	4.331		6.826
r-1, t-2, c-3, c-5-tetrafluoro	4	8	chair	all axial	-631.8424	-631.2657	2.410	2.019	0.02	5.207
	4	19	chair	all equatorial	-631.8463	-631.2689	0.000	0.000	1.00	2.797
	4	38	boat		-631.8404	-631.2639	3.677	3.195		6.474
	4	52	boat		-631.8395	-631.2628	4.262	3.839		7.059
	4	62	boat		-631.8391	-631.2624	4.482	4.087		7.278
r-1, t-2, c-3, t-5-tetrafluoro	4	9	chair	ax, ax, ax, eq	-631.8472	-631.2706	1.053	0.929	0.17	2.211
	4	18	chair	eq, eq, eq, ax	-631.8489	-631.2721	0.000	0.000	1.00	1.159
	4	39	boat		-631.8425	-631.2662	4.019	3.672		5.178
	4	54	boat		-631.8425	-631.2662	4.019	3.672		5.178
	4	61	boat		-631.8384	-631.2617	6.567	6.522		7.726
r-1, t-2, t-3, c-5-tetrafluoro	4	10	chair	ax, ax, eq, ax	-631.8482	-631.2716	0.000	0.000	1.00	1.582
	4	15	chair	eq, eq, ax, eq	-631.8481	-631.2712	0.057	0.295	0.91	1.639
	4	40	boat		-631.8394	-631.2627	5.551	5.577		7.133
	4	42	boat		-631.8372	-631.2606	6.901	6.897		8.483
	4	53	boat		-631.8400	-631.2632	5.189	5.263		6.771
	4	56	boat		-631.8384	-631.2619	6.156	6.138		7.738
	4	60	boat		-631.8433	-631.2668	3.108	3.038		4.690
	4	11	chair	ax, ax, eq, eq	-631.8488	-631.2721	0.000	0.000	1.00	1.212

r-1, t-2, t-3, t-5-tetrafluoro	4	14	chair	eq, eq, ax, ax	-631.8462	-631.2695	1.611	1.622	0.07	2.822
	4	41	boat		-631.8392	-631.2626	6.053	5.921		7.264
	4	43	boat		-631.8388	-631.2623	6.282	6.118		7.493
	4	55	boat		-631.8388	-631.2623	6.282	6.118		7.493
	4	58	boat		-631.8415	-631.2649	4.599	4.481		5.810
r-1, c-2, c-3, c-5-tetrafluoro	4	12	chair	ax, eq, ax, ax	-631.8396	-631.2628	4.172	3.853	0.001	7.017
	4	17	chair	eq, ax, eq, eq	-631.8462	-631.2689	0.000	0.000	1.00	2.845
			no boats considered							
r-1, c-2, c-3, t-5-tetrafluoro	4	13	chair	ax, eq, ax, eq	-631.8450	-631.2682	3.182	3.171	0.005	3.636
	4	16	chair	eq, ax, eq, ax	-631.8500	-631.2732	0.000	0.000	1.00	0.454
	4	57	boat		-631.8370	-631.2602	8.142	8.202		8.596
	4	59	boat		-631.8383	-631.2617	7.334	7.244		7.788
r-1, t-2, t-4, c-5-tetrafluoro	4	1	chair	all axial	-631.8470	-631.2703	0.558	0.195	0.39	2.361
	4	7	chair	all equatorial	-631.8479	-631.2706	0.000	0.000	1.00	1.803
	4	44	boat		-631.8415	-631.2649	4.023	3.612		5.826
	4	67	boat		-631.8417	-631.2651	3.862	3.476		5.665
r-1, t-2, t-4, t-5-tetrafluoro	4	2	chair	ax, ax, ax, eq	-631.8484	-631.2717	0.146	0.000	0.78	1.481
	4	6	chair	eq, eq, eq, ax	-631.8486	-631.2717	0.000	0.038	1.00	1.335
	4	45	boat		-631.8389	-631.2621	6.124	6.071		7.459
	4	47	boat		-631.8383	-631.2618	6.490	6.219		7.825
	4	50	boat		-631.8380	-631.2611	6.691	6.702		8.025
	4	68	boat		-631.8401	-631.2631	5.329	5.387		6.664
	4	69	boat		-631.8406	-631.2638	5.036	4.964		6.371
r-1, t-2, c-4, t-5-tetrafluoro	4	3	chair	ring flip -> self	-631.8507	-631.2741	0.000	0.000		0.000
	4	46	boat		-631.8407	-631.2642	6.330	6.208		6.330
	4	51	boat		-631.8418	-631.2654	5.613	5.443		5.613
	4	72	boat		-631.8379	-631.2608	8.033	8.311		8.033
	4	73	boat		-631.8370	-631.2597	8.623	9.010		8.623
r-1, c-2, t-4, t-5-tetrafluoro	4	4	chair	ring flip -> self	-631.8503	-631.2735	0.000	0.000		0.296
	4	48	boat		-631.8436	-631.2668	4.184	4.244		4.480
	4	71	boat		-631.8436	-631.2668	4.184	4.244		4.480

r-1, c-2, c-4, c-5-tetrafluoro	4	5	chair	ring flip -> self	-631.8453	-631.2684	0.000	0.000		3.429
	4	49	boat		-631.8380	-631.2608	4.555	4.720		7.984
	4	70	boat		-631.8380	-631.2608	4.555	4.720		7.984
r-1, t-2, c-3, t-4, c-5-pentafluoro	5	1	chair	all axial	-730.9648	-730.2999	2.922	2.295	0.01	4.981
	5	20	chair	all equatorial	-730.9695	-730.3035	0.000	0.000	1.00	2.059
	5	21	boat		-730.9644	-730.2996	3.151	2.491		5.209
r-1, t-2, c-3, t-4, t-5-pentafluoro	5	2	chair	ax, ax, ax, ax, eq	-730.9690	-730.3042	1.457	1.107	0.09	2.316
	5	14	chair	eq, eq, eq, eq, ax	-730.9714	-730.3059	0.000	0.000	1.00	0.859
	5	22	boat		-730.9650	-730.3003	3.984	3.507		4.842
	5	32	boat		-730.9595	-730.2946	7.459	7.130		8.317
	5	33	boat		-730.9612	-730.2960	6.403	6.245		7.261
r-1, t-2, c-3, c-4, c-5-pentafluoro	5	3	chair	ax, ax, ax, eq, ax	-730.9647	-730.2997	3.277	2.771	0.004	5.052
	5	18	chair	eq, eq, eq, ax, eq	-730.9699	-730.3042	0.000	0.000	1.00	1.774
	5	23	boat		-730.9588	-730.2937	6.983	6.532		8.757
	5	38	boat		-730.9602	-730.2950	6.105	5.740		7.879
r-1, t-2, c-3, c-4, t-5-pentafluoro	5	4	chair	ax, ax, ax, eq, eq	-730.9701	-730.3051	1.601	1.486	0.07	1.670
	5	8	chair	eq, eq, eq, ax, ax	-730.9726	-730.3074	0.000	0.000	1.00	0.069
	5	24	boat		-730.9643	-730.2998	5.230	4.806		5.299
	5	27	boat		-730.9666	-730.3020	3.768	3.393		3.838
r-1, t-2, t-3, t-4, c-5-pentafluoro	5	5	chair	ax, ax, eq, ax, ax	-730.9690	-730.3041	1.198	0.720	0.13	2.337
	5	19	chair	eq, eq, ax, eq, eq	-730.9709	-730.3053	0.000	0.000	1.00	1.138
	5	25	boat		-730.9642	-730.2993	4.229	3.731		5.367
	5	37	boat		-730.9609	-730.2960	6.303	5.789		7.441
r-1, t-2, t-3, t-4, t-5-pentafluoro	5	6	chair	ax, ax, eq, ax, eq	-730.9696	-730.3045	0.000	0.000	1.00	1.950
	5	11	chair	eq, eq, ax, eq, ax	-730.9676	-730.3022	1.266	1.427	0.12	3.216
	5	26	boat		-730.9592	-730.2942	6.570	6.464		8.520
	5	36	boat		-730.9586	-730.2931	6.948	7.155		8.897
r-1, t-2, t-3, c-4, c-5-pentafluoro	5	7	chair	ax, ax, eq, eq, ax	-730.9710	-730.3059	0.359	0.250	0.55	1.077
	5	16	chair	eq, eq, ax, ax, eq	-730.9716	-730.3063	0.000	0.000	1.00	0.718

c-5-pentafluoro	5	29	boat		-730.9642	-730.2995	4.629	4.295		5.347
	5	35	boat		-730.9625	-730.2976	5.711	5.472		6.429
r-1, c-2, c-3, t-4, t-5-pentafluoro	5	9	chair	ax, eq, ax, ax, eq	-730.9698	-730.3047	1.858	1.617	0.04	1.858
	5	12	chair	eq, ax, eq, eq, ax	-730.9727	-730.3073	0.000	0.000	1.00	0.000
	5	28	boat		-730.9637	-730.2988	5.661	5.308		5.661
	5	30	boat		-730.9598	-730.2949	8.093	7.806		8.093
	5	34	boat		-730.9599	-730.2949	8.026	7.802		8.026
r-1, c-2, c-3, c-4, c-5-pentafluoro	5	10	chair	ax, eq, ax, eq, ax	-730.9612	-730.2959	2.669	2.396	0.01	7.229
	5	17	chair	eq, ax, eq, ax, eq	-730.9655	-730.2997	0.000	0.000	1.00	4.561
			no boats considered							
r-1, c-2, t-3, c-4, c-5-pentafluoro	5	13	chair	ax, eq, eq, eq, ax	-730.9683	-730.3029	0.092	0.318	0.86	2.768
	5	15	chair	eq, ax, ax, ax, eq	-730.9685	-730.3034	0.000	0.000	1.00	2.676
	5	31	boat		-730.9629	-730.2979	3.478	3.466		6.154
r-1, t-2, c-3, t-4, c-5, t-6-hexafluoro	6	1	chair	all axial	-830.0830	-829.3297	4.680	3.624	0.0004	6.975
	6	12	chair	all equatorial	-830.0904	-829.3354	0.000	0.000	1.00	2.295
	6	13	boat		-830.0864	-829.3332	2.520	1.371		4.815
r-1, t-2, c-3, t-4, c-5, c-6-hexafluoro	6	2	chair	ax, ax, ax, ax, ax, eq	-830.0860	-829.3327	3.770	3.090	0.002	5.079
	6	11	chair	eq, eq, eq, eq, eq, ax	-830.0920	-829.3376	0.000	0.000	1.00	1.309
	6	14	boat		-830.0833	-829.3297	5.428	4.937		6.737
	6	15	boat		-830.0802	-829.3267	7.421	6.840		8.730
	6	17	boat		-830.0829	-829.3296	5.722	5.054		7.031
r-1, t-2, c-3, t-4, t-5, c-6-hexafluoro	6	20	boat		-830.0835	-829.3300	5.344	4.800		6.653
	6	3	chair	ax, ax, ax, ax, eq, eq	-830.0905	-829.3370	2.001	1.732	0.03	2.248
	6	8	chair	eq, eq, eq, eq, ax, ax	-830.0937	-829.3398	0.000	0.000	1.00	0.247
	6	16	boat		-830.0854	-829.3320	5.206	4.874		5.453
	6	18	boat		-830.0853	-829.3324	5.273	4.675		5.520
r-1, t-2, c-3, c-4, c-5, c-6-hexafluoro	6	22	boat		-830.0792	-829.3250	9.098	9.298		9.345
	6	4	chair	ax, ax, ax, eq, ax, eq	-830.0850	-829.3314	1.662	1.129	0.06	5.686
	6	9	chair	eq, eq, eq, ax, eq, ax	-830.0877	-829.3332	0.000	0.000	1.00	4.024
			no boats considered							

1_1

C	-0.285995	-0.623242	1.265580
C	0.350280	-1.183774	0.000000
C	-0.285995	-0.623242	-1.265580
C	-0.285995	0.910331	-1.260600
C	-0.972961	1.449936	0.000000
C	-0.285995	0.910331	1.260600
H	0.247275	-1.015268	-2.142059
H	0.315022	-2.282975	0.000000
H	-1.320666	-0.995307	1.312494
H	0.247275	-1.015268	2.142059
H	0.752839	1.267749	-1.288409
H	-0.785243	1.285450	-2.164657
H	-0.963263	2.548916	0.000000
H	-2.028587	1.134472	0.000000
H	0.752839	1.267749	1.288409
H	-0.785243	1.285450	2.164657
H	-1.320666	-0.995307	-1.312494
F	1.720931	-0.836411	0.000000

1_2

C	-0.582796	0.896662	0.000000
C	0.094989	0.381626	1.259630
C	0.094989	-1.153721	1.263086
C	0.769434	-1.703373	0.000000
C	0.094989	-1.153721	-1.263086
C	0.094989	0.381626	-1.259630
H	0.600745	-1.526442	2.164138
H	1.128788	0.756293	1.274509
H	-0.419442	0.779946	2.144424
H	-1.642676	0.597651	0.000000
H	1.830015	-1.408285	0.000000
H	0.736678	-2.801861	0.000000
H	0.600745	-1.526442	-2.164138
H	-0.943410	-1.517433	-1.304016
H	1.128788	0.756293	-1.274509
H	-0.419442	0.779946	-2.144424
H	-0.943410	-1.517433	1.304016
F	-0.561884	2.303686	0.000000

1_3

C	-1.159864	0.194262	0.317609
C	-0.263510	1.436597	0.297543
C	1.231451	1.081310	0.188448
C	1.417748	-0.174631	-0.669817
C	0.779967	-1.398878	0.021637
C	-0.435252	-1.011289	0.892397
H	1.787494	1.930788	-0.230194
H	-0.577070	2.051560	-0.556208
H	-0.451102	2.024622	1.206627
H	-0.109996	-0.737114	1.906513
H	0.938783	-0.009050	-1.643734
H	2.483737	-0.361313	-0.856540
H	1.523836	-1.897052	0.658462
H	0.469913	-2.128193	-0.736500
H	-1.126841	-1.857803	0.991575
H	1.645754	0.893078	1.190266

H	-2.095003	0.397725	0.857695
F	-1.545860	-0.119053	-1.008319

1_4

C	-0.970341	-0.067501	-0.339774
C	-0.399677	1.304269	0.030407
C	1.102331	1.212534	0.377292
C	1.770800	0.087387	-0.421233
C	1.185453	-1.285745	-0.017762
C	-0.285469	-1.174034	0.441629
H	1.592853	2.175633	0.183920
H	-0.565187	2.006966	-0.796747
H	-0.970773	1.673837	0.892369
H	-0.343019	-0.930999	1.511675
H	-0.865382	-0.260984	-1.417373
H	1.607148	0.267063	-1.493860
H	2.857532	0.090597	-0.264089
H	1.781585	-1.721232	0.794874
H	1.255488	-1.978099	-0.867614
H	-0.816816	-2.122033	0.290224
H	1.225394	1.004011	1.449581
F	-2.353045	-0.074025	-0.078479

1_5

C	0.338629	-1.103974	0.635969
C	1.090027	0.210359	0.408676
C	0.201419	1.283385	-0.222537
C	-1.237791	1.130104	0.283148
C	-1.848752	-0.196639	-0.222978
C	-0.769514	-1.286549	-0.403268
H	0.604215	2.282622	-0.013311
H	-0.325411	-1.219686	-1.405974
H	-0.102541	-1.091635	1.643145
H	-1.234876	1.150023	1.382874
H	-1.851134	1.980503	-0.041857
H	-2.362248	-0.027305	-1.179357
H	-2.610937	-0.542763	0.488848
H	-1.217172	-2.285929	-0.323074
H	1.067329	-1.924488	0.609271
H	0.225543	1.141139	-1.311579
H	1.522361	0.566370	1.354693
F	2.182306	-0.027663	-0.453082

2_1

C	-0.227575	1.450302	0.000000
C	0.227575	0.732181	1.262992
C	-0.227575	-0.732181	1.262992
C	0.227575	-1.450302	0.000000
C	-0.227575	-0.732181	-1.262992
C	0.227575	0.732181	-1.262992
H	0.164934	-1.256287	2.143703
H	1.323957	0.779399	1.304068
H	-0.164934	1.256287	2.143703
H	0.110852	2.495950	0.000000
H	-0.110852	-2.495950	0.000000
H	0.164934	-1.256287	-2.143703
H	-1.323957	-0.779399	-1.304068
H	1.323957	0.779399	-1.304068

H	-0.164934	1.256287	-2.143703
H	-1.323957	-0.779399	1.304068
F	-1.642103	1.495305	0.000000
F	1.642103	-1.495305	0.000000

2_2

C	0.473205	-1.539876	0.000000
C	-0.164811	-0.979301	1.264791
C	-0.164811	0.555320	1.257095
C	-0.851804	1.064983	0.000000
C	-0.164811	0.555320	-1.257095
C	-0.164811	-0.979301	-1.264791
H	-0.676349	0.945803	2.146104
H	-1.196613	-1.357595	1.316639
H	0.370568	-1.361502	2.143035
H	0.434153	-2.638394	0.000000
H	-1.909261	0.755337	0.000000
H	-0.676349	0.945803	-2.146104
H	0.867650	0.927709	-1.267566
H	-1.196613	-1.357595	-1.316639
H	0.370568	-1.361502	-2.143035
H	0.867650	0.927709	1.267566
F	-0.843913	2.469610	0.000000
F	1.840764	-1.190569	0.000000

2_3

C	-0.236350	1.435402	0.000000
C	0.241781	0.728290	1.259873
C	-0.241781	-0.728290	1.259873
C	0.236350	-1.435402	0.000000
C	-0.241781	-0.728290	-1.259873
C	0.241781	0.728290	-1.259873
H	0.124626	-1.260051	2.146954
H	1.340543	0.764576	1.279815
H	-0.124626	1.260051	2.146954
H	-1.335636	1.495270	0.000000
H	1.335636	-1.495270	0.000000
H	0.124626	-1.260051	-2.146954
H	-1.340543	-0.764576	-1.279815
H	1.340543	0.764576	-1.279815
H	-0.124626	1.260051	-2.146954
H	-1.340543	-0.764576	1.279815
F	0.241781	2.756055	0.000000
F	-0.241781	-2.756055	0.000000

2_4

C	-1.279901	-0.396414	0.408891
C	0.000000	-0.921595	1.052575
C	1.279901	-0.396414	0.408891
C	1.256817	1.114152	0.212336
C	0.000000	1.553620	-0.545534
C	-1.256817	1.114152	0.212336
H	2.146515	-0.693871	1.017144
H	0.000000	-0.606026	2.106125
H	0.000000	-2.018643	1.031540
H	-2.146515	-0.693871	1.017144

H	1.276023	1.585091	1.207184
H	2.168702	1.418585	-0.317629
H	0.000000	2.643295	-0.679128
H	0.000000	1.096919	-1.543294
H	-1.276023	1.585091	1.207184
H	-2.168702	1.418585	-0.317629
F	-1.454107	-1.007786	-0.845868
F	1.454107	-1.007786	-0.845868

2_5

C	-1.197333	-0.744272	0.406546
C	0.279494	-1.068441	0.600455
C	1.149348	-0.188559	-0.286839
C	0.888960	1.288758	-0.042575
C	-0.590976	1.600846	-0.304738
C	-1.493197	0.738810	0.586026
H	0.546152	-0.883165	1.650427
H	0.462622	-2.127742	0.381740
H	-1.816496	-1.351809	1.080880
H	1.143627	1.520201	1.002234
H	1.541014	1.890003	-0.689402
H	-0.791553	2.664802	-0.124536
H	-0.828498	1.399087	-1.358264
H	-1.324205	0.990021	1.643704
H	-2.552756	0.921269	0.364511
H	0.972486	-0.431061	-1.343469
F	-1.562217	-1.114841	-0.907617
F	2.498865	-0.480099	-0.021392

2_6

C	-0.169752	-0.441752	1.244849
C	0.516758	-0.988107	0.000000
C	-0.169752	-0.441752	-1.244849
C	-0.169752	1.078467	-1.265910
C	-0.851452	1.616413	0.000000
C	-0.169752	1.078467	1.265910
H	1.567713	-0.668992	0.000000
H	0.486380	-2.084847	0.000000
H	-1.205091	-0.812885	1.295486
H	0.872431	1.425583	-1.308595
H	-0.682271	1.433797	-2.169211
H	-0.830450	2.713385	0.000000
H	-1.910951	1.318234	0.000000
H	0.872431	1.425583	1.308595
H	-0.682271	1.433797	2.169211
H	-1.205091	-0.812885	-1.295486
F	0.488855	-0.932288	2.382862
F	0.488855	-0.932288	-2.382862

2_7

C	-0.727271	-0.919602	0.234820
C	0.727271	-0.919602	-0.234820
C	1.087157	0.344469	-0.997886
C	0.742185	1.603094	-0.192495
C	-0.742185	1.603094	0.192495
C	-1.087157	0.344469	0.997886
H	2.154550	0.312799	-1.253253
H	0.921957	-1.817995	-0.835945

H	-0.921957	-1.817995	0.835945
H	1.356469	1.628345	0.718598
H	0.989113	2.498217	-0.778801
H	-0.989113	2.498217	0.778801
H	-1.356469	1.628345	-0.718598
H	-0.516965	0.334273	1.937385
H	-2.154550	0.312799	1.253253
H	0.516965	0.334273	-1.937385
F	1.523494	-1.013712	0.923247
F	-1.523494	-1.013712	-0.923247

2_8

C	-0.398809	-1.003780	-0.330640
C	-0.907113	0.421163	-0.476088
C	-0.138780	1.387514	0.409341
C	1.353305	1.331080	0.047448
C	1.895535	-0.098348	0.173818
C	1.081681	-1.074132	-0.686742
H	-0.541862	2.399246	0.274203
H	-0.796548	0.707924	-1.533237
H	-1.005018	-1.684343	-0.944280
H	1.489203	1.679957	-0.988214
H	1.920526	2.014037	0.693459
H	2.951300	-0.133370	-0.126251
H	1.840936	-0.417454	1.223400
H	1.194324	-0.821921	-1.751580
H	1.432592	-2.105343	-0.552300
H	-0.287717	1.096648	1.457020
F	-0.560935	-1.411571	1.003978
F	-2.273805	0.465308	-0.178983

2_9

C	-0.453480	0.607808	-0.649581
C	0.453480	-0.607808	-0.649581
C	1.319411	-0.646930	0.602361
C	0.453480	-0.617830	1.867327
C	-0.453480	0.617830	1.867327
C	-1.319411	0.646930	0.602361
H	1.950605	-1.544100	0.568941
H	-0.166138	-1.512879	-0.730787
H	0.166138	1.512879	-0.730787
H	-0.169278	-1.524268	1.908756
H	1.095973	-0.625271	2.757628
H	-1.095973	0.625271	2.757628
H	0.169278	1.524268	1.908756
H	-1.986208	-0.227277	0.587368
H	-1.950605	1.544100	0.568941
H	1.986208	0.227277	0.587368
F	-1.280529	0.569816	-1.779172
F	1.280529	-0.569816	-1.779172

2_10

C	-0.298451	-1.053430	0.121379
C	-1.109609	0.175723	-0.313747
C	-0.328413	1.476958	-0.177082
C	1.130899	1.228998	-0.579302
C	1.818499	0.285846	0.432472
C	0.817699	-0.693154	1.082147
H	-0.793354	2.259224	-0.789880

H	-1.427918	0.012994	-1.352026
H	0.342642	-0.236601	1.962094
H	1.152986	0.777985	-1.580555
H	1.673953	2.180109	-0.642397
H	2.300129	0.875321	1.223949
H	2.610299	-0.278987	-0.073904
H	1.324542	-1.603738	1.425383
H	-0.988619	-1.792868	0.548240
H	-0.377688	1.802798	0.871124
F	0.266928	-1.629332	-1.034611
F	-2.267008	0.238011	0.480474

2_11

C	-0.700547	-0.644567	-0.248882
C	-0.690886	0.738903	0.389991
C	0.731292	1.226164	0.670495
C	1.712948	0.665248	-0.361733
C	1.794886	-0.873528	-0.239898
C	0.462779	-1.481959	0.254053
H	0.720962	2.323361	0.674369
H	0.427888	-1.509442	1.351955
H	1.369995	0.950279	-1.365878
H	2.707885	1.109063	-0.230740
H	2.593980	-1.151004	0.459582
H	2.060979	-1.305337	-1.213628
H	0.345436	-2.512976	-0.100465
H	1.027325	0.896884	1.676378
H	-0.650362	-0.529075	-1.340328
F	-1.916383	-1.279926	0.039248
F	-1.325205	1.639851	-0.484105
H	-1.292627	0.707358	1.308302

2_12

C	-1.131501	-0.857177	-0.305199
C	0.360775	-1.192600	-0.402596
C	1.235005	0.059496	-0.328327
C	0.638310	1.087431	0.615538
C	-0.688641	1.613674	0.025085
C	-1.429239	0.545195	-0.811165
H	0.622228	-1.845755	0.439055
H	0.561744	-1.743630	-1.330161
H	-1.109419	0.586954	-1.862480
H	0.463167	0.607770	1.586291
H	1.350666	1.908148	0.764300
H	-0.492154	2.485907	-0.612057
H	-1.333745	1.953575	0.842971
H	-2.510852	0.727238	-0.794334
H	-1.732482	-1.611348	-0.830670
H	1.364803	0.505704	-1.325745
F	-1.529476	-0.921646	1.049559
F	2.519230	-0.312874	0.101865

2_13

C	1.188690	-0.566626	0.461644
C	0.000000	-1.410793	0.000000
C	-1.188690	-0.566625	-0.461644
C	-0.744784	0.762240	-1.048441

C	0.000001	1.616349	0.000000
C	0.744784	0.762239	1.048441
H	0.336791	-2.057747	-0.819853
H	-0.336792	-2.057746	0.819854
H	0.081330	0.536453	1.893399
H	-0.081330	0.536454	-1.893399
H	-1.614546	1.304719	-1.439312
H	-0.713384	2.267465	0.518565
H	0.713386	2.267464	-0.518564
H	1.614546	1.304718	1.439313
H	1.812564	-1.132520	1.166425
F	2.015231	-0.300969	-0.657420
H	-1.812564	-1.132519	-1.166426
F	-2.015231	-0.300969	0.657419

2_14

C	0.741311	-1.023889	-0.299852
C	0.000000	0.000000	-1.165813
C	-0.741311	1.023889	-0.299852
C	0.000000	1.284214	1.000440
C	0.000000	0.000000	1.861793
C	0.000000	-1.284214	1.000440
H	0.703113	0.541272	-1.810709
H	-0.703113	-0.541272	-1.810709
H	-1.025878	-1.595092	0.759293
H	1.025878	1.595092	0.759293
H	-0.474752	2.112846	1.539667
H	-0.880715	-0.007676	2.515944
H	0.880715	0.007676	2.515944
H	0.474752	-2.112846	1.539667
H	-1.762513	0.682369	-0.078849
H	1.762513	-0.682369	-0.078849
F	0.876616	-2.218983	-1.024091
F	-0.876616	2.218983	-1.024091

2_15

C	1.581566	0.064673	-0.153730
C	0.848198	1.405414	-0.252523
C	-0.676459	1.233639	-0.403991
C	-1.131107	0.001900	0.361075
C	-0.557004	-1.275593	-0.257896
C	0.835291	-1.039272	-0.884365
H	-1.205549	2.119922	-0.033162
H	1.087337	1.977171	0.652930
H	1.245927	1.967837	-1.107117
H	0.734925	-0.723664	-1.932403
H	-0.839828	0.090680	1.415384
H	-1.259403	-1.607351	-1.033205
H	-0.506456	-2.063396	0.501821
H	1.424120	-1.964577	-0.876745
H	2.615820	0.160491	-0.510282
H	-0.948729	1.103251	-1.460872
F	1.674268	-0.303962	1.209855
F	-2.535498	-0.074363	0.338171

2_16

C	-1.415913	-0.248727	-0.127624
C	-0.456480	-1.431934	-0.331221
C	0.931795	-1.005428	-0.836962
C	1.415913	0.248727	-0.127624

C	0.456480	1.431934	-0.331221
C	-0.931795	1.005428	-0.836962
H	1.655162	-1.818257	-0.693646
H	-0.361404	-1.941346	0.634362
H	-0.898669	-2.146303	-1.037420
H	-0.896716	0.784848	-1.913749
H	0.898669	2.146303	-1.037420
H	0.361404	1.941346	0.634362
H	-1.655162	1.818257	-0.693646
H	-2.431968	-0.513208	-0.450217
H	0.896716	-0.784848	-1.913749
F	-1.513324	0.042516	1.248390
F	1.513324	-0.042516	1.248390
H	2.431968	0.513208	-0.450217

2_17

C	-0.029061	1.370952	-0.355535
C	1.319898	0.737341	0.008200
C	1.163738	-0.738386	0.432447
C	0.029061	-1.370952	-0.355535
C	-1.319898	-0.737341	0.008200
C	-1.163738	0.738386	0.432447
H	2.093836	-1.293846	0.261715
H	2.007306	0.822588	-0.842658
H	1.744729	1.322139	0.833402
H	-0.925928	0.812210	1.502057
H	-1.744729	-1.322139	0.833402
H	-2.007306	-0.822588	-0.842658
H	-2.093836	1.293846	0.261715
H	0.925928	-0.812210	1.502057
H	0.231726	-1.275269	-1.432593
H	-0.231726	1.275269	-1.432593
F	0.029061	2.749330	-0.092510
F	-0.029061	-2.749330	-0.092510

2_18

C	0.595284	0.475813	-0.918980
C	0.595284	1.392620	0.304199
C	-0.090568	0.761196	1.532119
C	0.090568	-0.761196	1.532119
C	-0.595284	-1.392620	0.304199
C	-0.595284	-0.475813	-0.918980
H	0.322897	1.197052	2.450786
H	1.647209	1.620504	0.521623
H	0.105302	2.336996	0.037556
H	1.163638	-0.992115	1.513865
H	-0.322897	-1.197052	2.450786
H	-1.647209	-1.620504	0.521623
H	-0.105302	-2.336996	0.037556
H	-0.632288	-1.055463	-1.850325
H	0.632288	1.055463	-1.850325
H	-1.163638	0.992115	1.513865
F	1.744789	-0.342538	-0.908615
F	-1.744789	0.342538	-0.908615

2_19

C	-0.331481	-1.051377	-0.160457
C	1.145754	-1.138812	-0.554201
C	1.855413	0.230930	-0.491009
C	1.235990	1.121025	0.595339

C	-0.248394	1.420884	0.285979
C	-0.879325	0.305877	-0.547944
H	2.926267	0.081529	-0.302762
H	1.616449	-1.852613	0.133290
H	1.221148	-1.561368	-1.565009
H	1.309202	0.601715	1.558959
H	1.797530	2.059665	0.684296
H	-0.355006	2.368980	-0.256084
H	-0.824556	1.503252	1.214649
H	-0.927904	-1.853370	-0.614435
H	1.773801	0.740469	-1.462320
F	-0.453873	-1.207916	1.233721
H	-0.672908	0.445806	-1.619240
F	-2.271879	0.334003	-0.404564

2_20

C	0.596017	0.467806	-0.607597
C	0.544496	1.408928	0.602756
C	-0.127307	0.755463	1.828222
C	0.127307	-0.755463	1.828222
C	-0.544496	-1.408928	0.602756
C	-0.596017	-0.467806	-0.607597
H	0.248776	1.219081	2.749033
H	1.564955	1.727905	0.848006
H	-0.009934	2.303509	0.291990
H	1.211968	-0.933017	1.802715
H	-0.248776	-1.219081	2.749033
H	-1.564955	-1.727905	0.848006
H	0.009934	-2.303509	0.291990
H	-1.211968	0.933017	1.802715
H	1.517235	-0.131425	-0.626774
F	0.596017	1.234771	-1.778361
H	-1.517235	0.131425	-0.626774
F	-0.596017	-1.234771	-1.778361

2_21

C	-0.943793	-0.982826	0.291353
C	-1.797773	0.274510	0.100497
C	-0.948207	1.559572	0.030799
C	0.432449	1.263234	-0.567447
C	1.210842	0.372013	0.396264
C	0.328377	-0.690037	1.070076
H	-1.468993	2.323195	-0.560108
H	-2.372849	0.140180	-0.824385
H	-2.520393	0.340901	0.925070
H	0.030047	-0.338669	2.067901
H	0.321406	0.727832	-1.517729
H	0.993867	2.186366	-0.758132
H	1.689347	0.985419	1.173248
H	0.919811	-1.604054	1.201863
H	-1.524752	-1.777659	0.779332
H	-0.817594	1.977700	1.040375
F	-0.583427	-1.490262	-0.975367
F	2.256620	-0.258627	-0.297599

2_22

C	1.271589	-0.588549	-0.420395
C	1.409077	0.934768	-0.512170
C	0.089600	1.662113	-0.189992
C	-0.693188	0.885886	0.871740

C	-1.128392	-0.478108	0.337183
C	-0.149915	-1.049124	-0.696765
H	0.294530	2.685985	0.147647
H	2.197999	1.233210	0.190185
H	1.754216	1.200299	-1.520493
H	-0.444015	-0.668220	-1.684134
H	-0.059975	0.730510	1.754775
H	-1.591716	1.428948	1.190599
H	-0.208677	-2.143469	-0.726386
H	1.985859	-1.086812	-1.088945
H	-0.528078	1.743182	-1.095464
F	1.614650	-1.006345	0.889541
F	-2.382746	-0.342991	-0.297338
H	-1.279900	-1.181518	1.164783

2_23

C	-1.056974	-0.407082	-0.307106
C	-1.261661	1.105676	-0.183344
C	0.042502	1.815506	0.244237
C	1.269670	1.047451	-0.262645
C	1.341208	-0.331785	0.399213
C	-0.045138	-0.903278	0.710189
H	0.054377	2.845370	-0.133562
H	-1.626032	1.507167	-1.137450
H	-2.048995	1.270491	0.563672
H	-0.361035	-0.584142	1.712823
H	1.190715	0.895723	-1.347794
H	2.197535	1.601963	-0.076362
H	0.008729	-1.998398	0.703464
H	0.091159	1.883044	1.340368
H	-0.726172	-0.681512	-1.317894
F	-2.286740	-1.056257	-0.107788
F	2.013580	-1.210775	-0.473241
H	1.940520	-0.295342	1.318727

2_24

C	1.248239	-0.250997	0.337269
C	1.164130	1.168103	-0.231780
C	-0.304994	1.614517	-0.403581
C	-1.196800	0.928434	0.635584
C	-1.225958	-0.585080	0.413185
C	0.095864	-1.112532	-0.156533
H	-0.382745	2.705858	-0.322032
H	1.707401	1.859020	0.425594
H	1.679876	1.163731	-1.200752
H	0.047080	-1.050111	-1.251464
H	-0.817269	1.133476	1.647225
H	-2.229118	1.297757	0.593129
H	0.255967	-2.161306	0.119022
H	-0.667062	1.344183	-1.404500
H	1.255729	-0.233619	1.436929
F	2.466642	-0.833574	-0.046467
H	-1.487423	-1.100614	1.347360
F	-2.249455	-0.892321	-0.504130

2_25

C	0.392454	0.655723	-1.118371
C	0.006962	1.511682	0.089934
C	-0.392454	0.658751	1.298163
C	0.392454	-0.658751	1.298163

C	-0.006962	-1.511682	0.089934
C	-0.392454	-0.655723	-1.118371
H	-0.236475	1.215492	2.230041
H	0.825640	2.198441	0.345604
H	-1.468300	-0.437342	-1.077228
H	1.468300	0.437342	-1.077228
H	1.468511	-0.451948	1.219689
H	0.236475	-1.215492	2.230041
H	-0.825640	-2.198441	0.345604
H	-0.212171	-1.238749	-2.029990
H	0.212171	1.238749	-2.029990
H	-1.468511	0.451948	1.219689
F	-1.091768	2.325685	-0.256275
F	1.091768	-2.325685	-0.256275

2_26

C	0.811127	-1.109761	0.655265
C	1.497266	0.210991	0.291517
C	0.491832	1.285301	-0.129247
C	-0.811127	1.109761	0.655265
C	-1.497266	-0.210991	0.291517
C	-0.491832	-1.285301	-0.129247
H	0.916048	2.287034	0.010545
H	2.117128	0.557261	1.130352
H	-0.292318	-1.160405	-1.201418
H	0.601017	-1.119068	1.734433
H	-0.601017	1.119068	1.734433
H	-1.513735	1.928311	0.456627
H	-0.916048	-2.287033	0.010545
H	1.513735	-1.928311	0.456628
H	0.292318	1.160405	-1.201418
F	2.382450	-0.014454	-0.781750
H	-2.117128	-0.557261	1.130352
F	-2.382450	0.014454	-0.781750

3_1

C	-1.278710	0.738264	-0.336532
C	0.000000	1.463744	-0.741782
C	1.278710	0.738264	-0.336532
C	1.267639	-0.731872	-0.741782
C	0.000000	-1.476527	-0.336532
C	-1.267639	-0.731872	-0.741782
H	2.142857	1.237179	-0.799176
H	0.000000	1.558457	-1.837671
H	0.000000	2.475060	-0.317138
H	-2.142857	1.237179	-0.799176
H	1.349664	-0.779229	-1.837671
H	2.143465	-1.237530	-0.317138
H	0.000000	-2.474358	-0.799176
H	-1.349664	-0.779229	-1.837671
H	-2.143465	-1.237530	-0.317138
F	-1.460846	0.843420	1.047097
F	0.000000	-1.686839	1.047097
F	1.460846	0.843420	1.047097

3_2

C	0.384322	-0.783754	1.279120
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C	0.955596	-1.387504	0.000000
C	0.384322	-0.783754	-1.279120
C	0.384322	0.740560	-1.255308
C	-0.301290	1.257543	0.000000
C	0.384322	0.740560	1.255308
H	0.950063	-1.150989	-2.146466
H	2.041038	-1.211928	0.000000
H	0.789494	-2.471651	0.000000
H	0.950063	-1.150989	2.146466
H	1.424603	1.095851	-1.263055
H	-0.117513	1.125166	-2.151308
H	1.424603	1.095851	1.263055
H	-0.117513	1.125166	2.151308
F	-0.938507	-1.226590	1.453505
F	-0.938507	-1.226590	-1.453505
H	-1.359800	0.971821	0.000000
F	-0.249055	2.660937	0.000000

3_3

C	-0.563177	1.489645	0.000000
C	0.068660	0.927898	1.267950
C	0.068660	-0.594339	1.242665
C	0.764556	-1.132518	0.000000
C	0.068660	-0.594339	-1.242665
C	0.068660	0.927898	-1.267950
H	1.107316	1.280558	1.332437
H	-0.475294	1.293252	2.147172
H	-0.515853	2.586245	0.000000
H	1.811642	-0.799921	0.000000
H	0.747269	-2.229141	0.000000
H	1.107316	1.280558	-1.332437
H	-0.475294	1.293252	-2.147172
F	-1.933862	1.146814	0.000000
H	-0.962276	-0.969533	-1.292980
F	0.731449	-1.068474	-2.383813
F	0.731449	-1.068474	2.383813
H	-0.962276	-0.969533	1.292980

3_4

C	-1.244087	0.718274	0.323424
C	0.000000	1.455856	-0.153912
C	1.244087	0.718274	0.323424
C	1.260809	-0.727928	-0.153912
C	0.000000	-1.436548	0.323424
C	-1.260809	-0.727928	-0.153912
H	0.000000	1.488224	-1.251521
H	0.000000	2.484558	0.226195
H	1.288839	-0.744112	-1.251521
H	2.151690	-1.242279	0.226195
H	-1.288839	-0.744112	-1.251521
H	-2.151690	-1.242279	0.226195
H	-1.301623	0.751493	1.422167
F	-2.382935	1.375788	-0.157102
F	0.000000	-2.751577	-0.157102
H	0.000000	-1.502985	1.422167
F	2.382935	1.375788	-0.157102
H	1.301623	0.751493	1.422167

3_5

C	-1.380760	0.006788	-0.389235
C	-0.580829	1.133604	0.262628
C	0.506935	0.612568	1.192162
C	1.361506	-0.494663	0.583473
C	0.517964	-1.599781	-0.037379
C	-0.482873	-1.026489	-1.046012
H	-1.263926	1.794042	0.813554
H	-2.099797	0.430053	-1.102581
H	2.035058	-0.904617	1.349158
H	1.178823	-2.329578	-0.520948
H	-0.020823	-2.114891	0.769106
H	0.054073	-0.530372	-1.864534
H	-1.101873	-1.822546	-1.478042
F	-2.123707	-0.604313	0.640963
F	-0.019274	1.888707	-0.775708
H	0.012970	0.206522	2.085272
H	1.145040	1.447400	1.507035
F	2.188402	0.052477	-0.415460

3_6

C	1.483003	-0.355369	0.054496
C	0.887741	1.003878	-0.311472
C	-0.548635	0.891392	-0.797636
C	-1.403700	0.122991	0.201425
C	-0.834301	-1.260713	0.469967
C	0.595102	-1.131637	1.013151
H	1.520225	1.497624	-1.060190
H	2.490196	-0.216407	0.468687
H	-1.471912	-1.793734	1.186042
H	-0.828811	-1.828382	-0.469597
H	0.591239	-0.591690	1.970073
H	1.037484	-2.119712	1.190043
F	1.616932	-1.072287	-1.147822
F	0.927748	1.788874	0.856435
H	-0.548754	0.351383	-1.753521
H	-0.960976	1.893766	-0.965436
F	-2.702252	0.005268	-0.318215
H	-1.485804	0.687202	1.140734

3_7

C	0.993319	0.771912	-0.486369
C	0.805218	-0.732514	-0.395128
C	-0.138914	-1.109953	0.736865
C	-1.482369	-0.411654	0.555842
C	-1.337206	1.095637	0.398368
C	-0.350328	1.450864	-0.721533
H	-0.280082	-2.196892	0.756775
H	0.406129	-1.082797	-1.356368
H	1.725561	1.016092	-1.267429
H	-2.159065	-0.655454	1.385531
H	-2.322132	1.532279	0.192307
H	-0.978097	1.505360	1.351426
H	-0.747161	1.119340	-1.690064
H	-0.202909	2.536401	-0.773272
H	0.303824	-0.796041	1.690182
F	1.526705	1.238599	0.728193
F	2.041980	-1.355531	-0.203962
F	-2.089173	-0.923517	-0.615048

3_8

C	1.234231	0.763688	-0.210162
C	0.954898	-0.699827	-0.512088
C	-0.314890	-1.180660	0.174483
C	-1.484880	-0.318144	-0.284956
C	-1.247033	1.155155	0.009815
C	0.055692	1.622458	-0.655288
H	-0.496555	-2.232992	-0.074097
H	0.860660	-0.800666	-1.604291
H	2.173012	1.074271	-0.688068
H	-2.096291	1.746850	-0.353398
H	-1.177815	1.288158	1.096796
H	-0.027647	1.559721	-1.750147
H	0.260996	2.669206	-0.401655
H	-0.197404	-1.088083	1.260725
F	1.407677	0.918643	1.172927
F	2.039701	-1.484871	-0.119299
F	-2.651171	-0.746248	0.362773
H	-1.652923	-0.460204	-1.364295

3_9

C	1.253033	0.413300	0.377199
C	0.628885	-0.971180	0.456603
C	-0.779379	-0.887728	1.039664
C	-1.661585	0.151763	0.350813
C	-0.969909	1.501369	0.198399
C	0.407789	1.356401	-0.460944
H	-1.256559	-1.873323	0.979185
H	-1.614794	2.168301	-0.386748
H	-0.861746	1.941383	1.201286
H	0.303893	0.942511	-1.470695
H	0.908280	2.329474	-0.533918
H	-0.700235	-0.617894	2.102502
H	1.344362	0.800949	1.404279
F	2.545783	0.313562	-0.141378
H	1.263774	-1.634078	1.060833
F	0.576255	-1.522007	-0.826783
H	-2.599942	0.265103	0.912076
F	-2.017598	-0.314441	-0.925085

3_10

C	-1.264930	0.404094	-0.494571
C	-0.723407	-1.008244	-0.332642
C	0.770546	-1.038575	-0.630429
C	1.507851	-0.038871	0.254576
C	0.955636	1.370978	0.099347
C	-0.547206	1.388813	0.415043
H	1.161135	-2.050084	-0.467879
H	1.499705	2.056028	0.760928
H	1.129696	1.698193	-0.936115
H	-0.726846	1.097134	1.457541
H	-0.964500	2.391763	0.266434
H	0.938177	-0.772127	-1.683188
F	2.865958	-0.047382	-0.100116
H	1.448235	-0.354233	1.304616
H	-1.131477	0.694979	-1.547803
F	-2.636877	0.410901	-0.233190
H	-1.282893	-1.703835	-0.971714

F -0.924877 -1.422074 0.994333

3_11

C -1.043551 0.650560 -0.254161
C -0.735162 -0.762159 0.203063
C 0.522755 -1.295059 -0.474484
C 1.711590 -0.367267 -0.265344
C 1.398222 1.061445 -0.688010
C 0.136314 1.575265 0.013435
H 0.749910 -2.296139 -0.089441
H 2.255395 1.705714 -0.457255
H 1.259814 1.069248 -1.779049
H 0.306539 1.620136 1.096683
H -0.116023 2.586395 -0.328101
H 0.331469 -1.382697 -1.553027
H -1.299475 0.631891 -1.324213
F -2.165575 1.125455 0.431762
H 2.594484 -0.749314 -0.795218
F 2.036969 -0.364716 1.107512
H -0.632528 -0.771228 1.295775
F -1.803683 -1.604152 -0.125180

3_12

C 1.193094 -0.527192 -0.299622
C 0.788786 0.808960 0.295923
C -0.644101 1.165198 -0.080321
C -1.600981 0.058325 0.342036
C -1.213629 -1.273852 -0.280806
C 0.223947 -1.625798 0.119491
H -0.922811 2.114893 0.391460
H 0.915150 0.760118 1.387331
H -1.908477 -2.056426 0.047499
H -1.298094 -1.184937 -1.373078
H 0.294672 -1.750740 1.209538
H 0.537258 -2.571345 -0.338519
H -0.707762 1.292628 -1.169436
F 1.642036 1.810247 -0.174555
F -2.899241 0.406577 -0.053284
H -1.615944 -0.033376 1.438791
H 1.236089 -0.431690 -1.394252
F 2.478006 -0.858266 0.141222

3_13

C 1.285851 -0.336425 0.120995
C 0.000000 -1.158364 0.022885
C -1.285851 -0.336425 0.120995
C -1.254918 0.906724 -0.753255
C 0.000000 1.743499 -0.483635
C 1.254918 0.906724 -0.753255
H -2.131332 -0.985903 -0.144280
H 0.000000 -1.942168 0.790698
H 2.131332 -0.985903 -0.144280
H -1.266329 0.576105 -1.801654
H -2.170712 1.484234 -0.573765
H 0.000000 2.638664 -1.118196
H 0.000000 2.078054 0.561509
H 1.266329 0.576105 -1.801654

H	2.170712	1.484234	-0.573765
F	1.449030	0.036321	1.462231
F	0.000000	-1.770178	-1.240349
F	-1.449030	0.036321	1.462231

3_14

C	-1.186241	-0.812641	0.049756
C	0.330395	-1.012994	0.053274
C	1.027164	0.182968	-0.573230
C	0.683049	1.475696	0.146781
C	-0.837163	1.690109	0.088515
C	-1.581177	0.500145	0.707305
H	0.608896	-1.937975	-0.467537
H	-1.670314	-1.666936	0.540432
H	1.020366	1.402609	1.188726
H	1.217789	2.306755	-0.329308
H	-1.108527	2.613160	0.615789
H	-1.151391	1.808828	-0.957685
H	-1.337344	0.419504	1.775428
H	-2.667923	0.624930	0.618726
H	0.710193	0.238997	-1.623838
F	-1.598408	-0.813060	-1.295702
F	0.719560	-1.143851	1.391810
F	2.407968	-0.037486	-0.562236

3_15

C	-0.219544	-1.277680	-0.202106
C	-0.843756	0.000000	-0.744528
C	-0.219544	1.277680	-0.202106
C	1.287715	1.262141	-0.437960
C	1.922447	0.000000	0.158247
C	1.287715	-1.262141	-0.437960
H	-0.696833	2.141130	-0.686407
H	-0.675569	0.000000	-1.832743
H	-0.696833	-2.141130	-0.686407
H	1.470723	1.300379	-1.522256
H	1.720591	2.168642	0.003157
H	3.003370	0.000000	-0.030883
H	1.774705	0.000000	1.245312
H	1.470723	-1.300379	-1.522256
H	1.720591	-2.168642	0.003157
F	-0.467340	-1.396358	1.167323
F	-2.218838	0.000000	-0.531558
F	-0.467340	1.396358	1.167323

3_16

C	0.917156	-0.992110	-0.323742
C	-0.554139	-0.648066	-0.507918
C	-0.949966	0.547486	0.339627
C	-0.071685	1.748539	0.011467
C	1.413341	1.412569	0.194754
C	1.802860	0.199697	-0.659060
H	-0.736978	-0.412762	-1.566562
H	1.164716	-1.877561	-0.924221
H	-0.264422	2.037129	-1.032154
H	-0.370282	2.590910	0.647672
H	2.028190	2.278453	-0.080652
H	1.616894	1.188554	1.250109
H	1.684465	0.434044	-1.727064
H	2.850745	-0.079404	-0.492736

F	1.127408	-1.341057	1.021056
F	-1.334735	-1.753565	-0.180217
F	-2.285466	0.867368	0.069572
H	-0.883593	0.277244	1.401123

3_17

C	-1.237042	-0.128643	-0.521048
C	0.000000	-0.949798	-0.187115
C	1.237042	-0.128643	-0.521048
C	1.271234	1.160883	0.283760
C	0.000000	1.976565	0.000349
C	-1.271234	1.160883	0.283760
H	1.332480	0.905652	1.348967
H	2.169300	1.730111	0.014386
H	0.000000	2.888166	0.610171
H	0.000000	2.296632	-1.052874
H	-1.332480	0.905652	1.348967
H	-2.169300	1.730111	0.014386
H	-1.220585	0.095379	-1.598557
H	0.000000	-1.905074	-0.728328
H	1.220585	0.095379	-1.598557
F	-2.379542	-0.893234	-0.277406
F	0.000000	-1.245699	1.178090
F	2.379542	-0.893234	-0.277406

3_18

C	-0.210341	-0.171908	1.256070
C	0.432507	-0.738521	0.000000
C	-0.210341	-0.171908	-1.256070
C	-0.210341	1.348947	-1.257317
C	-0.906413	1.880963	0.000000
C	-0.210341	1.348947	1.257317
H	0.831227	1.699071	-1.284825
H	-0.705443	1.702375	-2.170185
H	-0.895045	2.977685	0.000000
H	-1.961816	1.569869	0.000000
H	0.831227	1.699071	1.284825
H	-0.705443	1.702375	2.170185
H	-1.235337	-0.562794	1.333905
H	-1.235337	-0.562794	-1.333905
F	0.494419	-0.641966	2.368071
F	0.494419	-0.641966	-2.368071
H	1.509059	-0.518477	0.000000
F	0.284332	-2.125568	0.000000

3_19

C	-0.959060	-0.968873	0.067619
C	0.567577	-0.853999	0.173260
C	1.068037	0.534223	-0.191464
C	0.090766	1.592206	0.292212
C	-1.235678	1.479169	-0.491275
C	-1.538524	0.026422	-0.919339
H	0.874554	-1.091573	1.199617
H	-1.087600	-0.194628	-1.897280
H	-0.083273	1.445960	1.365568
H	0.542603	2.581782	0.157766
H	-1.195397	2.111731	-1.387179
H	-2.051743	1.858165	0.133875
H	-2.618788	-0.133789	-1.018622

H	-1.209310	-2.005145	-0.193394
H	1.201419	0.592888	-1.280900
F	-1.501910	-0.713514	1.340415
F	1.137524	-1.798399	-0.688911
F	2.327589	0.731881	0.385659

3_20

C	0.611732	-1.090002	0.331808
C	-0.698185	-0.800735	-0.416274
C	-0.978558	0.689520	-0.591599
C	0.324637	1.393707	-0.935735
C	1.312601	1.337776	0.252183
C	1.106153	0.093351	1.140411
H	-0.610624	-1.248382	-1.415224
H	0.350484	0.294596	1.909459
H	0.754526	0.887588	-1.811037
H	0.121550	2.432522	-1.220949
H	1.195491	2.235587	0.869519
H	2.335483	1.345594	-0.141832
H	2.039132	-0.181228	1.647742
H	0.468151	-1.983779	0.951930
F	1.586749	-1.405684	-0.638725
F	-1.761760	-1.411933	0.244754
H	-1.755424	0.839265	-1.352873
F	-1.488217	1.221676	0.602693

3_21

C	1.252365	0.705808	-0.012616
C	1.055322	-0.781993	-0.330949
C	-0.366713	-1.260684	-0.043014
C	-1.352481	-0.139052	-0.340897
C	-1.168862	1.032362	0.628422
C	0.303803	1.185965	1.068789
H	-0.607147	-2.148715	-0.638430
H	1.328600	-0.939620	-1.382110
H	0.506249	0.576411	1.960279
H	-1.238020	0.194502	-1.380340
H	-1.798927	0.835279	1.504761
H	-1.528488	1.955828	0.161418
H	0.526882	2.227352	1.329222
H	2.303687	0.871379	0.254062
H	-0.437542	-1.527970	1.019623
F	0.996985	1.428447	-1.195260
F	1.952513	-1.516233	0.457411
F	-2.660154	-0.634312	-0.222917

3_22

C	-0.848699	0.976433	0.052155
C	-1.064577	-0.527293	0.284827
C	-0.022098	-1.402830	-0.403724
C	1.370204	-0.813098	-0.236127
C	1.482019	0.597342	-0.835821
C	0.114223	1.253365	-1.087255
H	-0.059864	-2.422945	-0.004030
H	-1.074290	-0.702254	1.366158
H	-0.341981	0.855110	-2.004691
H	2.043795	0.551776	-1.777122
H	2.065719	1.202330	-0.132860
H	0.224617	2.336380	-1.222884
H	-1.828479	1.437730	-0.126318

H	-0.255365	-1.448854	-1.476105
F	-0.327898	1.539946	1.227808
F	-2.329770	-0.875758	-0.217459
H	2.125437	-1.480949	-0.669526
F	1.648109	-0.756614	1.145545

3_23

C	-1.228253	0.793558	-0.166090
C	-1.078293	-0.665255	-0.600517
C	0.375576	-1.153558	-0.559930
C	1.237985	-0.296720	0.355005
C	1.268426	1.161505	-0.113887
C	-0.076107	1.604405	-0.738579
H	0.388792	-2.199332	-0.232521
H	-0.066791	1.448397	-1.826737
H	2.068378	1.248563	-0.859914
H	1.529076	1.811895	0.727904
H	-0.248022	2.672897	-0.565692
H	-2.210823	1.179225	-0.467352
H	0.806758	-1.110700	-1.569312
F	-1.181595	0.873987	1.233767
H	0.886268	-0.371165	1.389428
F	2.548649	-0.803742	0.337374
F	-1.887485	-1.470114	0.203743
H	-1.465760	-0.744576	-1.625760

3_24

C	1.222669	0.312600	-0.568503
C	0.693784	-1.050815	-0.169628
C	-0.797806	-1.138188	-0.503930
C	-1.495755	0.223600	-0.405489
C	-0.862965	1.098541	0.665399
C	0.597739	1.423427	0.280056
H	-0.932499	-1.563309	-1.506039
H	1.209006	1.531910	1.182401
H	-0.893186	0.554334	1.616431
H	-1.448587	2.018202	0.779707
H	0.655158	2.366060	-0.277317
H	-1.265562	-1.818571	0.217531
H	0.995215	0.451856	-1.636057
F	2.614197	0.352688	-0.449373
F	0.873742	-1.213815	1.214845
H	1.269684	-1.848912	-0.654822
H	-1.470675	0.745815	-1.373589
F	-2.850667	0.010863	-0.113880

3_25

C	-0.894645	-0.553158	-0.496734
C	-0.729232	0.949911	-0.401986
C	0.752287	1.317482	-0.493373
C	1.667462	0.250524	0.114275
C	0.984560	-0.530391	1.225862
C	-0.281685	-1.255432	0.715460
H	1.041507	1.460918	-1.541564
H	-1.042193	-1.272596	1.503847
H	0.714297	0.188881	2.009077
H	1.692316	-1.248462	1.656245
H	-0.053578	-2.292175	0.445855
H	0.891854	2.271735	0.028781
H	-0.414819	-0.881606	-1.427601

F	-2.251461	-0.881788	-0.595001
F	-1.230486	1.382910	0.840949
H	-1.325105	1.456330	-1.171612
F	2.026004	-0.663232	-0.906198
H	2.606723	0.702358	0.458203

3_26

C	-1.227089	-0.439345	-0.259362
C	-0.807476	0.878993	0.385621
C	0.684323	0.909876	0.720406
C	1.465078	0.102377	-0.303088
C	1.094267	-1.384486	-0.230511
C	-0.363315	-1.587963	0.236069
H	1.024305	1.951805	0.737923
H	-0.420955	-1.622327	1.332270
H	1.782942	-1.861365	0.477546
H	1.253270	-1.851960	-1.209824
H	-0.766365	-2.534606	-0.141756
H	0.848890	0.479826	1.717218
H	-1.147844	-0.337182	-1.350772
F	-2.573065	-0.686978	0.032475
H	1.281899	0.508119	-1.307555
F	2.839953	0.244488	-0.066416
F	-1.101904	1.925993	-0.503248
H	-1.415714	1.039448	1.284856

3_27

C	0.967956	0.488609	-0.312975
C	0.743269	-0.759814	0.527292
C	-0.704607	-0.877553	1.025089
C	-1.682597	-0.114403	0.146714
C	-1.350787	1.379061	0.095786
C	0.160039	1.649777	0.246733
H	-0.969545	-1.940176	1.073099
H	0.427219	1.776267	1.305546
H	-1.901421	1.894655	0.892804
H	-1.723576	1.765044	-0.860723
H	0.445743	2.571380	-0.273173
H	-0.775946	-0.465770	2.041014
H	0.696407	0.278672	-1.354029
F	2.331078	0.812576	-0.290207
F	1.079414	-1.892557	-0.221832
H	1.437056	-0.724618	1.378384
H	-2.717912	-0.273580	0.475890
F	-1.601343	-0.639568	-1.160255

3_28

C	-0.558633	-1.064215	0.116465
C	-1.454617	0.102951	-0.322060
C	-0.745720	1.452654	-0.248832
C	0.737268	1.275993	-0.600231
C	1.424615	0.476746	0.505896
C	0.523324	-0.623298	1.083909
H	-1.233489	2.173097	-0.915609
H	-1.806006	-0.109397	-1.339970
H	0.018539	-0.250426	1.985874
H	0.840181	0.717365	-1.538689
H	1.231130	2.246014	-0.729609
H	1.741856	1.146202	1.317734
H	1.146443	-1.475407	1.380014

H	-1.192624	-1.847008	0.552816
H	-0.844413	1.834566	0.777153
F	0.040504	-1.601624	-1.035453
F	-2.578774	0.125510	0.519085
F	2.598377	-0.097219	-0.005921

3_29

C	-0.848833	0.944595	-0.289779
C	-1.388702	-0.408935	0.196423
C	-0.279395	-1.416774	0.476981
C	0.915452	-0.684158	1.094904
C	1.548069	0.274627	0.084992
C	0.527178	0.829795	-0.915702
H	-0.647808	-2.214849	1.132292
H	-1.994517	-0.222188	1.092734
H	0.454890	0.124880	-1.754705
H	0.588099	-0.108475	1.970686
H	1.686216	-1.388881	1.428259
H	0.851852	1.796460	-1.317376
H	-1.576652	1.382523	-0.984030
H	0.020563	-1.878658	-0.472885
F	-0.764276	1.803114	0.826371
F	-2.241608	-0.916897	-0.795218
H	2.072380	1.084684	0.605784
F	2.528368	-0.420705	-0.652007

3_30

C	0.693784	-1.050815	-0.169628
C	1.222669	0.312600	-0.568503
C	0.597739	1.423427	0.280056
C	-0.862965	1.098541	0.665400
C	-1.495755	0.223600	-0.405489
C	-0.797806	-1.138188	-0.503930
H	1.209006	1.531910	1.182401
H	-0.932499	-1.563309	-1.506039
H	-0.893186	0.554334	1.616431
H	-1.448587	2.018202	0.779708
H	-1.265562	-1.818571	0.217531
H	1.269684	-1.848912	-0.654822
H	0.655158	2.366060	-0.277317
F	0.873742	-1.213815	1.214845
F	-2.850667	0.010863	-0.113880
H	-1.470675	0.745815	-1.373589
H	0.995215	0.451856	-1.636057
F	2.614197	0.352688	-0.449373

3_31

C	-0.748032	1.009795	-0.401116
C	-1.235305	-0.424033	-0.636661
C	-0.231448	-1.482459	-0.164843
C	0.719923	-0.931592	0.899160
C	1.531116	0.238268	0.344977
C	0.746041	1.083519	-0.671833
H	-0.794616	-2.346103	0.208127
H	0.940285	0.671774	-1.671702
H	0.148675	-0.587116	1.768513
H	1.421494	-1.704096	1.237255
H	1.090787	2.123495	-0.664975
H	-1.318834	1.712090	-1.022252
H	0.357375	-1.823305	-1.027090

F	-0.981915	1.383562	0.931624
H	-1.417505	-0.535177	-1.715290
F	-2.466459	-0.595459	0.001697
H	1.910714	0.862015	1.162727
F	2.667024	-0.269722	-0.321478

3_32

C	-0.594932	-0.763283	-0.427851
C	-1.239790	0.621538	-0.391346
C	-0.187323	1.702391	-0.091346
C	1.241556	1.223019	-0.378198
C	1.593254	0.003767	0.481636
C	0.390129	-0.916952	0.716185
H	-0.406407	2.620368	-0.648688
H	-0.110790	-0.655484	1.656876
H	1.345459	0.933833	-1.432054
H	1.960285	2.030520	-0.195280
H	0.739868	-1.952654	0.789869
H	-0.283353	1.941062	0.976390
F	-1.584772	-1.742017	-0.373523
H	-0.076444	-0.885011	-1.389133
H	-1.782145	0.808707	-1.327181
H	2.021012	0.312853	1.444060
F	-2.197472	0.641881	0.631845
F	2.601705	-0.719538	-0.183804

3_33

C	-0.909868	-0.631846	-0.526579
C	-1.110333	0.849093	-0.208204
C	0.241975	1.579679	-0.161209
C	1.347308	0.796368	-0.877438
C	1.565044	-0.576393	-0.235901
C	0.255953	-1.202855	0.265326
H	0.148868	2.592583	-0.569683
H	0.128403	-0.943869	1.323375
H	1.100598	0.661156	-1.939786
H	2.296785	1.343865	-0.836635
H	0.274471	-2.294543	0.178314
H	0.509618	1.676226	0.898743
F	-2.081843	-1.333858	-0.255997
H	-0.723782	-0.732501	-1.606001
H	-1.807158	1.293439	-0.931187
F	-1.720616	0.957036	1.047523
H	2.077971	-1.242239	-0.942867
F	2.430654	-0.427444	0.862891

3_34

C	0.641374	0.833292	-0.160111
C	1.300735	-0.473865	0.266334
C	0.267042	-1.518498	0.693128
C	-1.046939	-1.335282	-0.072382
C	-1.683114	0.009837	0.292314
C	-0.634864	1.075855	0.627328
H	0.695898	-2.513082	0.522384
H	-0.408544	1.051211	1.701944
H	-0.846434	-1.333500	-1.151717
H	-1.745987	-2.155132	0.129568
H	-1.042237	2.065875	0.392971
H	0.086797	-1.423267	1.772982
F	1.533451	1.892985	0.039400

H	0.427906	0.787305	-1.235802
F	-2.448780	0.452038	-0.802274
H	-2.381143	-0.098024	1.132881
H	2.014606	-0.264242	1.073957
F	2.041300	-0.974487	-0.816995

3_35

C	-0.851392	0.777319	0.269529
C	-1.178010	-0.531636	-0.441581
C	0.062375	-1.410928	-0.605687
C	1.046911	-1.171128	0.540067
C	1.593064	0.256022	0.481056
C	0.556914	1.247679	-0.064518
H	-0.261323	-2.457448	-0.654079
H	0.672163	1.297834	-1.155077
H	0.540716	-1.326373	1.503029
H	1.893357	-1.867018	0.499036
H	0.716894	2.254094	0.337701
H	0.551210	-1.172446	-1.559629
F	-1.775443	1.758667	-0.104267
H	-0.967694	0.624929	1.351335
H	-1.641732	-0.303447	-1.410246
F	-2.137119	-1.220631	0.320644
F	2.707927	0.281877	-0.377910
H	1.958955	0.566689	1.468525

3_36

C	-0.327196	-1.004604	-0.270469
C	-1.210288	0.251033	-0.326796
C	-0.458495	1.533122	0.005134
C	0.919468	1.480363	-0.668350
C	1.793168	0.367769	-0.053626
C	0.971647	-0.796302	0.498014
H	-1.037548	2.397415	-0.342089
H	-1.615154	0.299099	-1.347152
H	0.783028	1.291156	-1.742165
H	1.424985	2.448770	-0.574539
H	2.386683	0.757083	0.783350
H	2.495902	-0.019852	-0.801018
H	1.555110	-1.725952	0.509395
H	-0.907752	-1.830477	0.157928
H	-0.347625	1.608692	1.093131
F	0.040801	-1.354726	-1.580273
F	-2.290645	0.085267	0.547005
F	0.597904	-0.532121	1.828792

3_37

C	-0.058132	-0.923471	0.316503
C	1.361164	-0.349521	0.199948
C	1.374989	1.111719	-0.246857
C	0.157112	1.849963	0.328268
C	-1.161553	1.266129	-0.229334
C	-0.991705	-0.199535	-0.628333
H	2.312479	1.585352	0.067897
H	1.840997	-0.471049	1.179518
H	0.166331	1.754892	1.421541
H	0.226251	2.919197	0.095818
H	-1.503182	1.833122	-1.103919
H	-1.951548	1.314563	0.528718
H	-0.043742	-2.001362	0.114035

H	1.346324	1.136050	-1.344665
F	-0.494475	-0.739285	1.636168
F	2.073014	-1.127715	-0.724581
H	-0.561834	-0.291801	-1.635981
F	-2.236686	-0.834186	-0.663158

3_38

C	0.477623	-0.708707	-0.482600
C	-1.007431	-0.905329	-0.260627
C	-1.771062	0.360479	-0.658259
C	-0.940272	1.642163	-0.432533
C	0.026892	1.459327	0.742379
C	1.043925	0.354933	0.452282
H	-2.071260	0.280813	-1.711193
H	-0.361408	1.881550	-1.335366
H	-1.608497	2.492592	-0.250682
H	-0.535977	1.188403	1.643845
H	0.581526	2.381999	0.952063
H	-2.688777	0.379320	-0.057687
H	-1.358450	-1.788988	-0.807929
F	-1.221415	-1.172076	1.106771
F	1.164315	-1.911102	-0.315721
H	0.633294	-0.381615	-1.520116
H	1.392213	-0.126708	1.373289
F	2.172576	0.913783	-0.174392

3_39

C	0.218318	-0.811104	-0.202800
C	-1.183054	-0.551930	0.352919
C	-1.418400	0.917395	0.690539
C	-0.691714	1.816011	-0.313394
C	0.835243	1.626452	-0.188740
C	1.208187	0.222817	0.303224
H	-2.500655	1.095478	0.692497
H	-1.026780	1.550353	-1.324941
H	-0.954392	2.869092	-0.157247
H	1.263094	2.365872	0.498877
H	1.321057	1.767917	-1.162176
H	-1.049462	1.114598	1.707245
F	0.634746	-2.088035	0.174111
H	0.185687	-0.784104	-1.300220
H	-1.334072	-1.195158	1.229411
F	-2.116983	-0.952775	-0.616712
F	2.485616	-0.100498	-0.161185
H	1.253636	0.169883	1.400145

3_40

C	-1.678742	-0.475188	-0.161192
C	-0.483616	-1.416400	-0.313774
C	0.850416	-0.671701	-0.432782
C	0.823385	0.618722	0.362616
C	-0.226233	1.581612	-0.207693
C	-1.427474	0.855475	-0.849773
H	-0.437658	-2.063152	0.570476
H	-0.626723	-2.058637	-1.191030
H	-1.230973	0.645489	-1.910600
H	0.636080	0.387244	1.418356
H	0.278216	2.198913	-0.961038
H	-0.568088	2.248665	0.590163
H	-2.323892	1.484717	-0.801045

H	-2.598452	-0.956130	-0.518267
H	1.094515	-0.434736	-1.478405
F	-1.879476	-0.217015	1.213675
F	1.869673	-1.503712	0.037700
F	2.079865	1.231006	0.292734

3_41

C	-1.335165	-0.885058	-0.151767
C	0.117439	-1.382713	-0.059625
C	1.115033	-0.339997	-0.555104
C	0.782189	1.039541	-0.025355
C	-0.572504	1.499447	-0.583564
C	-1.467927	0.335511	-1.051526
H	0.338829	-1.598364	0.991155
H	0.247519	-2.308077	-0.632847
H	-1.194593	0.026461	-2.070733
H	-0.407274	2.191349	-1.418778
H	-1.068219	2.060229	0.216581
H	-2.516460	0.655893	-1.080883
H	-1.995669	-1.691798	-0.495440
H	1.114874	-0.283562	-1.653726
F	-1.789185	-0.530591	1.131075
F	2.406275	-0.713981	-0.173825
H	1.586274	1.744597	-0.271975
F	0.722947	0.978225	1.373672

3_42

C	-1.667462	0.250524	0.114275
C	-0.752287	1.317482	-0.493373
C	0.729232	0.949911	-0.401986
C	0.894645	-0.553158	-0.496734
C	0.281685	-1.255432	0.715460
C	-0.984560	-0.530391	1.225862
H	-1.041507	1.460918	-1.541564
H	-0.891854	2.271735	0.028782
H	-0.714297	0.188881	2.009077
H	1.042193	-1.272596	1.503847
H	0.053578	-2.292175	0.445855
H	-1.692317	-1.248462	1.656245
H	-2.606723	0.702358	0.458203
F	-2.026004	-0.663232	-0.906198
H	0.414819	-0.881606	-1.427601
F	2.251461	-0.881788	-0.595001
F	1.230486	1.382910	0.840949
H	1.325105	1.456330	-1.171612

3_43

C	1.307273	-0.795271	-0.104201
C	0.140292	-0.972638	-1.084829
C	-1.171750	-0.363561	-0.604987
C	-0.968440	0.938086	0.161041
C	-0.028010	0.774661	1.361167
C	0.833845	-0.499829	1.308801
H	0.424357	-0.508326	-2.036046
H	-0.039703	-2.038578	-1.271571
H	0.253437	-1.365305	1.651661
H	-0.614842	0.779917	2.286899
H	0.615809	1.661674	1.373009
H	1.702812	-0.392198	1.969538
H	1.958282	-1.678965	-0.123888

F	2.105384	0.284450	-0.533767
F	-1.809738	-1.252277	0.285416
H	-1.859722	-0.209214	-1.445892
H	-1.939611	1.342123	0.472907
F	-0.426766	1.847849	-0.762601

3_44

C	-1.573173	0.018739	-0.351562
C	-0.658242	1.206622	-0.034810
C	0.754935	0.765714	0.364909
C	1.153857	-0.494235	-0.379120
C	0.230843	-1.665066	-0.006714
C	-1.167932	-1.205246	0.450589
H	-0.571266	1.869862	-0.903420
H	-1.114687	1.778291	0.781501
H	-1.165652	-0.940568	1.516498
H	0.724756	-2.220890	0.798830
H	0.145976	-2.340581	-0.865908
H	-1.900906	-2.008534	0.311179
F	2.470389	-0.833425	-0.054961
H	1.140861	-0.284532	-1.458191
H	0.838035	0.582670	1.444849
F	1.649297	1.794717	0.061391
F	-2.896340	0.374887	-0.057593
H	-1.548951	-0.220501	-1.424626

3_45

C	-1.350939	-0.200396	0.350248
C	-0.254495	-1.234225	0.063024
C	0.974288	-0.580836	-0.574247
C	1.188819	0.818626	-0.036039
C	0.041028	1.723798	-0.489546
C	-1.294511	0.960914	-0.632728
H	0.061743	-1.729605	0.986978
H	-0.662871	-1.994116	-0.613584
H	-1.404249	0.555596	-1.648141
H	0.308939	2.190061	-1.445765
H	-0.046309	2.526234	0.252494
H	-2.141080	1.634650	-0.456431
H	0.858838	-0.499602	-1.664604
F	2.101493	-1.374222	-0.347323
F	-2.602306	-0.828723	0.250883
H	-1.266490	0.174852	1.377271
H	2.167499	1.209595	-0.340946
F	1.200683	0.759062	1.370713

3_46

C	1.495755	0.223600	-0.405489
C	0.797806	-1.138188	-0.503930
C	-0.693784	-1.050815	-0.169628
C	-1.222669	0.312600	-0.568503
C	-0.597739	1.423427	0.280056
C	0.862965	1.098541	0.665400
H	0.932499	-1.563309	-1.506039
H	1.265562	-1.818571	0.217531
H	0.893186	0.554334	1.616431
H	-1.209006	1.531910	1.182401
H	-0.655158	2.366060	-0.277317
H	1.448586	2.018202	0.779708
F	2.850667	0.010863	-0.113880

H	1.470675	0.745815	-1.373589
H	-0.995215	0.451856	-1.636057
F	-2.614197	0.352688	-0.449373
F	-0.873742	-1.213815	1.214845
H	-1.269684	-1.848912	-0.654822

3_47

C	-1.301139	-0.281278	-0.286070
C	-0.541362	0.940536	-0.809323
C	0.912715	0.979506	-0.336040
C	1.454797	-0.419171	-0.063947
C	0.659835	-1.135619	1.026894
C	-0.814516	-0.685572	1.095773
H	-0.578016	0.973245	-1.903826
H	-1.035734	1.842046	-0.426255
H	-0.919191	0.177800	1.764125
H	1.146580	-0.961448	1.993120
H	0.731276	-2.209341	0.811716
H	-1.444938	-1.494308	1.483893
F	-2.668399	0.035325	-0.231309
H	-1.203054	-1.125777	-0.979920
F	1.002046	1.673689	0.886226
H	1.548038	1.515203	-1.051969
H	2.524080	-0.387472	0.178740
F	1.334017	-1.122387	-1.280845

3_48

C	-0.341670	1.463671	0.242035
C	1.151531	1.116224	0.220017
C	1.389087	-0.391276	0.321493
C	0.281377	-1.172188	-0.368116
C	-1.015395	-0.985656	0.421443
C	-1.155186	0.428473	1.004684
H	1.571430	1.468643	-0.729788
H	1.671070	1.639061	1.032679
H	-0.806567	0.429846	2.047297
H	0.134029	-0.782749	-1.381836
H	0.548204	-2.233341	-0.430570
H	-1.072451	-1.717841	1.238863
H	-2.217286	0.699951	1.007464
H	-0.498549	2.467552	0.658429
H	1.460332	-0.703308	1.374710
F	-0.819713	1.509744	-1.082174
F	2.626446	-0.699786	-0.259257
F	-2.101031	-1.256992	-0.421523

3_49

C	0.219547	1.533678	-0.405668
C	-1.165121	0.900959	-0.581950
C	-1.149139	-0.600947	-0.292886
C	-0.168175	-0.929668	0.817980
C	1.260810	-0.634413	0.359340
C	1.340716	0.532713	-0.634859
H	-1.853886	1.382450	0.122837
H	-1.535874	1.089924	-1.597022
H	1.234103	0.122066	-1.648006
H	-0.403320	-0.319126	1.698194
H	-0.240698	-1.987880	1.094475
H	2.317043	1.026275	-0.572664
H	0.332298	2.409406	-1.057157

H	-0.888157	-1.172049	-1.194726
F	0.339998	2.015336	0.918825
F	-2.441077	-1.006694	0.071204
H	1.901853	-0.453239	1.229353
F	1.779391	-1.776615	-0.284143

3_50

C	-0.148642	1.421966	0.423570
C	1.240601	1.151753	-0.157088
C	1.450065	-0.313084	-0.543701
C	0.146425	-0.999489	-0.915582
C	-0.799673	-1.032258	0.287584
C	-0.695403	0.217150	1.171146
H	1.372290	1.792345	-1.037752
H	2.011144	1.424480	0.574590
H	-0.016453	0.009586	2.008159
H	-0.334531	-0.421706	-1.713847
H	0.334537	-2.014993	-1.282417
H	-1.688321	0.438762	1.579449
H	-0.132561	2.310742	1.068271
F	-1.026451	1.725738	-0.639103
F	-2.113805	-1.160716	-0.191963
H	-0.609016	-1.923120	0.897543
H	2.192976	-0.400533	-1.346326
F	1.996889	-0.997443	0.570706

3_51

C	0.852188	-0.983598	-0.310075
C	-0.638759	-1.313506	-0.170650
C	-1.428107	-0.103105	0.338589
C	-0.832351	1.202631	-0.169099
C	0.578267	1.396735	0.402783
C	1.277105	0.068530	0.701101
H	-1.060485	-1.615437	-1.136871
H	-0.740604	-2.156873	0.522979
H	1.014077	-0.272664	1.711842
H	-0.757644	1.159133	-1.263464
H	-1.481998	2.044859	0.093655
H	2.361853	0.222302	0.666543
H	0.555167	2.015806	1.308508
H	1.084395	-0.630230	-1.323277
F	1.599591	-2.153626	-0.116660
F	-2.756969	-0.206510	-0.093014
H	-1.463875	-0.095172	1.437183
F	1.339495	2.107042	-0.542881

4_1

C	-0.629061	-1.273132	0.433375
C	0.629061	-1.273132	-0.433375
C	0.768196	0.000000	-1.254627
C	0.629061	1.273132	-0.433375
C	-0.629061	1.273132	0.433375
C	-0.768196	0.000000	1.254627
H	1.732000	0.000000	-1.777602
H	0.612953	-2.150945	-1.092476
H	-0.612953	-2.150945	1.092476
H	0.612953	2.150945	-1.092476
H	-0.612953	2.150945	1.092476
H	0.031563	0.000000	2.006726

H	-1.732000	0.000000	1.777602
H	-0.031563	0.000000	-2.006726
F	-1.721264	-1.419716	-0.432788
F	1.721264	-1.419716	0.432788
F	1.721264	1.419716	0.432788
F	-1.721264	1.419716	-0.432788

4_2

C	1.502777	-0.496800	0.148928
C	1.208565	0.891403	-0.418894
C	-0.226118	1.029378	-0.902891
C	-1.186400	0.670751	0.221172
C	-0.973693	-0.758251	0.693249
C	0.463876	-0.946277	1.169987
H	-0.408581	2.055814	-1.241037
H	1.923589	1.120275	-1.218623
H	2.501260	-0.493114	0.605410
H	0.610828	-0.353253	2.082559
H	0.634464	-2.000159	1.419643
H	-0.381888	0.345011	-1.745412
F	1.539274	-1.381602	-0.934234
F	1.436123	1.807793	0.626804
H	-1.687140	-1.001111	1.492266
H	-1.035341	1.340405	1.078638
F	-2.503368	0.834154	-0.209845
F	-1.237721	-1.633132	-0.365252

4_3

C	0.614513	0.453717	-1.472830
C	-0.614513	-0.453717	-1.472830
C	-0.699664	-1.288640	-0.207018
C	-0.629686	-0.422389	1.046307
C	0.629686	0.422389	1.046307
C	0.699664	1.288640	-0.207018
H	-1.629286	-1.869330	-0.204119
H	-0.607729	-1.091097	-2.365753
H	0.607729	1.091097	-2.365753
H	-0.143203	1.991821	-0.200717
H	1.629286	1.869330	-0.204119
H	0.143203	-1.991821	-0.200717
F	1.737547	-0.387169	-1.559089
F	-1.737547	0.387169	-1.559089
H	-1.505302	0.234882	1.127442
F	-0.629686	-1.261028	2.164021
F	0.629686	1.261028	2.164021
H	1.505302	-0.234882	1.127442

4_4

C	-1.096212	-0.593052	-0.776676
C	-1.100162	-0.583651	0.744074
C	0.314251	-0.601254	1.311729
C	1.096212	0.593052	0.776676
C	1.100162	0.583651	-0.744074
C	-0.314251	0.601254	-1.311729
H	0.275617	-0.560641	2.405952
H	-2.124649	-0.615199	-1.158582

H	-0.810159	1.533296	-1.013990
H	-0.275617	0.560641	-2.405952
H	0.810159	-1.533296	1.013990
F	-0.470849	-1.771330	-1.220084
H	-1.630200	0.318728	1.076198
F	-1.809516	-1.687380	1.219345
F	0.470849	1.771330	1.220084
H	2.124649	0.615199	1.158582
H	1.630200	-0.318728	-1.076198
F	1.809516	1.687380	-1.219345

4_5

C	0.767613	-0.395035	1.276273
C	-0.753430	-0.400572	1.229400
C	-1.277994	0.327263	0.000000
C	-0.753430	-0.400572	-1.229400
C	0.767613	-0.395035	-1.276273
C	1.344644	-1.006486	0.000000
H	-2.373785	0.320122	0.000000
H	1.114613	-0.945709	2.161165
H	1.137570	-2.085960	0.000000
H	2.432904	-0.875609	0.000000
H	-0.922253	1.363377	0.000000
F	1.214128	0.919777	1.412793
H	-1.083024	-1.451587	1.215283
F	-1.264557	0.174405	2.390294
F	-1.264557	0.174405	-2.390294
H	-1.083024	-1.451587	-1.215283
H	1.114613	-0.945709	-2.161165
F	1.214128	0.919777	-1.412793

4_6

C	-1.204759	-1.015170	-0.159998
C	-1.382879	0.437478	-0.572841
C	-0.365003	1.334250	0.115824
C	1.047840	0.873103	-0.225129
C	1.254809	-0.582645	0.153315
C	0.205039	-1.477807	-0.500974
H	-0.501738	2.373024	-0.204801
H	-1.967286	-1.643340	-0.637954
H	0.343388	-1.452438	-1.590644
H	0.349345	-2.511713	-0.168278
H	-0.514739	1.281036	1.200711
F	-1.391078	-1.121127	1.225747
H	-1.267689	0.490512	-1.666172
F	-2.674476	0.864231	-0.271355
H	1.230702	-0.677042	1.246282
F	2.517706	-0.996956	-0.278596
F	1.963510	1.668680	0.464045
H	1.256776	0.991256	-1.298910

4_7

C	-0.629456	0.423603	1.260262
C	0.629456	-0.423603	1.260262
C	0.698085	-1.277072	0.000000
C	0.629456	-0.423603	-1.260262
C	-0.629456	0.423603	-1.260262
C	-0.698085	1.277072	0.000000

H	0.145496	1.980652	0.000000
H	-1.623576	1.863550	0.000000
F	-0.629456	1.264756	2.373163
H	-1.503068	-0.238217	1.348320
H	-0.145496	-1.980652	0.000000
H	1.623576	-1.863550	0.000000
F	0.629456	-1.264756	2.373163
H	1.503068	0.238217	1.348320
F	-0.629456	1.264756	-2.373163
H	-1.503068	-0.238217	-1.348320
H	1.503068	0.238217	-1.348320
F	0.629456	-1.264756	-2.373163

4_8

C	-0.270837	0.514962	1.285221
C	-0.836726	1.117237	0.000000
C	-0.270837	0.514962	-1.285221
C	-0.270837	-1.006923	-1.265711
C	0.329994	-1.607990	0.000000
C	-0.270837	-1.006923	1.265711
H	-0.877086	0.877929	-2.126649
H	-0.691016	2.204385	0.000000
H	-0.877086	0.877929	2.126649
H	-1.315607	-1.339175	-1.335926
H	0.264374	-1.380586	-2.146788
H	0.169502	-2.695440	0.000000
H	-1.315607	-1.339175	1.335926
H	0.264374	-1.380586	2.146788
F	1.022604	1.006807	1.459341
F	-2.215466	0.848501	0.000000
F	1.022604	1.006807	-1.459341
F	1.716771	-1.415141	0.000000

4_9

C	0.670857	-0.081546	1.284942
C	1.436270	0.237111	0.000000
C	0.670857	-0.081546	-1.284942
C	-0.761886	0.427928	-1.253782
C	-1.478812	-0.050944	0.000000
C	-0.761886	0.427928	1.253782
H	1.220093	0.350139	-2.131788
H	2.398306	-0.289742	0.000000
H	1.220093	0.350139	2.131788
H	-0.741542	1.525823	-1.255236
H	-1.289362	0.089601	-2.153440
H	-0.741542	1.525823	1.255236
H	-1.289362	0.089601	2.153440
F	0.670857	-1.472937	1.446645
F	1.678201	1.617788	0.000000
F	0.670857	-1.472937	-1.446645
F	-2.782879	0.464688	0.000000
H	-1.562404	-1.144400	0.000000

4_10

C	0.498451	1.394565	-0.015367
C	-0.939675	0.891398	-0.145895
C	-0.952487	-0.576202	-0.531523
C	-0.246858	-1.426111	0.513080
C	1.200148	-0.968870	0.666100

C	1.317081	0.528556	0.933701
H	-1.504013	1.490399	-0.871141
H	0.486916	2.434519	0.335773
H	-0.764292	-1.319031	1.474408
H	-0.272466	-2.480577	0.215962
H	0.955118	0.720928	1.952440
H	2.369622	0.831794	0.882988
F	1.059672	1.391348	-1.298017
F	-1.541307	1.058693	1.108667
H	-0.456477	-0.674871	-1.504866
F	-2.274272	-1.003179	-0.679843
F	1.892776	-1.284096	-0.517265
H	1.693815	-1.528063	1.471978

4_11

C	-0.041730	1.525758	0.129710
C	-1.236885	0.573834	0.207437
C	-0.961534	-0.685921	-0.596530
C	0.295654	-1.393029	-0.112639
C	1.477175	-0.439863	-0.249449
C	1.255197	0.844521	0.539575
H	-2.153228	1.063798	-0.144304
H	-0.235230	2.407468	0.752591
H	0.174266	-1.678133	0.939282
H	0.465744	-2.297471	-0.707948
H	1.193317	0.597777	1.607347
H	2.094011	1.534456	0.390247
F	0.052689	1.960636	-1.204667
F	-1.410905	0.249467	1.556076
F	2.633980	-1.068477	0.227262
H	1.654348	-0.206043	-1.308202
H	-0.854489	-0.389810	-1.649265
F	-2.060875	-1.539831	-0.510712

4_12

C	-0.391114	0.373101	1.276081
C	-1.035920	0.893696	0.000000
C	-0.391114	0.373101	-1.276081
C	-0.391114	-1.153711	-1.272643
C	0.190706	-1.765217	0.000000
C	-0.391114	-1.153711	1.272643
H	-0.955793	0.754698	2.138588
H	-1.429651	-1.500238	-1.373949
H	0.169548	-1.517622	-2.141736
H	-1.429651	-1.500238	1.373949
H	0.169548	-1.517622	2.141736
F	0.907247	0.854254	1.400089
F	1.579963	-1.609769	0.000000
H	0.000034	-2.847953	0.000000
H	-2.078833	0.538786	0.000000
F	-1.064610	2.282587	0.000000
F	0.907247	0.854254	-1.400089
H	-0.955793	0.754698	-2.138588

4_13

C	-0.271902	0.514982	1.278013
C	-0.903695	1.051468	0.000000

C	-0.271902	0.514982	-1.278013
C	-0.271902	-1.009994	-1.260897
C	0.407246	-1.530734	0.000000
C	-0.271902	-1.009994	1.260897
H	-0.825486	0.905513	2.142279
H	-1.308059	-1.375482	-1.284361
H	0.243118	-1.385093	-2.152802
H	-1.308059	-1.375482	1.284361
H	0.243118	-1.385093	2.152802
F	1.042325	0.970988	1.397717
H	-1.954448	0.722233	0.000000
F	-0.894789	2.440370	0.000000
F	1.042325	0.970988	-1.397717
H	-0.825486	0.905513	-2.142279
F	0.340306	-2.931448	0.000000
H	1.468152	-1.254464	0.000000

4_14

C	-0.133307	-1.365302	0.405791
C	1.074881	-0.438997	0.456037
C	0.798137	0.854205	-0.287810
C	-0.399352	1.565175	0.332106
C	-1.641972	0.684438	0.351039
C	-1.374533	-0.684698	0.970959
H	0.093797	-2.288895	0.955085
H	-0.145263	1.838083	1.366087
H	-0.606910	2.489119	-0.219761
H	-1.237637	-0.550295	2.053321
H	-2.244602	-1.334221	0.819184
F	-0.361661	-1.729047	-0.924231
H	1.306949	-0.205841	1.506085
F	2.177564	-1.087959	-0.086158
H	0.639561	0.642893	-1.351344
F	1.914105	1.688950	-0.178490
F	-2.096566	0.520630	-0.966337
H	-2.449998	1.187070	0.899556

4_15

C	-0.255115	-1.398528	-0.323162
C	-1.162380	-0.191501	-0.522047
C	-0.722407	0.972694	0.348648
C	0.733051	1.328206	0.066342
C	1.637385	0.117479	0.257613
C	1.197122	-1.050579	-0.616971
H	-0.611201	-2.231732	-0.941884
H	0.818554	1.673389	-0.973129
H	1.046364	2.146771	0.724495
H	1.300524	-0.765739	-1.672947
H	1.831014	-1.925484	-0.432473
F	-0.351908	-1.810005	1.016852
H	-1.125875	0.115438	-1.577429
F	-2.474110	-0.544647	-0.226681
F	2.947822	0.472751	-0.085669
H	1.652807	-0.188883	1.311411
H	-0.881747	0.714563	1.403142
F	-1.521402	2.081350	0.061752

4_16

C	-1.234693	-0.281646	-0.471147
C	0.000000	-1.155529	-0.311264

C	1.234693	-0.281646	-0.471147
C	1.271713	0.804491	0.595365
C	0.000000	1.644277	0.541982
C	-1.271713	0.804491	0.595365
H	0.000000	-1.982716	-1.032457
H	1.350738	0.331483	1.581723
H	2.145994	1.447009	0.442100
H	-1.350738	0.331483	1.581723
H	-2.145994	1.447009	0.442100
F	0.000000	-1.719150	0.968456
H	1.218697	0.166038	-1.473750
F	2.380782	-1.071934	-0.384310
F	0.000000	2.362496	-0.676231
H	0.000000	2.391728	1.344929
H	-1.218697	0.166038	-1.473750
F	-2.380782	-1.071934	-0.384310

4_17

C	0.714162	0.229970	1.235231
C	0.661904	1.118406	0.000000
C	0.714162	0.229970	-1.235231
C	-0.461277	-0.737171	-1.265116
C	-0.445400	-1.588960	0.000000
C	-0.461277	-0.737171	1.265116
H	1.483940	1.845705	0.000000
H	-1.396460	-0.166634	-1.308107
H	-0.394193	-1.376371	-2.152848
H	-1.396460	-0.166634	1.308107
H	-0.394193	-1.376371	2.152848
F	-0.534553	1.835068	0.000000
F	-1.561806	-2.430446	0.000000
H	0.441491	-2.241618	0.000000
H	1.667276	-0.320420	-1.221638
F	0.714162	1.021716	-2.381080
F	0.714162	1.021716	2.381080
H	1.667276	-0.320420	1.221638

4_18

C	0.296772	1.253888	0.151651
C	1.097906	0.000000	-0.160314
C	0.296772	-1.253888	0.151651
C	-1.046028	-1.260154	-0.566971
C	-1.840563	0.000000	-0.257158
C	-1.046028	1.260154	-0.566971
H	-0.871016	-1.309749	-1.650385
H	-1.614403	-2.149820	-0.272748
H	-0.871016	1.309749	-1.650385
H	-1.614403	2.149820	-0.272748
H	1.396107	0.000000	-1.218391
F	2.259970	0.000000	0.607227
H	0.162479	-1.330734	1.238024
F	1.031447	-2.369230	-0.257998
F	-2.157285	0.000000	1.117510
H	-2.793410	0.000000	-0.801372
H	0.162479	1.330734	1.238024
F	1.031447	2.369230	-0.257998

4_19

C	-0.452480	-1.254849	0.257147
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C	-1.174989	0.000000	-0.209353
C	-0.452480	1.254849	0.257147
C	1.012901	1.254156	-0.155520
C	1.699773	0.000000	0.365155
C	1.012901	-1.254156	-0.155520
H	1.081188	1.269673	-1.251371
H	1.504152	2.153544	0.233290
H	1.081188	-1.269673	-1.251371
H	1.504152	-2.153544	0.233290
H	-1.255267	0.000000	-1.305141
F	-2.465838	0.000000	0.313410
F	3.034512	0.000000	-0.050647
H	1.709293	0.000000	1.465609
H	-0.556635	1.334016	1.348983
F	-1.083514	2.368702	-0.296748
F	-1.083514	-2.368702	-0.296748
H	-0.556635	-1.334016	1.348983

4_20

C	0.249522	1.462378	0.311869
C	-0.126731	0.754574	-0.990036
C	0.126731	-0.754574	-0.990036
C	-0.249522	-1.462378	0.311869
C	0.249522	-0.723984	1.541300
C	-0.249522	0.723984	1.541300
H	-0.428868	-1.201602	-1.824240
H	0.428868	1.201602	-1.824240
H	-0.140646	2.487993	0.273450
H	0.140646	-2.487993	0.273450
H	-0.087381	-1.255422	2.439302
H	1.346821	-0.742986	1.526171
H	-1.346821	0.742986	1.526171
H	0.087381	1.255422	2.439302
F	1.649448	1.544920	0.353587
F	-1.492571	0.963503	-1.197306
F	1.492571	-0.963503	-1.197306
F	-1.649448	-1.544920	0.353587

4_21

C	1.577906	0.331987	-0.068111
C	0.874740	-1.027513	-0.059592
C	-0.610795	-0.955213	0.300843
C	-1.312799	0.122435	-0.509896
C	-0.660077	1.479658	-0.312777
C	0.789097	1.399321	-0.810828
H	-1.081967	-1.931953	0.129753
H	1.388466	-1.707640	0.630612
H	2.573006	0.199526	-0.513621
H	-1.219847	2.238566	-0.871727
H	-0.685595	1.743110	0.751069
H	0.807448	1.143573	-1.879600
H	1.301659	2.361256	-0.690553
F	1.760208	0.724136	1.262807
F	0.966186	-1.549760	-1.357597
F	-0.707624	-0.664103	1.659824
H	-1.264941	-0.170008	-1.568745
F	-2.659511	0.158563	-0.145592

4_22

C	-1.513154	-0.465159	0.310201
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C	-0.158174	-1.170774	0.215662
C	0.748083	-0.440221	-0.764238
C	0.910573	1.043059	-0.469186
C	-0.460277	1.708994	-0.412279
C	-1.360945	1.015043	0.616694
H	-0.287710	-2.210503	-0.111741
H	-2.133416	-0.970099	1.061266
H	-0.330127	2.767189	-0.156951
H	-0.919147	1.657895	-1.408408
H	-0.921064	1.105463	1.617869
H	-2.353959	1.479929	0.637300
F	-2.146226	-0.625904	-0.937350
F	0.390558	-1.192352	1.494873
F	1.986125	-1.070406	-0.825847
H	0.276290	-0.521332	-1.753841
H	1.550034	1.494117	-1.240060
F	1.560929	1.227739	0.754262

4_23

C	1.700690	0.079490	-0.054963
C	0.599682	1.138865	-0.052423
C	-0.727349	0.555355	-0.515132
C	-1.132411	-0.634088	0.337159
C	-0.045707	-1.702007	0.298756
C	1.299687	-1.134935	0.766433
H	0.870874	1.998497	-0.677580
H	2.635540	0.521066	0.312586
H	-0.349887	-2.546000	0.928841
H	0.041839	-2.068687	-0.732085
H	1.239948	-0.820007	1.816687
H	2.086565	-1.894712	0.688823
F	1.906395	-0.297666	-1.392680
F	0.476142	1.590131	1.267235
H	-1.334806	-0.298012	1.362379
F	-2.319032	-1.168378	-0.171976
F	-1.699947	1.549177	-0.460195
H	-0.629652	0.232391	-1.560076

4_24

C	1.321713	0.849106	-0.208441
C	0.928944	-0.521851	-0.745862
C	-0.388862	-1.040599	-0.184264
C	-1.475965	-0.011696	-0.472719
C	-1.137185	1.331465	0.153233
C	0.186204	1.844048	-0.432869
H	2.244243	1.175826	-0.707567
H	-1.947803	2.041383	-0.048321
H	-1.046943	1.205245	1.238372
H	0.082393	2.016560	-1.514323
H	0.465808	2.799148	0.026589
F	1.601809	0.773917	1.155555
H	-0.636839	-2.008691	-0.640092
H	0.804722	-0.415948	-1.834766
F	-0.292540	-1.240661	1.186690
F	1.941396	-1.446077	-0.525770
F	-2.695365	-0.488095	0.004684
H	-1.572372	0.091881	-1.564786

4_25

C	-0.289214	1.433698	-0.483203
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C	0.214335	0.728929	0.769466
C	-0.214335	-0.728929	0.769466
C	0.289214	-1.433698	-0.483203
C	-0.209162	-0.738207	-1.741778
C	0.209162	0.738207	-1.741778
H	-0.002490	2.492639	-0.450893
H	0.199885	-1.253308	-2.618804
H	-1.303023	-0.818055	-1.781954
H	1.303023	0.818055	-1.781954
H	-0.199885	1.253308	-2.618804
F	-1.695050	1.392414	-0.478711
H	1.309563	0.787759	0.806524
F	-0.289214	1.367035	1.898513
H	-1.309563	-0.787759	0.806524
F	0.289214	-1.367035	1.898513
H	0.002490	-2.492639	-0.450893
F	1.695050	-1.392414	-0.478711

4_26

C	-1.520287	-0.603263	-0.235712
C	-0.848823	0.740602	-0.469200
C	0.515533	0.816715	0.199694
C	1.399650	-0.337707	-0.248522
C	0.730864	-1.686422	-0.027188
C	-0.630256	-1.734802	-0.730652
H	-2.507744	-0.609421	-0.715107
H	1.391354	-2.477441	-0.400946
H	0.596340	-1.840169	1.050515
H	-0.509444	-1.637555	-1.819221
H	-1.127511	-2.692292	-0.537300
F	-1.729691	-0.766121	1.141703
H	-0.724937	0.890333	-1.551708
F	-1.658540	1.765088	0.006348
F	2.596700	-0.287566	0.467645
H	1.650716	-0.192592	-1.309861
H	0.404802	0.809988	1.290946
F	1.118901	2.019533	-0.164345

4_27

C	-0.679332	-1.281133	0.268543
C	-0.005912	-0.764945	-0.994934
C	0.005912	0.764945	-0.994934
C	0.679332	1.281133	0.268543
C	-0.005912	0.768479	1.526224
C	0.005912	-0.768479	1.526224
H	0.510577	1.154095	-1.887726
H	-0.510577	-1.154095	-1.887726
H	0.516114	1.160658	2.406518
H	-1.036182	1.146343	1.545908
H	1.036182	-1.146343	1.545908
H	-0.516114	-1.160658	2.406518
F	1.325854	-1.191592	-1.034578
F	-1.325854	1.191592	-1.034578
H	1.726690	0.950687	0.245707
F	0.676048	2.676951	0.244644
H	-1.726690	-0.950687	0.245707
F	-0.676048	-2.676951	0.244644

4_28

C	-1.487510	0.253190	-0.528832
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C	-0.639569	-0.968560	-0.206655
C	0.821627	-0.666618	-0.508746
C	1.302485	0.522407	0.307171
C	0.423939	1.742547	0.048218
C	-1.058014	1.444036	0.313880
H	-0.978891	-1.848800	-0.767277
H	0.771372	2.569604	0.677879
H	0.566241	2.045853	-0.999068
H	-1.224322	1.202744	1.370713
H	-1.675932	2.312989	0.060242
F	-0.765759	-1.264440	1.153188
H	1.314750	0.249966	1.369819
F	2.615211	0.820639	-0.068286
F	1.590575	-1.790157	-0.230043
H	0.937736	-0.438920	-1.578339
H	-1.374137	0.481681	-1.599465
F	-2.830535	-0.047946	-0.308718

4_29

C	0.431567	-1.402944	-0.492793
C	-0.096788	-0.755275	0.776637
C	0.096788	0.755275	0.776637
C	-0.431567	1.402944	-0.492793
C	0.157338	0.749238	-1.733238
C	-0.157338	-0.749238	-1.733238
H	-0.253820	1.236294	-2.624843
H	1.244131	0.913449	-1.736957
H	-1.244131	-0.913449	-1.736957
H	0.253820	-1.236294	-2.624843
H	-1.163707	-0.991974	0.891061
F	0.571700	-1.283931	1.878023
F	-0.096788	2.757756	-0.470716
H	-1.529085	1.337176	-0.498657
H	1.163707	0.991974	0.891061
F	-0.571700	1.283931	1.878023
H	1.529085	-1.337176	-0.498657
F	0.096788	-2.757756	-0.470716

4_30

C	1.573812	-0.396430	0.129015
C	0.840588	0.946620	0.158309
C	-0.641307	0.823138	-0.184607
C	-1.193173	-0.527691	0.238654
C	-0.500897	-1.666409	-0.521159
C	0.962455	-1.340294	-0.887286
H	0.944102	1.393911	1.154380
H	1.018183	-0.838462	-1.863214
H	-1.087631	-0.639243	1.324751
H	-1.080444	-1.846052	-1.434570
H	-0.548777	-2.576747	0.085000
H	1.557300	-2.257974	-0.957875
H	2.638470	-0.210271	-0.057875
H	-0.778515	0.953708	-1.266867
F	1.458956	-0.968236	1.409231
F	1.452660	1.791983	-0.772357
F	-1.340704	1.845011	0.453223
F	-2.561085	-0.559032	-0.043573

4_31

C	1.061414	1.043935	0.088721
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C	-0.463829	0.992458	0.276587
C	-1.097140	-0.196821	-0.429075
C	-0.266270	-1.450703	-0.237890
C	1.111312	-1.291339	-0.894757
C	1.530381	0.180865	-1.069917
H	-0.696460	0.953931	1.346115
H	1.092984	0.601222	-1.986573
H	1.110870	-1.790883	-1.871190
H	1.827451	-1.817505	-0.253961
H	2.619661	0.259919	-1.166017
H	1.343758	2.094557	-0.055371
H	-1.170695	0.020906	-1.503987
F	1.677937	0.599657	1.264386
F	-1.015120	2.162565	-0.258449
F	-2.390907	-0.391331	0.046266
H	-0.809447	-2.317444	-0.634138
F	-0.113390	-1.668121	1.139254

4_32

C	-1.395002	-0.680447	0.133857
C	-1.018299	0.650298	-0.538490
C	0.457436	1.009342	-0.357631
C	1.258210	-0.270363	-0.511462
C	1.027642	-1.205111	0.678097
C	-0.417576	-1.102282	1.216228
H	-1.224907	0.547476	-1.611761
H	-0.470977	-0.346742	2.009024
H	1.737047	-0.920875	1.462694
H	1.256936	-2.230821	0.370213
H	-0.743683	-2.059826	1.638314
H	-2.420562	-0.599539	0.513834
F	-1.394947	-1.666994	-0.874990
F	-1.811083	1.674204	-0.033235
H	0.950889	-0.749851	-1.451124
F	2.617362	0.028013	-0.629056
F	0.662723	1.540204	0.917747
H	0.774303	1.772710	-1.078977

4_33

C	-1.366846	-0.436909	0.285114
C	-0.653914	0.658516	-0.501175
C	0.683878	0.999620	0.117455
C	1.635518	-0.203209	0.045988
C	0.894499	-1.540344	0.039938
C	-0.377499	-1.435345	0.890217
H	-0.476070	0.299318	-1.524077
H	-0.122184	-1.107464	1.905457
H	1.552749	-2.335543	0.407599
H	0.629746	-1.784324	-0.997196
H	-0.879394	-2.406500	0.967872
H	-1.997309	0.023017	1.054836
F	-2.220725	-1.110977	-0.603307
F	-1.455657	1.793917	-0.586041
F	0.495601	1.327180	1.468788
H	1.135721	1.865585	-0.380331
H	2.319281	-0.126828	0.900821
F	2.396741	-0.085812	-1.123907

4_34

C	1.429324	0.611082	0.363344
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C	0.995657	-0.855768	0.334005
C	-0.503314	-1.037761	0.051892
C	-1.071824	0.165791	-0.671207
C	-0.957755	1.430338	0.182077
C	0.341067	1.445729	1.022871
H	0.151536	1.022688	2.018190
H	-0.525606	0.272726	-1.615922
H	-1.828461	1.460690	0.846313
H	-1.002181	2.306109	-0.473474
H	0.700183	2.471631	1.159858
H	2.397706	0.705508	0.870521
F	1.620571	1.069355	-0.948900
F	-2.411925	-0.068750	-0.990357
H	1.187009	-1.288563	1.324658
F	1.742399	-1.556342	-0.606320
H	-0.666787	-1.960902	-0.516564
F	-1.152415	-1.171636	1.288746

4_35

C	1.323100	0.061672	-0.611640
C	0.670419	-0.907520	0.351652
C	-0.852478	-0.877860	0.169394
C	-1.356715	0.478376	-0.311458
C	-0.504010	1.606807	0.250417
C	0.940354	1.508097	-0.290210
H	1.041128	-1.928966	0.203897
H	1.646487	1.879345	0.460272
H	-1.351362	0.490640	-1.410486
H	-0.507057	1.533643	1.344387
H	-0.960035	2.564585	-0.023366
H	1.062271	2.115677	-1.194472
H	-1.325544	-1.119793	1.129048
F	0.962932	-0.526719	1.666087
F	-1.201742	-1.862099	-0.759925
F	-2.685909	0.634639	0.091051
H	0.998142	-0.222945	-1.623146
F	2.710491	-0.082446	-0.578887

4_36

C	1.172372	-0.402442	0.467489
C	0.445175	0.932392	0.265210
C	-0.911677	0.717680	-0.410718
C	-1.474105	-0.666139	-0.165327
C	-0.551991	-1.728115	-0.772399
C	0.940633	-1.330146	-0.715225
H	0.311299	1.459974	1.216632
H	1.247352	-0.809013	-1.631454
H	-0.853695	-1.907791	-1.811465
H	-0.728491	-2.656183	-0.216064
H	1.573063	-2.218789	-0.612829
H	-0.763568	0.835951	-1.493267
F	1.210918	1.749701	-0.568769
F	-1.812868	1.695157	0.002473
H	-2.493153	-0.735885	-0.564391
F	-1.575350	-0.869325	1.224840
F	2.531334	-0.158178	0.642505
H	0.798440	-0.863826	1.389216

4_37

C	1.164297	0.516009	-0.253907
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C	0.706772	-0.831901	0.279456
C	-0.816310	-0.919014	0.456678
C	-1.567822	0.109726	-0.378726
C	-1.135280	1.537539	-0.054167
C	0.342274	1.629252	0.379941
H	0.425665	1.538851	1.470635
H	-1.779539	1.931644	0.739780
H	-1.318442	2.135558	-0.955251
H	0.772794	2.594855	0.092547
H	1.166280	-0.990628	1.264163
F	1.127136	-1.854878	-0.568587
H	-1.141532	-1.938721	0.219149
F	-1.129823	-0.652543	1.796911
F	-1.259183	-0.184599	-1.719442
H	-2.651073	-0.017749	-0.262514
F	2.515013	0.688611	0.069225
H	1.083969	0.527192	-1.347117

4_38

C	-0.058853	-1.382848	0.077295
C	1.216433	-0.535638	0.186498
C	0.975100	0.919251	-0.186684
C	-0.418533	1.358522	0.237618
C	-1.460260	0.621656	-0.607814
C	-1.035470	-0.815716	-0.937244
H	1.597249	-0.590365	1.213789
H	-0.540028	-0.838335	-1.918101
H	-0.583147	1.105297	1.291454
H	-0.513897	2.443310	0.119734
H	-1.651142	1.165619	-1.542787
H	-1.931224	-1.443933	-1.001903
H	0.231039	-2.411079	-0.173839
H	1.107090	1.031738	-1.272540
F	-0.668737	-1.409474	1.339920
F	2.177500	-1.080181	-0.672445
F	1.939423	1.721685	0.426620
F	-2.673348	0.606458	0.091035

4_39

C	-0.277936	1.455201	-0.046608
C	-1.291118	0.302053	-0.049305
C	-0.613619	-1.059669	-0.033220
C	0.651015	-1.008928	0.807317
C	1.693227	-0.101854	0.149987
C	1.059143	1.052236	-0.638375
H	-1.942118	0.396343	0.828772
H	0.883619	0.708269	-1.666540
H	0.410168	-0.626983	1.806963
H	1.070094	-2.015574	0.913246
H	1.734095	1.913843	-0.683899
H	-0.720276	2.305588	-0.579564
H	-0.383270	-1.358933	-1.064363
F	-0.076019	1.851982	1.289137
F	-2.078399	0.417832	-1.199194
F	-1.498980	-2.008125	0.485199
F	2.457024	-0.865022	-0.752982
H	2.390768	0.273198	0.907163

4_40

C	0.242159	1.270611	0.339395
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C	1.273450	0.431062	-0.431074
C	0.850858	-1.025345	-0.612956
C	-0.641479	-1.073619	-0.901171
C	-1.429770	-0.644170	0.342909
C	-0.709699	0.427845	1.167978
H	1.382722	0.880788	-1.426704
H	-0.119737	-0.059614	1.953518
H	-0.871416	-0.366393	-1.708531
H	-0.944522	-2.075652	-1.223208
H	-1.459199	1.069575	1.645484
H	0.778848	1.999393	0.959533
F	-0.501756	1.991817	-0.611936
F	2.505365	0.488918	0.214274
H	-1.641660	-1.511054	0.979296
F	-2.675382	-0.156349	-0.082273
F	1.106503	-1.741741	0.567822
H	1.449272	-1.499151	-1.400852

4_41

C	-0.819976	1.103432	-0.408416
C	-1.393236	-0.135259	0.297922
C	-0.329885	-1.170797	0.656805
C	0.896164	-0.448710	1.194035
C	1.543388	0.465122	0.142110
C	0.574138	0.888482	-0.964768
H	-1.865554	0.207508	1.227833
H	0.528223	0.086018	-1.709369
H	0.586773	0.154502	2.058078
H	1.646290	-1.170559	1.535464
H	0.924833	1.802913	-1.456510
H	-1.525714	1.420363	-1.185214
F	-0.753788	2.138319	0.550231
F	-2.373072	-0.719639	-0.499276
F	0.021135	-1.899140	-0.485048
H	-0.733694	-1.892646	1.378725
H	1.966511	1.345818	0.639450
F	2.622257	-0.204823	-0.454194

4_42

C	-0.130871	-1.138582	-0.455927
C	-1.230177	-0.089564	-0.273233
C	-0.630034	1.237231	0.201738
C	0.842196	1.380484	-0.157309
C	1.673667	0.272005	0.505660
C	0.889498	-1.034074	0.664187
H	-1.793536	0.062590	-1.202304
H	0.372660	-1.055381	1.632470
H	0.965274	1.302900	-1.244787
H	1.196936	2.370717	0.147843
H	2.063074	0.598442	1.477754
H	1.588889	-1.876473	0.630078
H	-0.765754	1.285220	1.290864
F	-2.129401	-0.538607	0.695843
F	-1.348099	2.300765	-0.350390
F	2.792369	0.033581	-0.311052
F	-0.700948	-2.405216	-0.503226
H	0.361495	-0.967714	-1.423178

4_43

C	1.174148	-0.250088	-0.616975
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C	0.391617	-0.978855	0.454471
C	-1.117094	-0.864068	0.184687
C	-1.488559	0.304095	-0.729842
C	-0.630421	1.530917	-0.449948
C	0.872852	1.245669	-0.606990
H	0.674685	-2.037712	0.494771
H	1.396722	1.699333	0.241311
H	-1.328429	-0.004485	-1.771614
H	-2.549354	0.551832	-0.611978
H	1.256708	1.698203	-1.528383
H	-1.617046	-0.782510	1.156053
F	0.671393	-0.409418	1.697646
F	-1.547391	-2.051456	-0.425158
F	-0.891593	1.946471	0.868494
H	-0.934146	2.361810	-1.098447
F	2.543133	-0.453445	-0.442224
H	0.905727	-0.701860	-1.582957

4_44

C	1.126723	-1.000115	0.052976
C	1.536372	0.454194	0.313601
C	0.392077	1.438044	0.064863
C	-0.952402	0.781716	0.354171
C	-1.221164	-0.338016	-0.642068
C	0.057011	-1.100350	-1.017738
H	0.504596	2.337437	0.679625
H	1.915394	0.521472	1.340732
H	0.479498	-0.680450	-1.940424
H	-0.989969	0.373352	1.370927
H	-1.681068	0.102846	-1.536629
H	-0.202598	-2.147034	-1.212821
H	2.020672	-1.578657	-0.210869
H	0.421858	1.741382	-0.990292
F	0.624851	-1.516254	1.259295
F	2.594121	0.764137	-0.552077
F	-1.961894	1.743724	0.251527
F	-2.157088	-1.223072	-0.098198

4_45

C	-1.377765	0.774824	0.083670
C	-1.383038	-0.761049	0.099397
C	0.020506	-1.363411	0.019910
C	1.005244	-0.408510	0.678936
C	1.162507	0.859422	-0.159329
C	-0.200234	1.357422	-0.674130
H	0.056411	-2.342821	0.508350
H	-1.908966	-1.081119	1.007675
H	-0.289052	1.023523	-1.716447
H	0.653899	-0.123780	1.679009
H	-0.253219	2.451491	-0.667026
H	-2.329530	1.120680	-0.337296
H	0.293660	-1.490078	-1.034947
F	-1.328193	1.215707	1.422039
F	-2.131967	-1.195526	-1.001522
F	2.246246	-1.019284	0.834927
F	1.960097	0.561831	-1.271478
H	1.697836	1.625363	0.414272

4_46

C	-0.968495	1.049239	0.126128
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C	-1.443920	-0.400383	-0.064304
C	-0.347996	-1.331278	-0.575161
C	0.968497	-1.049235	0.126188
C	1.443936	0.400374	-0.064298
C	0.348020	1.331262	-0.575188
H	-0.638321	-2.379095	-0.437892
H	-1.848134	-0.749271	0.892244
H	0.210270	1.156313	-1.650592
H	0.638341	2.379082	-0.437929
H	-1.760947	1.718459	-0.230233
H	-0.210219	-1.156346	-1.650564
F	-0.800203	1.286768	1.500076
F	-2.489979	-0.401403	-0.999405
F	0.800151	-1.286691	1.500142
H	1.760960	-1.718477	-0.230108
F	2.489989	0.401345	-0.999407
H	1.848163	0.749292	0.892233

4_47

C	-1.088837	-1.055119	0.246745
C	-1.544706	0.382137	0.501392
C	-0.388192	1.390157	0.437652
C	0.837402	0.833345	-0.274424
C	1.354716	-0.409560	0.439110
C	0.221854	-1.298407	0.978244
H	-0.734844	2.295999	-0.071170
H	0.064956	-1.092965	2.045974
H	0.530352	-2.345072	0.880743
H	-1.871595	-1.763101	0.547898
H	-0.088911	1.675099	1.455298
F	-0.883529	-1.239766	-1.124831
F	-2.536162	0.717937	-0.419900
H	-2.008820	0.412765	1.496669
H	2.008656	-0.084170	1.259283
H	0.623794	0.589983	-1.319696
F	1.840322	1.810383	-0.264934
F	2.148590	-1.148982	-0.442258

4_48

C	1.272666	0.860198	-0.079423
C	1.079924	-0.449075	0.662581
C	0.000003	-1.311412	-0.000013
C	-1.079934	-0.449070	-0.662577
C	-1.272659	0.860205	0.079422
C	0.000005	1.707743	-0.000004
H	0.478993	-1.949659	-0.749420
H	0.029301	2.351641	0.886611
H	-0.029276	2.351639	-0.886621
H	2.146182	1.400630	0.304621
H	-0.478974	-1.949701	0.749364
F	1.540250	0.571286	-1.431297
F	2.284192	-1.154541	0.703574
H	0.806789	-0.209127	1.697641
H	-0.806811	-0.209123	-1.697639
F	-2.284205	-1.154539	-0.703554
F	-1.540243	0.571298	1.431294
H	-2.146176	1.400634	-0.304624

4_49

C	-0.909219	1.101298	0.039820
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C	-1.335937	-0.148689	-0.707777
C	-0.577478	-1.386566	-0.225265
C	0.909223	-1.101297	0.039881
C	1.335946	0.148652	-0.707776
C	0.577492	1.386546	-0.225303
H	-1.026469	-1.720249	0.716406
H	0.689876	2.188937	-0.963112
H	1.026465	1.720224	0.716378
H	-1.541334	1.949298	-0.251631
H	-0.689827	-2.188964	-0.963073
F	-1.119466	0.895789	1.406577
F	-2.706068	-0.361336	-0.558063
H	-1.161001	0.029636	-1.779295
H	1.161008	-0.029717	-1.779287
F	2.706078	0.361304	-0.558076
F	1.119431	-0.895703	1.406632
H	1.541349	-1.949312	-0.251498

4_50

C	1.111232	0.628440	-0.440880
C	1.215819	-0.894844	-0.383003
C	-0.157083	-1.520588	-0.083045
C	-1.306554	-0.555753	-0.349039
C	-1.194809	0.710628	0.496342
C	0.260288	1.138545	0.709421
H	-0.314739	-2.439936	-0.656668
H	1.660163	-1.278470	-1.309626
H	0.646377	0.724828	1.649019
H	-1.352314	-0.266372	-1.407369
H	-1.705075	0.543775	1.453026
H	0.303275	2.231342	0.769275
H	-0.166891	-1.785013	0.982125
F	2.089778	-1.241390	0.653206
F	-2.511784	-1.200403	-0.057187
F	-1.885941	1.736784	-0.166096
F	2.385205	1.184567	-0.405063
H	0.660523	0.915253	-1.402295

4_51

C	-1.244626	-0.587876	-0.129135
C	-1.213994	0.894414	0.237081
C	0.186154	1.359379	0.642518
C	1.244643	0.587873	-0.129150
C	1.214000	-0.894416	0.237077
C	-0.186141	-1.359358	0.642562
H	0.276987	2.432946	0.443580
H	-0.333679	-1.201286	1.719032
H	-0.276984	-2.432934	0.443680
H	0.333713	1.201366	1.718993
F	-1.640612	1.638369	-0.872883
H	-1.935439	1.074208	1.044026
H	1.935472	-1.074222	1.043994
H	1.082841	0.687363	-1.210601
F	2.510479	1.109024	0.150793
F	1.640562	-1.638382	-0.872902
F	-2.510464	-1.109029	0.150788
H	-1.082801	-0.687379	-1.210581

4_52

C	1.218677	-0.486598	0.454099
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C	0.913977	1.013171	0.324033
C	-0.488559	1.296305	-0.207760
C	-1.454712	0.285267	0.394469
C	-1.166572	-1.133594	-0.103762
C	0.314845	-1.357942	-0.410234
H	-0.797540	2.313651	0.057091
H	1.044655	1.443626	1.326061
H	-1.399137	0.326851	1.490842
H	-1.724128	-1.291920	-1.034978
H	-1.510859	-1.872069	0.628526
H	0.586503	-2.414911	-0.299382
H	2.275895	-0.660373	0.222860
H	-0.485430	1.198185	-1.299126
F	0.983036	-0.869783	1.784452
F	1.862204	1.600480	-0.514896
F	-2.767698	0.629799	0.049089
F	0.587360	-0.998572	-1.740530

4_53

C	1.234483	0.185921	0.345965
C	0.385303	1.455443	0.207934
C	-1.057841	1.157689	-0.208758
C	-1.499226	-0.202445	0.322373
C	-0.660858	-1.341891	-0.272050
C	0.750183	-0.866419	-0.627548
H	-1.733456	1.939984	0.153551
H	0.426850	1.985696	1.167099
H	-1.443971	-0.216049	1.417637
H	-1.166280	-1.711313	-1.171731
H	-0.575483	-2.168733	0.440891
H	2.293438	0.420969	0.187544
H	-1.108456	1.144454	-1.305267
F	1.083831	-0.287279	1.656974
F	0.981609	2.272230	-0.760156
F	-2.844576	-0.400086	-0.014351
F	1.625470	-1.952566	-0.645570
H	0.778100	-0.415492	-1.629289

4_54

C	1.291118	0.302053	-0.049305
C	0.613619	-1.059669	-0.033220
C	-0.651015	-1.008928	0.807317
C	-1.693227	-0.101854	0.149987
C	-1.059143	1.052236	-0.638375
C	0.277936	1.455201	-0.046608
H	-1.070094	-2.015574	0.913246
H	0.383270	-1.358933	-1.064363
H	-1.734095	1.913843	-0.683899
H	-0.883619	0.708269	-1.666540
H	1.942118	0.396343	0.828772
H	-0.410168	-0.626983	1.806963
F	2.078399	0.417832	-1.199194
F	1.498980	-2.008125	0.485199
H	0.720276	2.305588	-0.579564
F	0.076019	1.851982	1.289137
F	-2.457024	-0.865022	-0.752982
H	-2.390768	0.273198	0.907163

4_55

C	-0.391664	-0.978839	0.454487
C	1.117053	-0.864128	0.184694
C	1.488578	0.304020	-0.729827
C	0.630496	1.530887	-0.449957
C	-0.872792	1.245693	-0.606997
C	-1.174154	-0.250048	-0.616969
H	2.549384	0.551707	-0.611955
H	1.617014	-0.782609	1.156059
H	-1.256630	1.698237	-1.528392
H	-1.396642	1.699383	0.241300
H	-0.674784	-2.037680	0.494814
H	1.328444	-0.004547	-1.771602
F	-0.671403	-0.409366	1.697656
F	1.547278	-2.051535	-0.425160
F	0.891684	1.946472	0.868466
H	0.934257	2.361742	-1.098486
H	-0.905756	-0.701848	-1.582942
F	-2.543158	-0.453337	-0.442227

4_56

C	-1.248336	0.548905	0.288385
C	-1.057112	-0.615899	-0.690258
C	0.409713	-1.031132	-0.851030
C	1.256011	-0.606657	0.339967
C	1.236477	0.914380	0.527514
C	-0.101848	1.543489	0.132632
H	0.455026	-2.118146	-0.981109
H	2.007156	1.351527	-0.119372
H	1.476751	1.172989	1.564322
H	-2.229234	1.018143	0.147072
H	0.822659	-0.557341	-1.749898
F	-1.196079	0.083715	1.606040
F	-0.080103	1.905394	-1.229010
H	-0.295046	2.458689	0.704166
H	0.918273	-1.116842	1.248586
F	2.581788	-1.010201	0.120437
F	-1.823263	-1.691471	-0.234774
H	-1.466098	-0.314477	-1.661273

4_57

C	1.138783	0.634395	-0.044285
C	-0.055857	1.388134	-0.637681
C	-1.334213	0.538444	-0.660351
C	-1.287517	-0.603302	0.349322
C	-0.099786	-1.541146	0.089031
C	1.074216	-0.793894	-0.551106
H	-2.191420	1.190549	-0.459645
H	-0.432918	-2.346546	-0.575748
H	0.251216	-1.988156	1.024720
H	2.089168	1.116301	-0.303726
H	-1.470408	0.103065	-1.659539
F	1.045221	0.630168	1.349045
H	-1.253046	-0.206789	1.369377
F	-2.475983	-1.339495	0.238556
F	-0.258532	2.554793	0.096234
H	0.207888	1.690123	-1.660254
H	0.972695	-0.759334	-1.645821

F 2.268523 -1.460466 -0.279273

4_58

C 1.176476 -0.083738 -0.495675
C 0.413720 -1.374545 -0.271850
C -1.062554 -1.181198 -0.626487
C -1.538759 0.253307 -0.365495
C -0.784207 0.883502 0.794826
C 0.700481 1.015604 0.451930
H -1.233622 -1.455233 -1.674401
H 0.869576 -2.190639 -0.845304
H -1.420366 0.875438 -1.263665
H -0.899639 0.251460 1.682601
H -1.184425 1.879209 1.016514
H -1.650202 -1.861201 0.001398
F 0.528042 -1.724188 1.086080
F -2.909451 0.228065 -0.081656
F 0.921428 2.249280 -0.182612
H 1.319497 0.999794 1.355607
F 2.544526 -0.289159 -0.340267
H 1.007322 0.247593 -1.530144

4_59

C -0.692433 0.142924 0.842659
C -0.488816 -1.168028 0.068214
C 0.759756 -1.102359 -0.823961
C 1.797680 -0.133322 -0.282588
C 1.264893 1.298538 -0.167686
C -0.248681 1.356734 0.050825
H 1.198391 -2.098530 -0.947123
H -0.425616 -1.993537 0.787492
H 1.489766 1.854912 -1.085280
H 1.787325 1.790136 0.661761
H 0.434973 -0.739364 -1.806645
F -1.596803 -1.424651 -0.735915
H -0.551668 2.276730 0.566174
F -0.889277 1.361982 -1.197455
F 2.177727 -0.577271 1.008105
H 2.710591 -0.154837 -0.889917
H -0.071610 0.101557 1.747590
F -2.016820 0.261718 1.240950

4_60

C 0.899221 0.215684 -0.564134
C 0.682915 -1.265631 -0.324391
C -0.806767 -1.605514 -0.356066
C -1.685631 -0.449940 0.131287
C -0.968300 0.428629 1.144743
C 0.327237 1.033557 0.587354
H -1.115147 -1.862732 -1.376363
H 1.255720 -1.857046 -1.048604
H -0.728965 -0.190625 2.017746
H -1.620935 1.247569 1.467520
H -0.959233 -2.488094 0.276406
F 1.193111 -1.584467 0.950903
F -2.025299 0.346800 -0.982807
H -2.632037 -0.828648 0.537405
H 1.088186 1.105531 1.372914

F	0.085793	2.333645	0.129668
F	2.259970	0.484760	-0.704928
H	0.398187	0.506691	-1.495306

4_61

C	-1.167067	0.264299	-0.194814
C	-0.248170	1.371775	0.330568
C	1.138017	0.866861	0.719736
C	1.595743	-0.185811	-0.275860
C	0.694781	-1.425965	-0.216898
C	-0.715942	-1.103274	0.288154
H	1.832024	1.714792	0.737822
H	1.165031	-2.158416	0.449017
H	0.600112	-1.883782	-1.208336
H	1.105622	0.429363	1.726648
H	1.605432	0.247276	-1.284678
F	2.913089	-0.564252	0.008489
F	-0.110478	2.342103	-0.673997
H	-0.742992	1.854575	1.181762
H	-0.775653	-1.135557	1.384600
F	-1.599143	-2.071011	-0.189319
F	-2.470813	0.506642	0.232702
H	-1.167646	0.283092	-1.293031

4_62

C	-0.618294	0.743370	-0.241176
C	0.676217	1.099016	0.485581
C	1.438524	-0.130331	0.993475
C	1.136315	-1.368651	0.165143
C	-0.350280	-1.723448	0.211566
C	-1.248443	-0.492837	0.378442
H	2.510111	0.098635	0.980657
H	-0.538786	-2.431213	1.027389
H	-0.616070	-2.217675	-0.730100
H	1.148695	-0.337301	2.032960
F	1.489412	1.837000	-0.377489
H	0.419793	1.760307	1.323828
H	1.748728	-2.222130	0.482656
F	1.492683	-1.097998	-1.170095
F	-2.477798	-0.743075	-0.230966
H	-1.460002	-0.285419	1.437651
F	-1.504447	1.814592	-0.133419
H	-0.415349	0.577408	-1.305502

4_63

C	-0.578422	-0.915329	-0.495595
C	-1.447925	0.348931	-0.426520
C	-0.734431	1.529078	0.222874
C	0.734431	1.529078	-0.222875
C	1.447925	0.348931	0.426520
C	0.578422	-0.915329	0.495595
H	-1.233199	2.464491	-0.054013
H	-1.733005	0.590015	-1.459385
H	0.800465	1.420552	-1.313199
H	1.233199	2.464491	0.054012
H	1.733005	0.590016	1.459384
H	1.212969	-1.796324	0.340059
H	-1.212969	-1.796324	-0.340058
H	-0.800465	1.420552	1.313198

F	-0.008475	-0.994448	-1.773203
F	-2.619505	0.055023	0.277218
F	2.619505	0.055023	-0.277218
F	0.008475	-0.994447	1.773204

4_64

C	-0.683878	0.999620	0.117455
C	-1.635518	-0.203209	0.045988
C	-0.894499	-1.540344	0.039938
C	0.377499	-1.435345	0.890217
C	1.366846	-0.436909	0.285114
C	0.653914	0.658516	-0.501175
H	-1.552749	-2.335543	0.407599
H	-2.319281	-0.126828	0.900821
H	0.122184	-1.107464	1.905457
H	0.879394	-2.406500	0.967872
H	-1.135721	1.865584	-0.380331
H	-0.629746	-1.784324	-0.997195
F	-0.495601	1.327180	1.468788
F	-2.396741	-0.085812	-1.123907
H	1.997309	0.023017	1.054836
F	2.220725	-1.110977	-0.603307
F	1.455657	1.793917	-0.586041
H	0.476071	0.299318	-1.524077

4_65

C	1.097140	-0.196821	-0.429075
C	0.266270	-1.450703	-0.237890
C	-1.111312	-1.291339	-0.894757
C	-1.530381	0.180865	-1.069917
C	-1.061414	1.043935	0.088721
C	0.463829	0.992458	0.276587
H	-1.110870	-1.790883	-1.871190
H	0.809447	-2.317444	-0.634138
H	-1.092984	0.601222	-1.986573
H	-2.619661	0.259919	-1.166017
H	-1.827451	-1.817505	-0.253961
F	0.113390	-1.668121	1.139254
H	-1.343758	2.094557	-0.055371
F	-1.677937	0.599657	1.264386
F	1.015120	2.162565	-0.258449
H	0.696460	0.953931	1.346115
H	1.170695	0.020906	-1.503987
F	2.390907	-0.391331	0.046266

4_66

C	0.740626	0.804523	-0.172220
C	1.453696	-0.420127	0.404812
C	0.520151	-1.617054	0.560510
C	-0.520150	-1.617055	-0.560508
C	-1.453695	-0.420128	-0.404812
C	-0.740626	0.804523	0.172220
H	1.127762	-2.529262	0.555844
H	-0.013473	-1.561027	-1.533679
H	-1.127761	-2.529262	-0.555842
H	0.013474	-1.561025	1.533681
F	2.494679	-0.763205	-0.472428
H	1.915977	-0.139878	1.359635

F	-2.494680	-0.763205	0.472427
H	-1.915975	-0.139879	-1.359636
H	-0.869893	0.816485	1.262783
F	-1.325659	1.964275	-0.330074
H	0.869893	0.816486	-1.262783
F	1.325658	1.964276	0.330074

4_67

C	-1.470328	0.740774	-0.177970
C	-0.248813	1.447642	0.403391
C	0.981121	0.539598	0.533243
C	0.981121	-0.539597	-0.533243
C	-0.248813	-1.447642	-0.403391
C	-1.470328	-0.740774	0.177971
H	0.006248	2.274158	-0.270809
H	-0.498862	1.872797	1.380730
H	1.031353	-0.064374	-1.520680
H	0.006248	-2.274158	0.270808
H	-0.498863	-1.872796	-1.380730
H	-2.399656	-1.230085	-0.136471
H	-2.399656	1.230085	0.136472
H	1.031353	0.064374	1.520680
F	-1.429237	0.800956	-1.584370
F	2.128018	1.326794	0.397463
F	2.128018	-1.326793	-0.397463
F	-1.429236	-0.800956	1.584370

4_68

C	-1.159964	-1.045492	-0.014099
C	0.227112	-1.549927	-0.408286
C	1.269708	-0.426734	-0.512872
C	0.928616	0.737209	0.401639
C	-0.428385	1.350178	0.026450
C	-1.377468	0.330652	-0.608207
H	0.562182	-2.255694	0.360251
H	0.167892	-2.090615	-1.359846
H	0.943961	0.393493	1.442449
H	-0.247710	2.173250	-0.673961
H	-0.915705	1.757533	0.917679
H	-1.951355	-1.740224	-0.320583
H	1.358567	-0.046640	-1.540758
F	-1.231892	-0.941530	1.385954
F	2.518673	-0.945864	-0.169450
F	1.914483	1.718860	0.274246
F	-2.697072	0.744074	-0.428526
H	-1.213266	0.253713	-1.692992

4_69

C	1.137862	0.380975	-0.912250
C	-0.264797	-0.027038	-1.384629
C	-1.089380	-0.703552	-0.290392
C	-0.920944	-0.001996	1.042621
C	0.535336	-0.097410	1.515047
C	1.540719	-0.310860	0.386697
H	-0.788029	0.886261	-1.688672
H	-0.200287	-0.691438	-2.252562
H	0.653497	-0.926231	2.223336
H	0.771333	0.834308	2.041090
H	1.886848	0.175128	-1.686212
H	-0.791647	-1.751363	-0.161531

F	1.182941	1.757342	-0.651198
F	-2.435063	-0.700513	-0.665903
H	2.543908	0.008588	0.693521
F	1.622807	-1.686804	0.087243
F	-1.270229	1.346151	0.885942
H	-1.612508	-0.421553	1.783706

4_70

C	-0.909227	-1.101295	0.039853
C	0.577478	-1.386560	-0.225287
C	1.335938	-0.148671	-0.707777
C	0.909227	1.101295	0.039853
C	-0.577478	1.386560	-0.225287
C	-1.335938	0.148671	-0.707777
H	1.026459	-1.720253	0.716385
H	0.689838	-2.188937	-0.963113
H	-0.689839	2.188937	-0.963114
H	-1.026459	1.720252	0.716385
H	-1.541345	-1.949302	-0.251569
H	1.161005	0.029675	-1.779294
F	-1.119452	-0.895746	1.406603
F	2.706071	-0.361326	-0.558063
F	1.119452	0.895746	1.406602
H	1.541344	1.949302	-0.251570
H	-1.161005	-0.029675	-1.779294
F	-2.706071	0.361325	-0.558063

4_71

C	1.272662	0.860200	0.079425
C	0.000000	1.707747	0.000000
C	-1.272662	0.860200	-0.079425
C	-1.079932	-0.449075	0.662570
C	0.000000	-1.311416	0.000000
C	1.079932	-0.449075	-0.662570
H	-0.029283	2.351644	0.886616
H	0.029283	2.351644	-0.886616
H	-0.478984	-1.949683	-0.749393
H	0.478984	-1.949683	0.749393
H	2.146177	1.400623	-0.304634
F	1.540242	0.571291	1.431288
F	-2.284209	-1.154536	0.703555
H	-0.806809	-0.209127	1.697635
H	-2.146177	1.400623	0.304634
F	-1.540242	0.571291	-1.431288
F	2.284209	-1.154536	-0.703555
H	0.806809	-0.209127	-1.697635

4_72

C	-1.251081	-0.323649	-0.689572
C	0.000002	-0.000004	-1.507979
C	1.251081	0.323649	-0.689572
C	1.251082	-0.323648	0.689573
C	0.000000	0.000000	1.507979
C	-1.251081	0.323650	0.689572
H	0.196345	-0.864102	-2.152938
H	-0.196339	0.864084	-2.152951
H	0.196342	0.864093	2.152946
H	-0.196343	-0.864094	2.152943
H	-2.153915	-0.026273	-1.237218

F	-1.338611	-1.708049	-0.475671
H	2.153917	0.026275	-1.237217
F	1.338606	1.708050	-0.475675
H	-2.153916	0.026276	1.237217
F	-1.338608	1.708050	0.475672
F	1.338610	-1.708048	0.475674
H	2.153916	-0.026273	1.237218

4_73

C	1.225498	0.654806	0.381494
C	0.000000	1.494191	0.000001
C	-1.225497	0.654806	-0.381494
C	-1.225498	-0.654806	0.381494
C	0.000000	-1.494191	0.000001
C	1.225497	-0.654806	-0.381494
H	-0.286452	2.139210	0.837929
H	0.286452	2.139211	-0.837927
H	-1.259208	-0.438827	1.458388
H	-0.286452	-2.139212	-0.837927
H	0.286452	-2.139209	0.837930
H	-1.259207	0.438827	-1.458388
F	-2.377267	1.380323	-0.078857
F	-2.377267	-1.380323	0.078856
F	2.377267	1.380323	0.078856
H	1.259208	0.438827	1.458388
H	1.259206	-0.438827	-1.458388
F	2.377267	-1.380323	-0.078858

5_1

C	1.272196	0.671783	-0.611255
C	1.286766	-0.625828	0.195087
C	0.000000	-0.911579	0.970178
C	-1.286767	-0.625828	0.195087
C	-1.272196	0.671784	-0.611255
C	0.000000	0.833838	-1.428656
H	0.000000	-1.971276	1.257233
H	2.126781	-0.611780	0.900645
H	2.148574	0.670850	-1.273017
H	-2.126781	-0.611780	0.900645
H	-2.148573	0.670850	-1.273017
H	0.000000	0.055983	-2.203767
H	0.000000	1.811744	-1.923813
F	1.421541	1.732578	0.282970
F	1.477005	-1.671442	-0.713525
F	0.000000	-0.133338	2.123328
F	-1.477005	-1.671442	-0.713525
F	-1.421540	1.732578	0.282970

5_2

C	1.005315	1.114950	-0.563859
C	1.456422	-0.319346	-0.281912
C	0.544195	-1.101368	0.667882
C	-0.949198	-0.891438	0.410430
C	-1.270447	0.587363	0.286529
C	-0.484492	1.221503	-0.850268
H	0.780992	-2.168938	0.580039
H	2.468486	-0.304229	0.141613

H	1.598186	1.505302	-1.400525
H	-1.534469	-1.349866	1.217516
H	-0.706769	0.696546	-1.786991
H	-0.763418	2.275293	-0.960067
F	1.314368	1.880751	0.569723
F	1.488439	-0.993601	-1.502958
F	0.812630	-0.685160	1.972909
F	-1.268575	-1.545041	-0.779569
F	-2.638893	0.743466	0.068300
H	-1.025500	1.072176	1.239968

5_3

C	1.570838	0.524287	-0.150604
C	1.211544	-0.924981	0.182361
C	-0.267798	-1.148054	0.504569
C	-1.142045	-0.511308	-0.565225
C	-0.861544	0.966405	-0.790668
C	0.609940	1.162144	-1.147041
H	-0.470856	-2.226628	0.543822
H	1.828296	-1.278411	1.017158
H	0.794598	0.708589	-2.130094
H	0.829445	2.233411	-1.222579
F	1.507551	-1.691540	-0.955138
F	-0.529843	-0.617447	1.757889
F	-1.184608	1.705100	0.342777
H	-1.505443	1.330263	-1.603233
H	-0.920030	-1.030594	-1.508898
F	-2.482320	-0.718250	-0.267716
H	2.589638	0.531544	-0.561107
F	1.592414	1.246678	1.040474

5_4

C	-1.443621	0.907705	-0.031140
C	-1.450117	-0.563330	0.389311
C	-0.185950	-1.320206	-0.016802
C	1.073661	-0.566371	0.388461
C	1.077748	0.836707	-0.190381
C	-0.138515	1.604951	0.315818
H	-0.185537	-2.318829	0.438237
H	-2.331348	-1.066885	-0.025480
H	-2.289694	1.409626	0.455581
H	-0.070721	1.689025	1.408496
H	-0.141017	2.617285	-0.103755
F	-1.655648	0.961179	-1.412173
F	-1.525785	-0.594153	1.787284
F	-0.208765	-1.476986	-1.400869
H	1.117325	-0.503719	1.484444
F	2.183005	-1.280455	-0.045895
F	2.229017	1.500122	0.237872
H	1.105345	0.789409	-1.285106

5_5

C	-0.620717	-0.794392	1.276895
C	0.240200	0.471017	1.273010
C	1.067388	0.536414	0.000000
C	0.240200	0.471017	-1.273010
C	-0.620717	-0.794392	-1.276895
C	-1.437794	-0.937210	0.000000

H	0.905742	0.482318	2.145349
H	-1.283837	-0.770271	2.150792
H	-2.196157	-0.143573	0.000000
H	-1.952627	-1.905018	0.000000
F	0.243622	-1.885302	1.433268
F	-0.620717	1.561019	1.376867
H	0.905742	0.482318	-2.145349
H	-1.283837	-0.770271	-2.150792
H	1.724863	-0.343510	0.000000
F	1.861829	1.676709	0.000000
F	-0.620717	1.561019	-1.376867
F	0.243622	-1.885302	-1.433268

5_6

C	-0.248601	1.631081	0.312262
C	-1.343888	0.569960	0.176196
C	-0.900271	-0.528823	-0.781526
C	0.443208	-1.144877	-0.415002
C	1.483689	-0.032398	-0.376561
C	1.107554	1.029044	0.648208
H	-2.269288	1.027060	-0.196423
H	-0.552263	2.365007	1.067903
H	1.051900	0.567219	1.641270
H	1.866969	1.818558	0.666155
F	-0.170532	2.298096	-0.924899
F	-1.595243	0.064014	1.446191
H	0.718740	-1.914378	-1.148093
H	-0.794498	-0.064685	-1.772566
F	-1.876621	-1.510865	-0.869570
F	0.377502	-1.761072	0.829133
F	2.728160	-0.574035	-0.065476
H	1.558891	0.412055	-1.378115

5_7

C	1.699850	0.298668	0.037077
C	0.586316	1.327297	-0.151525
C	-0.718504	0.666619	-0.570565
C	-1.144622	-0.356772	0.468496
C	-0.074401	-1.431766	0.620577
C	1.277270	-0.823820	0.977901
H	0.875343	2.093927	-0.880261
H	2.590248	0.805746	0.429808
H	1.220608	-0.408603	1.992646
H	2.041873	-1.609129	0.973111
F	2.022556	-0.205726	-1.225728
F	0.408962	1.956167	1.088396
H	-0.583046	0.175254	-1.541455
F	-1.698610	1.643287	-0.705047
H	-0.391768	-2.158009	1.380194
H	-1.303146	0.143147	1.432705
F	-2.342828	-0.946641	0.088363
F	0.031525	-2.127498	-0.588040

5_8

C	1.230818	-1.276296	-0.082294
C	1.523605	0.205849	0.144439
C	0.419157	1.067715	-0.445020

C	-0.944736	0.705519	0.123862
C	-1.235147	-0.772314	-0.093044
C	-0.131152	-1.659044	0.470570
H	2.492986	0.491384	-0.281381
H	2.024249	-1.882722	0.370420
H	-0.104568	-1.546580	1.561716
H	-0.346763	-2.707967	0.238600
F	1.261283	-1.496176	-1.469346
F	1.583054	0.400856	1.527607
H	0.404550	0.926897	-1.533844
F	0.694216	2.405037	-0.189252
H	-0.991301	0.951069	1.192181
F	-1.912536	1.459640	-0.533607
F	-2.434670	-1.092756	0.543295
H	-1.376541	-0.950060	-1.167039

5_9

C	0.817614	1.192126	-0.541092
C	1.203572	-0.273865	-0.688569
C	0.500229	-1.204462	0.292291
C	-1.015001	-1.010661	0.193829
C	-1.371165	0.452504	0.402083
C	-0.697821	1.346725	-0.631031
H	1.327473	1.776669	-1.317657
H	-1.041512	1.065242	-1.633962
H	-0.969848	2.392151	-0.449788
F	1.253749	1.685100	0.691617
H	0.898785	-0.587074	-1.697113
H	0.767598	-2.244139	0.065565
H	-1.536822	-1.644741	0.920375
F	2.578999	-0.430667	-0.584764
F	0.878990	-0.940820	1.604740
F	-1.402031	-1.416269	-1.089218
F	-2.755751	0.601762	0.325820
H	-1.055849	0.735726	1.413765

5_10

C	0.950560	0.363678	-1.280752
C	-0.544721	0.654313	-1.233176
C	-1.238025	0.085888	0.000000
C	-0.544721	0.654313	1.233176
C	0.950560	0.363678	1.280752
C	1.626237	0.854006	0.000000
H	1.379924	0.872725	-2.154851
H	1.625016	1.953184	0.000000
H	2.670539	0.521678	0.000000
F	1.176745	-0.995624	-1.451301
H	-0.658813	1.749318	-1.200347
H	-2.295678	0.384008	0.000000
F	-1.168948	0.201242	-2.384893
F	-1.197977	-1.295480	0.000000
H	-0.658813	1.749318	1.200347
H	1.379924	0.872725	2.154851
F	-1.168948	0.201242	2.384893
F	1.176745	-0.995624	1.451301

5_11

C	1.121775	1.211365	-0.179765
C	1.310557	-0.182564	-0.767141
C	0.330674	-1.207245	-0.210658

C	-1.095095	-0.721142	-0.448853
C	-1.314342	0.636832	0.197078
C	-0.324603	1.657128	-0.360363
H	1.813105	1.905795	-0.674843
H	-0.530260	1.798114	-1.430588
H	-0.472676	2.620620	0.139390
F	1.439341	1.215710	1.177229
H	1.128961	-0.103346	-1.850247
H	0.487233	-2.180722	-0.693433
F	2.613404	-0.620367	-0.586517
F	0.530346	-1.381575	1.152838
H	-1.281008	-0.638371	-1.530030
F	-1.985424	-1.653765	0.062612
F	-2.607635	1.071968	-0.098139
H	-1.229442	0.543927	1.285755

5_12

C	0.559843	-1.427411	0.452971
C	1.253758	-0.070597	0.500059
C	0.668813	0.868607	-0.544494
C	-0.831292	1.019512	-0.325575
C	-1.501371	-0.342740	-0.423963
C	-0.947291	-1.295092	0.629265
H	1.002630	-2.092457	1.204151
H	-1.173970	-0.900490	1.626982
H	-1.416172	-2.279506	0.525755
F	0.808296	-2.004309	-0.805018
H	1.127125	0.370451	1.496868
F	2.613340	-0.237935	0.270428
H	-1.261138	1.729307	-1.042952
H	0.864065	0.469286	-1.547983
F	1.275357	2.114194	-0.451176
F	-1.046182	1.538055	0.955450
F	-2.875798	-0.194910	-0.254292
H	-1.332412	-0.746126	-1.430933

5_13

C	1.270399	-1.028997	0.384163
C	1.241485	0.492240	0.433288
C	0.000000	1.061258	-0.238104
C	-1.241485	0.492240	0.433288
C	-1.270399	-1.028997	0.384163
C	0.000000	-1.619440	0.988733
H	2.160898	-1.390755	0.914921
H	0.000000	-1.430584	2.071436
H	0.000000	-2.704705	0.837065
F	1.393273	-1.433662	-0.945033
H	1.250392	0.813097	1.485920
F	2.380581	1.003064	-0.170658
H	0.000000	0.842948	-1.311845
F	0.000000	2.443180	-0.069899
H	-1.250392	0.813097	1.485920
F	-2.380581	1.003064	-0.170658
F	-1.393273	-1.433662	-0.945033
H	-2.160898	-1.390755	0.914921

5_14

C	-0.901351	-1.437010	-0.186078
C	-1.373796	-0.029980	-0.514561
C	-0.516334	1.018662	0.176747
C	0.961889	0.828451	-0.139671
C	1.431889	-0.594287	0.118655
C	0.552407	-1.614340	-0.594987
H	-1.557999	-2.171092	-0.668874
H	0.647729	-1.480040	-1.681041
H	0.891203	-2.626163	-0.347506
F	-1.004732	-1.632344	1.199408
H	-1.320450	0.118157	-1.602834
F	-2.697926	0.128295	-0.130103
H	-0.679682	0.980369	1.260569
F	-0.903292	2.278636	-0.270537
F	2.739956	-0.720795	-0.350405
H	1.449115	-0.778077	1.199792
H	1.147775	1.089508	-1.191198
F	1.698670	1.706025	0.648356

5_15

C	0.723583	0.499611	1.227784
C	-0.678091	-0.089516	1.283233
C	-1.454597	0.222620	0.000000
C	-0.678091	-0.089516	-1.283233
C	0.723583	0.499611	-1.227784
C	1.484462	0.019412	0.000000
H	-2.397647	-0.336373	0.000000
H	-1.224963	0.307039	2.148266
H	-1.224963	0.307039	-2.148266
H	1.547786	-1.074278	0.000000
H	2.495859	0.440330	0.000000
F	-0.604540	-1.472401	1.414545
F	-1.739216	1.594209	0.000000
F	-0.604540	-1.472401	-1.414545
F	1.409239	0.163845	-2.391658
H	0.623594	1.594513	-1.208040
H	0.623594	1.594513	1.208040
F	1.409239	0.163845	2.391658

5_16

C	-1.430309	0.378003	-0.558448
C	-1.202486	-0.909394	0.219532
C	0.240351	-1.375988	0.026976
C	1.222790	-0.289582	0.446741
C	0.977072	1.004907	-0.310824
C	-0.464000	1.469691	-0.121400
H	0.435477	-2.295808	0.590775
H	-1.911104	-1.684369	-0.096284
H	-0.633343	1.699520	0.937457
H	-0.638762	2.378716	-0.707009
F	-1.387560	-0.682236	1.585518
F	0.406769	-1.658710	-1.333254
H	1.109014	-0.103113	1.522726
F	2.516687	-0.743127	0.219790
F	1.837068	1.985586	0.182468
H	1.219454	0.856234	-1.371102
F	-2.744028	0.802155	-0.373088
H	-1.301665	0.149983	-1.624935

5_17

C	1.234987	-0.928854	-0.477412
C	1.273783	0.569307	-0.192330
C	0.000000	1.200804	-0.745975
C	-1.273783	0.569307	-0.192330
C	-1.234987	-0.928854	-0.477412
C	0.000000	-1.579414	0.132374
H	2.153836	1.030304	-0.660091
H	0.000000	-1.427452	1.217436
H	0.000000	-2.653511	-0.082805
F	1.369846	0.777535	1.175151
H	-2.153836	1.030304	-0.660091
H	0.000000	1.047612	-1.836437
F	0.000000	2.566907	-0.513218
F	-1.369846	0.777535	1.175151
F	-2.389866	-1.522129	0.019212
H	-1.240470	-1.070259	-1.569551
F	2.389866	-1.522129	0.019212
H	1.240470	-1.070258	-1.569551

5_18

C	1.509398	-0.432246	-0.589127
C	1.097086	0.948951	-0.102518
C	-0.360644	1.184316	-0.468411
C	-1.265529	0.130262	0.155792
C	-0.808127	-1.272071	-0.224692
C	0.666686	-1.507184	0.080920
H	1.736965	1.731430	-0.529042
H	0.827347	-1.464975	1.164297
H	0.963003	-2.498221	-0.279310
F	1.229049	1.003551	1.285367
H	-0.472621	1.154034	-1.562019
F	-0.750470	2.445468	-0.041568
H	-1.279735	0.242800	1.246689
F	-2.560448	0.324993	-0.316902
F	-1.572831	-2.198563	0.480771
H	-1.018879	-1.425126	-1.293437
F	2.857214	-0.640690	-0.316163
H	1.388076	-0.464946	-1.682500

5_19

C	0.793820	0.319541	1.269620
C	-0.472568	-0.520646	1.249138
C	-1.286062	-0.213953	0.000000
C	-0.472568	-0.520646	-1.249138
C	0.793820	0.319541	-1.269620
C	1.606011	0.082959	0.000000
H	1.957380	-0.957906	0.000000
H	2.487542	0.733060	0.000000
H	-0.200316	-1.585954	1.263267
H	-2.227770	-0.776274	0.000000
F	-1.244458	-0.263261	2.373359
F	-1.606911	1.147079	0.000000
H	-0.200316	-1.585954	-1.263267
F	-1.244458	-0.263261	-2.373359
F	1.567919	-0.053497	-2.368152
H	0.524337	1.375094	-1.395725
H	0.524337	1.375094	1.395725
F	1.567919	-0.053497	2.368152

5_20

C	0.472365	-0.896818	1.248772
C	-0.292095	0.415809	1.271090
C	-0.058284	1.220877	0.000000
C	-0.292095	0.415809	-1.271090
C	0.472365	-0.896818	-1.248772
C	0.137702	-1.698180	0.000000
H	-0.933335	-1.940943	0.000000
H	0.699151	-2.638793	0.000000
H	-1.364989	0.214670	1.395804
F	0.126381	1.179089	2.355220
H	0.968196	1.612865	0.000000
F	-0.921422	2.311211	0.000000
F	0.126381	-1.637635	-2.376290
H	1.549656	-0.686803	-1.313000
H	-1.364989	0.214670	-1.395804
F	0.126381	1.179089	-2.355220
F	0.126381	-1.637635	2.376290
H	1.549656	-0.686803	1.313000

5_21

C	0.587559	-1.523423	0.133098
C	1.483337	-0.283366	0.166751
C	0.728577	1.001581	-0.167111
C	-0.746838	0.903469	0.194531
C	-1.431417	-0.198252	-0.612000
C	-0.507901	-1.384918	-0.906765
H	1.937809	-0.189585	1.160090
H	-0.021525	-1.243068	-1.881548
H	-0.869233	0.706722	1.265868
H	-1.796834	0.243729	-1.547969
H	-1.114588	-2.295466	-0.961798
H	1.213745	-2.405825	-0.045784
H	0.829767	1.209112	-1.241583
F	0.007120	-1.655929	1.402601
F	2.502265	-0.463705	-0.773104
F	1.304075	2.064846	0.519826
F	-1.356395	2.122607	-0.089100
F	-2.552514	-0.636282	0.095522

5_22

C	-1.608756	-0.293725	-0.439528
C	-1.081414	0.615664	0.665286
C	0.395552	1.000335	0.478689
C	1.107322	0.145139	-0.559765
C	0.735526	-1.317100	-0.389997
C	-0.758827	-1.544188	-0.641852
H	-1.672472	1.538053	0.706903
H	-1.091270	-2.328860	0.046755
H	0.829594	0.479211	-1.566420
H	-0.926718	-1.896524	-1.666326
H	-2.655357	-0.555218	-0.243308
H	0.904313	0.888744	1.442734
F	-1.586716	0.475897	-1.617687
F	-1.239639	-0.070936	1.869854
F	0.471316	2.337574	0.090940
F	2.483293	0.302824	-0.420407
F	1.040583	-1.692586	0.927355
H	1.355951	-1.937108	-1.047832

5_23

C	-0.129991	1.502275	0.074365
C	-1.286494	0.493641	0.196374
C	-0.951463	-0.864929	-0.405481
C	0.473550	-1.259607	-0.066268
C	1.421583	-0.335260	-0.843532
C	0.892485	1.100403	-0.977955
H	-1.551543	0.373255	1.251960
H	0.403913	1.207519	-1.956268
H	1.741976	1.792287	-0.955698
H	-0.570630	2.475256	-0.178110
H	-1.064265	-0.810393	-1.498231
F	0.494597	1.637036	1.314003
F	-2.394248	1.006757	-0.487012
F	-1.845437	-1.822394	0.059618
H	1.552766	-0.763564	-1.847174
F	2.667891	-0.347394	-0.230131
F	0.667601	-1.116354	1.302761
H	0.656123	-2.312367	-0.314654

5_24

C	-0.426565	1.517414	0.002278
C	-1.354053	0.290781	-0.030515
C	-0.610627	-0.988996	-0.382540
C	0.725221	-1.056674	0.328624
C	1.646526	0.088983	-0.118027
C	0.890648	1.276289	-0.716149
H	-1.842691	0.181177	0.943619
H	0.672902	1.057137	-1.769976
H	1.508638	2.180041	-0.682221
H	-0.970127	2.359178	-0.443333
H	-0.432622	-1.015312	-1.466681
F	-0.156465	1.845446	1.336784
F	-2.336030	0.506788	-1.001777
F	-1.388993	-2.093515	-0.057078
F	0.511014	-0.951381	1.704688
H	1.216205	-2.017030	0.132167
H	2.239201	0.389214	0.753006
F	2.523985	-0.407470	-1.090241

5_25

C	0.960062	1.262648	0.106399
C	1.467187	-0.054660	-0.504533
C	0.470263	-1.203218	-0.341859
C	-0.926218	-0.649760	-0.557551
C	-1.321565	0.255040	0.605746
C	-0.129992	1.057305	1.144372
H	1.630959	0.120484	-1.575615
H	0.313227	0.518991	1.990116
H	-0.493944	2.027549	1.500401
H	1.815940	1.807964	0.521596
F	0.437355	2.030168	-0.949851
F	2.677841	-0.409986	0.075765
F	-2.321262	1.126185	0.161715
F	-1.839056	-1.691784	-0.687336
H	-0.948103	-0.062789	-1.485236
H	-1.760732	-0.363899	1.396214
H	0.684457	-2.023404	-1.037277
F	0.560652	-1.724475	0.952413

5_26

C	-1.385000	0.924127	-0.155451
C	-1.426176	-0.527938	0.353598
C	-0.046676	-1.191969	0.369640
C	0.940686	-0.145958	0.854676
C	1.152620	0.968452	-0.182736
C	-0.141178	1.253064	-0.960280
H	-1.819735	-0.505548	1.378028
H	-0.134662	0.610118	-1.848149
H	-0.177632	2.298154	-1.285960
H	-2.298467	1.115438	-0.730068
F	-1.415409	1.764893	0.978061
F	-2.291545	-1.274889	-0.434104
F	2.151817	-0.723582	1.199220
H	0.518515	0.313272	1.760165
H	-0.036529	-2.075780	1.019443
F	0.286321	-1.615254	-0.913738
F	2.142510	0.593528	-1.085458
H	1.519612	1.863410	0.334021

5_27

C	1.148108	1.014328	0.252100
C	1.210096	-0.346007	-0.439082
C	0.216645	-1.316741	0.164265
C	-1.218702	-0.827152	-0.067095
C	-1.310655	0.693905	-0.139036
C	-0.260772	1.342016	0.751618
H	0.960055	-0.213994	-1.501174
H	-0.380393	0.977305	1.778273
H	-0.392290	2.429326	0.751830
H	1.873007	1.033593	1.073291
F	1.545326	1.984581	-0.679613
F	2.498633	-0.863234	-0.369011
H	0.339588	-2.319498	-0.260938
F	0.435758	-1.399649	1.545043
F	-1.679516	-1.379722	-1.263843
H	-1.849336	-1.191392	0.753051
H	-1.184770	1.009618	-1.183414
F	-2.586221	1.092797	0.262142

5_28

C	-1.055297	-1.211704	-0.219505
C	-1.010025	-0.086805	0.798033
C	-0.107276	1.074448	0.340250
C	1.052456	0.558813	-0.512186
C	1.467233	-0.842872	-0.108877
C	0.333976	-1.841153	-0.361463
H	0.452516	-2.665930	0.350602
H	0.726409	0.544844	-1.559491
H	0.412873	-2.252441	-1.374228
H	-1.810879	-1.953090	0.066526
H	0.292339	1.603082	1.213610
F	-1.445242	-0.691595	-1.463019
F	-0.839062	1.987360	-0.405727
F	2.135502	1.426663	-0.406629
F	-2.283038	0.384293	1.073457
H	-0.591932	-0.498447	1.725416
H	2.386899	-1.131428	-0.630555
F	1.770215	-0.834604	1.267541

5_29

C	-1.095377	-1.124646	0.430566
C	-1.541247	0.326540	0.238290
C	-0.370813	1.278865	-0.049341
C	0.835788	0.541916	-0.595409
C	1.354696	-0.468233	0.422542
C	0.217639	-1.149203	1.200139
H	0.070037	-0.631257	2.156315
H	0.551225	0.017551	-1.514518
H	2.035984	0.047152	1.109324
H	0.514796	-2.181938	1.411487
H	-1.881846	-1.698722	0.935941
F	-0.902879	-1.717501	-0.821820
F	1.839043	1.454635	-0.909774
F	2.104790	-1.433575	-0.254332
F	-2.476926	0.405322	-0.784428
H	-2.010145	0.671963	1.168662
H	-0.692045	2.071995	-0.733820
F	-0.007597	1.876877	1.168787

5_30

C	-1.342826	0.984413	-0.345534
C	-1.379764	-0.538864	-0.499531
C	-0.060630	-1.225328	-0.109455
C	0.742804	-0.346272	0.827350
C	1.129362	0.995904	0.187866
C	0.025458	1.507750	-0.753128
H	0.259090	1.134332	-1.758433
H	0.108690	-0.140501	1.698817
H	0.020236	2.602079	-0.784651
H	-2.150682	1.439263	-0.930962
F	-1.578329	1.329988	0.994753
F	1.877003	-1.009430	1.269540
F	-2.426055	-1.062068	0.249782
H	-1.556933	-0.770541	-1.557724
H	-0.271784	-2.196503	0.353615
F	0.664935	-1.451104	-1.282842
F	2.302678	0.853520	-0.547972
H	1.342873	1.718110	0.984578

5_31

C	0.619426	-1.409294	-0.307508
C	1.294012	-0.073319	-0.567275
C	0.695478	1.034355	0.293169
C	-0.830801	0.919380	0.438000
C	-1.402426	0.090302	-0.695741
C	-0.871256	-1.343547	-0.672138
H	-1.049757	-1.812719	-1.645955
H	-1.424444	-1.905901	0.087843
H	1.137737	-2.197342	-0.866684
F	0.765106	-1.714703	1.050009
F	2.659061	-0.165407	-0.323112
H	1.167476	0.189305	-1.627246
H	1.148469	1.010634	1.290203
F	0.991155	2.261410	-0.306801
H	-1.137845	0.596185	-1.635918
F	-2.793215	0.071301	-0.626367
F	-1.133574	0.312525	1.653521
H	-1.265031	1.926435	0.441469

5_32

C	0.861172	-1.098255	-0.738973
C	1.356336	0.338793	-0.575671
C	0.329558	1.285112	0.064058
C	-0.792860	0.605235	0.841273
C	-1.425143	-0.588973	0.108110
C	-0.617937	-1.073395	-1.096510
H	-0.777257	-0.380856	-1.933224
H	-0.961333	-2.068131	-1.399763
H	1.464576	-1.616636	-1.494184
F	1.021719	-1.798278	0.459965
F	2.541068	0.360190	0.145734
H	1.555819	0.736785	-1.579874
H	0.853033	2.000895	0.708760
F	-0.295799	1.990565	-0.976130
F	-0.263080	0.179762	2.058515
H	-1.578898	1.343013	1.043057
H	-1.541310	-1.392693	0.843061
F	-2.701840	-0.224848	-0.332702

5_33

C	-1.253013	-0.645813	-0.455937
C	-1.117954	0.857194	-0.226992
C	0.326142	1.235696	0.132830
C	1.335166	0.145748	-0.198253
C	0.986900	-1.196754	0.451326
C	-0.516548	-1.399232	0.638008
H	-1.440633	1.425292	-1.107398
H	-0.836666	-1.021352	1.617054
H	1.398608	0.013493	-1.286332
H	1.521763	-1.273590	1.405315
H	-0.737406	-2.470737	0.590862
H	0.365078	1.450540	1.208882
F	-1.942254	1.221991	0.838213
F	0.687523	2.396307	-0.545147
F	2.590622	0.555797	0.241629
F	1.483014	-2.207996	-0.383609
F	-2.597532	-0.989379	-0.488359
H	-0.827255	-0.895165	-1.438816

5_34

C	0.642127	-1.071760	0.501184
C	1.292117	0.292868	0.233122
C	0.293114	1.262480	-0.408440
C	-1.143568	0.905643	-0.084150
C	-1.462341	-0.445073	-0.740466
C	-0.306908	-1.450689	-0.627435
H	1.697154	0.728751	1.153306
H	0.262651	-1.480084	-1.565176
H	-0.724961	-2.447591	-0.452644
H	0.429436	1.203394	-1.497700
F	2.350817	0.125675	-0.660899
F	0.567472	2.567848	-0.017680
H	-1.695066	-0.259336	-1.797372
F	-2.613829	-0.958392	-0.149442
F	-1.291470	0.812108	1.301770
H	-1.831107	1.687198	-0.428280
F	1.639145	-2.032583	0.625213
H	0.105431	-1.025046	1.454315

5_35

C	1.115264	-0.685799	0.592408
C	1.089963	0.744785	0.039835
C	-0.321453	1.122680	-0.418142
C	-1.400265	0.334303	0.291074
C	-1.257543	-1.165638	-0.008029
C	0.198273	-1.596694	-0.214494
H	1.450127	1.463264	0.785225
H	0.448562	-1.510707	-1.279213
H	0.342425	-2.638420	0.089521
H	-0.395158	0.893633	-1.490248
F	1.932715	0.821270	-1.068503
F	-0.531220	2.487657	-0.256436
F	-1.282249	0.517101	1.676266
H	-2.394878	0.680794	-0.011601
H	-1.723988	-1.709403	0.822398
F	-1.989033	-1.441104	-1.167507
H	0.797401	-0.656279	1.641723
F	2.417573	-1.167670	0.565767

5_36

C	1.119253	0.885281	-0.368205
C	1.187814	-0.628706	-0.646628
C	-0.142357	-1.319271	-0.281937
C	-1.287039	-0.350933	-0.512076
C	-1.218154	0.813219	0.478203
C	0.225208	1.194231	0.821202
H	1.407801	-0.800779	-1.708907
H	0.566573	0.628615	1.694815
H	0.259482	2.264178	1.053449
F	2.202979	-1.207010	0.092660
F	-1.855831	1.911365	-0.119218
F	-2.504536	-1.011423	-0.391967
H	-1.230560	0.048460	-1.534702
H	-1.788443	0.551966	1.375933
H	-0.285151	-2.243831	-0.853817
F	-0.128756	-1.668372	1.068842
F	2.402273	1.376140	-0.173319
H	0.716795	1.382166	-1.263103

5_37

C	-0.808514	1.201892	0.235776
C	-1.250691	-0.097501	-0.436077
C	-0.038408	-1.003206	-0.710403
C	1.030015	-0.866238	0.353135
C	1.624087	0.547213	0.297680
C	0.608289	1.597605	-0.165713
H	0.666376	1.681197	-1.258643
H	0.844698	2.579174	0.257746
H	0.420101	-0.688234	-1.659057
F	-0.445332	-2.317948	-0.855942
F	-2.163707	-0.752041	0.377782
H	-1.759734	0.137738	-1.379902
H	1.820489	-1.612674	0.212920
F	0.473741	-1.047007	1.622108
F	2.696480	0.531704	-0.600999
H	2.021200	0.779863	1.292758
H	-0.887851	1.064112	1.320775
F	-1.684954	2.227540	-0.124392

5_38

C	1.402538	0.662553	-0.355544
C	1.259665	-0.726685	0.258803
C	-0.205843	-1.164853	0.392756
C	-1.033846	-0.492084	-0.683240
C	-1.090784	1.032635	-0.510910
C	0.239562	1.564305	0.039709
H	0.157520	1.583816	1.132844
H	-0.538996	-0.709991	-1.642456
H	0.433847	2.582996	-0.311366
F	-2.311805	-1.020569	-0.743317
F	1.924634	-1.655051	-0.546071
H	1.720001	-0.732085	1.254169
H	-0.270617	-2.256262	0.307465
F	-0.663061	-0.795605	1.657175
F	-2.112195	1.375472	0.366615
H	-1.341364	1.486393	-1.478674
H	1.478600	0.561414	-1.447159
F	2.599456	1.232251	0.080680

5_39

C	0.825885	1.046559	-0.146909
C	1.348176	-0.364344	0.086253
C	0.226245	-1.395565	0.286785
C	-1.107633	-0.918878	-0.275821
C	-1.550875	0.357736	0.445969
C	-0.385508	1.310747	0.738107
H	-0.075891	1.195758	1.784481
H	-0.727222	2.341625	0.597602
F	2.144165	-0.763201	-0.984192
H	1.966171	-0.363848	0.993828
H	0.533069	-2.344108	-0.167958
F	0.037441	-1.596750	1.661663
H	-2.039050	0.068822	1.383737
F	-2.511971	0.988777	-0.343915
F	-0.894222	-0.651878	-1.628488
H	-1.878804	-1.695469	-0.208671
F	1.834567	1.955817	0.185871
H	0.594159	1.184802	-1.207772

5_40

C	1.057493	0.901889	-0.311322
C	1.256339	-0.419272	0.414603
C	-0.049921	-1.212557	0.567549
C	-1.110970	-0.826101	-0.455456
C	-1.419702	0.677663	-0.470736
C	-0.276103	1.521818	0.087134
H	-0.357646	1.549230	1.180606
H	-0.331209	2.547240	-0.292990
F	2.188773	-1.200960	-0.263169
H	1.643947	-0.213142	1.420840
H	0.177013	-2.283343	0.502312
F	-0.590816	-0.942744	1.828531
F	-0.598323	-1.177769	-1.710759
H	-2.037660	-1.385740	-0.283119
H	-1.633313	0.943601	-1.514237
F	-2.576323	0.913218	0.272145
H	1.111295	0.732260	-1.394389
F	2.097218	1.769283	0.027735

5_41

C	1.483330	0.006001	0.483013
C	0.505985	1.166784	0.263963
C	-0.862736	0.722520	-0.241027
C	-1.246326	-0.618578	0.365882
C	-0.268012	-1.728571	-0.040004
C	1.131069	-1.212260	-0.360313
H	0.372486	1.675005	1.227856
H	-1.300059	-0.509301	1.456900
H	-0.656598	-2.215391	-0.942242
H	-0.210809	-2.480052	0.754023
H	1.883478	-2.001018	-0.243003
H	2.503219	0.354806	0.285988
H	-0.858795	0.659723	-1.335408
F	1.396160	-0.395320	1.823323
F	1.063046	2.072736	-0.632963
F	-1.803073	1.681125	0.129994
F	-2.525047	-0.963539	-0.071659
F	1.180828	-0.783795	-1.696827

5_42

C	1.145891	0.806150	0.367321
C	-0.260552	1.358261	0.125596
C	-1.269997	0.278527	-0.268428
C	-0.876784	-1.090295	0.268106
C	0.494705	-1.528743	-0.266264
C	1.405494	-0.340718	-0.584803
H	-0.608202	1.857142	1.037773
H	-0.894561	-1.068488	1.363932
H	0.333153	-2.125483	-1.170656
H	1.000160	-2.156005	0.474694
H	1.888726	1.603962	0.253245
H	-1.344449	0.232925	-1.363635
F	1.200595	0.340318	1.686045
F	-0.182333	2.305231	-0.898037
F	-2.523006	0.632312	0.222388
F	-1.838232	-2.014569	-0.140804
F	2.738614	-0.738848	-0.518709
H	1.231880	0.036850	-1.602466

5_43

C	1.081414	0.615664	0.665286
C	-0.395552	1.000335	0.478689
C	-1.107322	0.145139	-0.559765
C	-0.735526	-1.317100	-0.389997
C	0.758827	-1.544188	-0.641852
C	1.608756	-0.293725	-0.439528
H	-0.904313	0.888744	1.442734
H	0.926718	-1.896524	-1.666326
H	1.091270	-2.328860	0.046755
H	1.672472	1.538053	0.706903
H	-0.829594	0.479211	-1.566420
F	1.239639	-0.070936	1.869854
F	-0.471316	2.337574	0.090940
F	-2.483293	0.302824	-0.420407
H	2.655357	-0.555218	-0.243307
F	1.586716	0.475897	-1.617687
F	-1.040583	-1.692586	0.927354
H	-1.355951	-1.937108	-1.047832

5_44

C	0.830801	0.919381	0.438000
C	-0.695478	1.034355	0.293168
C	-1.294012	-0.073320	-0.567275
C	-0.619426	-1.409294	-0.307508
C	0.871257	-1.343547	-0.672137
C	1.402426	0.090302	-0.695741
H	-1.148469	1.010634	1.290203
H	1.049758	-1.812719	-1.645954
H	1.424444	-1.905901	0.087843
H	1.265031	1.926435	0.441468
H	-1.167476	0.189304	-1.627246
F	1.133574	0.312526	1.653521
F	-0.991156	2.261410	-0.306801
F	-2.659061	-0.165407	-0.323113
F	-0.765106	-1.714703	1.050009
H	-1.137737	-2.197343	-0.866683
H	1.137845	0.596185	-1.635918
F	2.793215	0.071301	-0.626367

5_45

C	-1.375105	-0.472684	-0.363139
C	-0.807008	0.923647	-0.665133
C	0.666607	1.088754	-0.283708
C	1.366912	-0.219763	-0.601196
C	0.924122	-1.324117	0.358613
C	-0.583533	-1.293333	0.652477
H	-0.892768	1.060170	-1.751720
H	1.448916	-1.179482	1.309049
H	1.215301	-2.296085	-0.052663
H	-2.419376	-0.373166	-0.046101
F	-1.339263	-1.207477	-1.561756
F	-1.569303	1.897091	-0.040026
F	-0.825896	-0.728429	1.906579
F	2.748997	-0.057177	-0.514336
H	-0.995855	-2.309349	0.671202
H	1.137202	-0.487260	-1.641849
H	1.119801	1.923898	-0.832302
F	0.789333	1.367797	1.071416

5_46

C	1.285845	0.502525	0.289320
C	0.041812	1.387599	0.468654
C	-1.259299	0.662544	0.107155
C	-1.140993	-0.776987	0.577860
C	-0.094910	-1.537489	-0.245844
C	1.031877	-0.607784	-0.712852
H	0.001899	1.675801	1.526789
H	-0.594813	-1.983096	-1.111505
H	0.343455	-2.338027	0.358740
H	2.142290	1.119513	-0.005362
F	1.573032	-0.073775	1.535784
F	0.164684	2.534803	-0.301642
F	-2.378398	-1.409915	0.476074
H	-0.866451	-0.766749	1.640980
H	-2.129507	1.161123	0.550108
F	-1.434813	0.680015	-1.278106
F	2.201663	-1.343613	-0.898107
H	0.781631	-0.138642	-1.671531

5_47

C	1.354053	0.290782	-0.030514
C	0.610627	-0.988996	-0.382540
C	-0.725221	-1.056674	0.328623
C	-1.646525	0.088983	-0.118027
C	-0.890648	1.276290	-0.716149
C	0.426564	1.517414	0.002279
H	0.432623	-1.015311	-1.466682
H	-1.508638	2.180041	-0.682221
H	-0.672902	1.057138	-1.769975
H	1.842691	0.181177	0.943619
F	2.336030	0.506790	-1.001776
F	1.388994	-2.093515	-0.057078
H	-1.216205	-2.017030	0.132164
F	-0.511014	-0.951383	1.704688
H	0.970127	2.359179	-0.443331
F	0.156464	1.845445	1.336785
F	-2.523985	-0.407469	-1.090241
H	-2.239200	0.389213	0.753006

5_48

C	-0.624984	-1.038478	0.374462
C	0.894429	-0.860347	0.535393
C	1.459511	0.356425	-0.195782
C	0.537418	1.561149	-0.015186
C	-0.878673	1.293925	-0.546582
C	-1.164717	-0.192451	-0.762774
H	1.089501	-0.736364	1.606636
H	-1.042405	1.833617	-1.484786
H	-1.586684	1.674629	0.198135
H	-0.852182	-2.099096	0.214739
F	-1.239035	-0.638938	1.563951
F	1.557820	-1.999376	0.089560
H	2.475132	0.572423	0.155934
F	1.537806	0.104741	-1.569385
F	0.497883	1.820117	1.362851
H	0.979817	2.439489	-0.498706
H	-0.710972	-0.551498	-1.693399
F	-2.542265	-0.381494	-0.873171

5_49

C	-1.479080	0.518324	-0.132985
C	-0.265542	1.182993	0.538445
C	0.969876	0.255452	0.577482
C	0.969638	-0.735106	-0.573285
C	-0.262610	-1.648006	-0.494493
C	-1.476541	-0.978688	0.148726
H	1.021691	-0.193449	-1.524680
H	-0.003038	-2.519719	0.118286
H	-0.527745	-2.002973	-1.495314
H	-2.409376	-1.448412	-0.182503
H	-2.409344	1.005450	0.181354
H	0.964842	-0.306113	1.520155
F	-1.380961	0.656931	-1.519098
F	2.119239	1.027257	0.551353
F	2.114274	-1.530332	-0.485901
F	-1.418473	-1.115769	1.549826
F	0.028393	2.342927	-0.158763
H	-0.533721	1.466275	1.562610

5_50

C	-1.234740	-0.161827	-0.766799
C	-0.504696	1.098013	-0.276033
C	0.906434	0.768318	0.216901
C	1.466222	-0.473031	-0.460893
C	0.605357	-1.713883	-0.181557
C	-0.868561	-1.380920	0.055931
H	-0.433030	1.823895	-1.096227
H	1.562596	-0.276674	-1.538326
H	0.991115	-2.200475	0.721223
H	0.699730	-2.421312	-1.013156
H	-1.522924	-2.225206	-0.192377
H	0.876364	0.618840	1.302691
F	-1.219712	1.698601	0.747878
F	1.742376	1.849754	-0.049763
F	2.755280	-0.707430	0.014347
F	-1.063217	-1.095259	1.412882
H	-0.918332	-0.359451	-1.802497
F	-2.600906	0.056598	-0.781637

5_51

C	1.210096	-0.346007	-0.439082
C	0.216645	-1.316741	0.164265
C	-1.218702	-0.827152	-0.067095
C	-1.310655	0.693905	-0.139036
C	-0.260772	1.342016	0.751618
C	1.148108	1.014328	0.252100
H	0.339588	-2.319498	-0.260938
H	-1.184770	1.009618	-1.183414
H	-0.380393	0.977305	1.778273
H	-0.392290	2.429327	0.751830
H	-1.849336	-1.191392	0.753051
F	0.435758	-1.399649	1.545043
F	-1.679516	-1.379722	-1.263843
F	-2.586221	1.092797	0.262142
F	1.545326	1.984580	-0.679613
H	1.873007	1.033593	1.073291
F	2.498633	-0.863234	-0.369011
H	0.960055	-0.213994	-1.501174

5_52

C	1.010025	-0.086805	0.798033
C	0.107276	1.074448	0.340250
C	-1.052456	0.558813	-0.512186
C	-1.467233	-0.842872	-0.108877
C	-0.333976	-1.841153	-0.361463
C	1.055297	-1.211704	-0.219505
H	-0.292339	1.603082	1.213610
H	-0.412874	-2.252441	-1.374228
H	-0.452516	-2.665930	0.350602
H	-0.726409	0.544844	-1.559491
F	0.839062	1.987360	-0.405727
F	-2.135502	1.426663	-0.406629
H	1.810879	-1.953090	0.066526
F	1.445242	-0.691595	-1.463019
F	-1.770215	-0.834604	1.267541
H	-2.386899	-1.131428	-0.630555
H	0.591932	-0.498447	1.725416
F	2.283038	0.384293	1.073457

5_53

C	-0.835787	0.541919	-0.595409
C	0.370810	1.278872	-0.049336
C	1.541249	0.326551	0.238292
C	1.095380	-1.124638	0.430574
C	-0.217641	-1.149218	1.200134
C	-1.354692	-0.468244	0.422531
H	0.692049	2.072002	-0.733810
H	-0.070060	-0.631297	2.156328
H	-0.514791	-2.181963	1.411447
H	2.010159	0.671987	1.168653
F	0.007586	1.876869	1.168789
F	2.476921	0.405326	-0.784436
F	0.902893	-1.717498	-0.821812
H	1.881850	-1.698709	0.935954
H	-2.035981	0.047136	1.109314
F	-2.104789	-1.433581	-0.254347
F	-1.839046	1.454641	-0.909758
H	-0.551232	0.017567	-1.514527

6_1

C	-0.374711	1.277686	0.683284
C	-0.959582	0.923090	-0.683282
C	-0.138929	-0.084229	-1.487740
C	0.374711	-1.277686	-0.683284
C	0.959582	-0.923090	0.683282
C	0.138929	0.084229	1.487740
H	-0.760719	-0.461209	-2.309797
H	-1.051425	1.845023	-1.271599
H	-1.149673	1.785455	1.271602
H	1.149673	-1.785455	-1.271602
H	1.051425	-1.845023	1.271599
H	0.760719	0.461209	2.309797
F	0.688502	2.154017	0.483916
F	-2.228252	0.385639	-0.483914
F	0.960590	0.582391	-2.021406
F	-0.688502	-2.154017	-0.483916
F	2.228252	-0.385639	0.483914
F	-0.960590	-0.582391	2.021407

6_2

C	0.441276	0.503717	1.272129
C	-0.407570	-0.769441	1.290635
C	-1.189208	-1.029132	0.000000
C	-0.407570	-0.769441	-1.290635
C	0.441276	0.503717	-1.272129
C	1.270233	0.562870	0.000000
H	-1.509388	-2.079093	0.000000
H	-1.116388	-0.721106	2.126134
H	1.108787	0.505599	2.143577
H	-1.116388	-0.721106	-2.126134
H	1.108787	0.505599	-2.143577
F	-0.407570	1.595548	1.378082
F	0.458486	-1.847083	1.491772
F	-2.315165	-0.214367	0.000000
F	0.458486	-1.847083	-1.491772

F	-0.407570	1.595548	-1.378082
F	2.069973	1.697074	0.000000
H	1.924203	-0.320351	0.000000

6_3

C	-0.921098	1.154619	-0.143700
C	-0.656295	0.395092	-1.443607
C	0.656295	-0.395092	-1.443607
C	0.921098	-1.154619	-0.143700
C	0.707410	-0.277466	1.082523
C	-0.707410	0.277466	1.082523
H	0.635515	-1.107783	-2.277112
H	-0.635515	1.107783	-2.277112
H	-1.942005	1.555846	-0.147920
H	1.942005	-1.555846	-0.147920
F	-0.033217	2.229613	-0.099612
F	-1.707324	-0.499294	-1.637451
F	1.707324	0.499294	-1.637451
F	0.033217	-2.229613	-0.099612
F	-0.921098	1.038018	2.223502
H	-1.431122	-0.546664	1.075777
H	1.431122	0.546664	1.075777
F	0.921098	-1.038018	2.223502

6_4

C	0.807355	-0.168203	1.287621
C	1.625871	-0.028020	0.000000
C	0.807355	-0.168203	-1.287621
C	-0.437347	0.708965	-1.231424
C	-1.300656	0.461620	0.000000
C	-0.437347	0.708965	1.231424
H	1.427742	0.139772	-2.139507
H	2.431746	-0.770856	0.000000
H	1.427742	0.139772	2.139507
F	0.477723	-1.502352	1.455031
F	2.187962	1.256303	0.000000
F	0.477723	-1.502352	-1.455031
H	-0.092068	1.752361	-1.192219
F	-1.185823	0.549776	-2.386364
F	-1.185823	0.549776	2.386364
H	-0.092068	1.752361	1.192219
H	-2.153892	1.153460	0.000000
F	-1.809605	-0.824218	0.000000

6_5

C	-1.277347	-0.925377	-0.026467
C	0.000000	-1.651587	0.398876
C	1.277347	-0.925377	-0.026467
C	1.239978	0.542980	0.372599
C	0.000000	1.248449	-0.158522
C	-1.239978	0.542980	0.372599
H	2.149119	-1.411478	0.429063
H	0.000000	-2.666868	-0.014017
H	-2.149119	-1.411478	0.429063
F	-1.394120	-1.031800	-1.408002
F	0.000000	-1.725563	1.796174
F	1.394120	-1.031800	-1.408002
H	0.000000	1.275918	-1.254118

F	0.000000	2.556269	0.313459
H	1.243845	0.611286	1.469271
F	2.382103	1.171943	-0.098162
F	-2.382103	1.171943	-0.098162
H	-1.243845	0.611286	1.469271

6_6

C	0.764150	1.277588	0.052754
C	-0.764150	1.277588	-0.052754
C	-1.238494	0.000000	-0.731542
C	-0.764150	-1.277588	-0.052754
C	0.764150	-1.277588	0.052754
C	1.238494	0.000000	0.731542
H	-1.101857	2.146469	-0.630660
H	1.101857	2.146469	0.630660
F	1.279525	1.390087	-1.235450
F	-1.279525	1.390087	1.235450
H	1.101857	-2.146469	0.630659
F	1.279525	-1.390087	-1.235450
H	-0.812876	0.000000	-1.744174
F	-2.622159	0.000000	-0.835901
H	-1.101857	-2.146469	-0.630659
F	-1.279525	-1.390087	1.235450
F	2.622159	0.000000	0.835901
H	0.812876	0.000000	1.744174

6_7

C	-0.452383	-1.471081	0.156921
C	1.045843	-1.166215	0.200116
C	1.354482	0.011713	-0.717981
C	0.518651	1.248206	-0.414169
C	-0.962991	0.891224	-0.497967
C	-1.283827	-0.234279	0.474515
H	1.617694	-2.043750	-0.125596
H	-0.702355	-2.281089	0.851584
F	-0.745152	-1.905628	-1.141751
F	1.388248	-0.891350	1.517793
H	1.116982	-0.309956	-1.741848
F	2.704453	0.319507	-0.664005
H	0.759789	2.050750	-1.122716
F	0.799577	1.721339	0.862396
F	-2.629974	-0.562168	0.387804
H	-1.069844	0.093308	1.499068
H	-1.217289	0.579157	-1.519192
F	-1.719777	2.010986	-0.190004

6_8

C	-0.401002	-0.649797	-1.441273
C	0.401002	0.649797	-1.441273
C	0.082738	1.460379	-0.194167
C	0.361357	0.671234	1.076643
C	-0.361357	-0.671234	1.076643
C	-0.082738	-1.460379	-0.194167
H	0.195740	1.242743	-2.339998
H	-0.195740	-1.242743	-2.339998
F	-1.754821	-0.302993	-1.446510
F	1.754821	0.302993	-1.446510

H	1.441203	0.515109	1.192300
F	-0.082738	1.411546	2.166230
H	-0.976398	1.746974	-0.218475
F	0.843950	2.620600	-0.195392
F	-0.843950	-2.620600	-0.195392
H	0.976398	-1.746974	-0.218475
H	-1.441203	-0.515109	1.192300
F	0.082738	-1.411546	2.166230

6_9

C	0.813060	1.269700	-0.195251
C	1.424652	0.000000	-0.776396
C	0.813060	-1.269700	-0.195251
C	-0.693259	-1.247145	-0.431304
C	-1.342267	0.000000	0.156418
C	-0.693259	1.247145	-0.431304
H	1.257332	2.153792	-0.670429
F	1.062077	1.355767	1.165854
H	1.228777	0.000000	-1.860063
F	2.796507	0.000000	-0.593815
F	1.062077	-1.355767	1.165854
H	1.257332	-2.153792	-0.670429
F	-2.688790	0.000000	-0.190482
H	-1.264003	0.000000	1.249586
F	-1.261844	-2.379369	0.127186
H	-0.892516	-1.273034	-1.513094
H	-0.892516	1.273034	-1.513094
F	-1.261844	2.379369	0.127186

6_10

C	-0.645633	-1.302158	0.000000
C	-0.622558	-0.438167	1.255135
C	0.622558	0.438167	1.255135
C	0.645633	1.302158	0.000000
C	0.622558	0.438167	-1.255135
C	-0.622558	-0.438167	-1.255135
H	-1.518760	-1.965200	0.000000
F	0.496545	-2.110125	0.000000
H	-1.517493	0.195533	1.294516
F	-0.622558	-1.258247	2.373238
F	0.622558	1.258247	2.373238
H	1.517493	-0.195533	1.294516
H	1.518760	1.965200	0.000000
F	-0.496545	2.110125	0.000000
F	-0.622558	-1.258247	-2.373238
H	-1.517493	0.195533	-1.294516
H	1.517493	-0.195533	-1.294516
F	0.622558	1.258247	-2.373238

6_11

C	-0.193944	-1.533962	0.000000
C	-0.568357	-0.739209	1.240201
C	0.189310	0.579418	1.277654
C	-0.030022	1.381532	0.000000
C	0.189310	0.579418	-1.277654
C	-0.568357	-0.739209	-1.240201
H	-0.682872	-2.515530	0.000000
F	1.186767	-1.743832	0.000000
H	-1.650058	-0.541769	1.239830
F	-0.273553	-1.478047	2.374876

F	-0.273553	1.333440	2.349983
H	1.258547	0.391035	1.429969
H	1.258547	0.391035	-1.429969
F	-0.273553	1.333440	-2.349983
H	-1.053485	1.782296	0.000000
F	0.842082	2.462687	0.000000
F	-0.273553	-1.478047	-2.374876
H	-1.650058	-0.541769	-1.239830

6_12

C	-0.380147	-1.273380	-0.632588
C	-1.070075	-0.788002	0.632588
C	-0.171647	0.120758	1.456753
C	0.380147	1.273380	0.632588
C	1.070075	0.788002	-0.632588
C	0.171647	-0.120758	-1.456753
H	-1.996861	-0.258716	0.371902
F	-1.414878	-1.890359	1.402558
F	-0.910704	0.640698	2.510504
H	0.656237	-0.461674	1.883855
H	1.996861	0.258716	-0.371902
F	1.414877	1.890359	-1.402558
H	-0.431130	1.966854	0.371901
F	1.301196	1.970337	1.402557
F	0.910704	-0.640698	-2.510504
H	-0.656237	0.461674	-1.883855
H	0.431130	-1.966854	-0.371901
F	-1.301196	-1.970337	-1.402557

6_13

C	-0.571861	-1.378831	-0.502644
C	-1.461216	-0.136026	-0.385451
C	-0.734973	1.070262	0.201027
C	0.734973	1.070262	-0.201027
C	1.461216	-0.136026	0.385451
C	0.571861	-1.378831	0.502644
H	-1.810605	0.121380	-1.393476
H	0.830058	1.064668	-1.294097
H	1.810605	0.121380	1.393476
H	1.191632	-2.276366	0.396386
H	-1.191632	-2.276366	-0.396386
H	-0.830058	1.064668	1.294097
F	0.011630	-1.377195	-1.773290
F	-2.569076	-0.436401	0.399357
F	-1.334628	2.231140	-0.273127
F	1.334628	2.231140	0.273127
F	2.569076	-0.436401	-0.399358
F	-0.011630	-1.377195	1.773290

6_14

C	-0.555678	-1.336048	0.369192
C	0.965061	-1.254696	0.209600
C	1.447822	0.121289	-0.255731
C	0.491237	1.237367	0.145508
C	-0.915867	1.033305	-0.424520
C	-1.205536	-0.453557	-0.675335
H	1.437215	-1.495859	1.168876
H	0.420972	1.296700	1.238034

H	-1.004548	1.592286	-1.364557
H	-0.886738	-2.376143	0.269838
H	1.570323	0.111617	-1.347412
F	-0.876668	-0.887058	1.650077
F	1.353335	-2.208400	-0.732849
F	2.696361	0.375447	0.299337
F	1.002025	2.443965	-0.320359
F	-1.843294	1.558041	0.461233
F	-2.568676	-0.668818	-0.749850
H	-0.767205	-0.733167	-1.645357

6_15

C	1.212855	-1.013461	0.506253
C	1.455189	0.444139	0.087843
C	0.179168	1.181604	-0.310346
C	-0.978942	0.696677	0.550515
C	-1.284885	-0.802537	0.332652
C	-0.046184	-1.585245	-0.131044
H	1.902230	0.965184	0.944624
H	-0.715921	0.854074	1.605136
H	2.096651	-1.608133	0.251482
H	-0.034265	1.038316	-1.375161
F	1.024798	-1.055272	1.895160
F	2.364148	0.470398	-0.962529
F	0.367521	2.542414	-0.086707
F	-2.111433	1.442387	0.285119
H	-0.162794	-2.655488	0.075143
F	0.110570	-1.431609	-1.506778
F	-2.272879	-0.955832	-0.622823
H	-1.653639	-1.233392	1.270555

6_16

C	-0.982054	-1.186415	0.307640
C	0.458948	-1.503901	-0.106201
C	1.342143	-0.261203	-0.252964
C	0.781345	0.899656	0.555713
C	-0.605676	1.303294	0.033893
C	-1.447105	0.086820	-0.363319
H	0.902246	-2.164699	0.647928
H	0.704165	0.613470	1.610945
H	-1.635807	-2.026161	0.046677
H	1.408906	0.022605	-1.311269
F	-1.012177	-1.027446	1.697842
F	0.410283	-2.183741	-1.323846
F	2.624670	-0.562160	0.190173
F	1.633522	1.985441	0.469868
F	-0.444400	2.099661	-1.098892
H	-1.137991	1.895159	0.786748
H	-1.340363	-0.052183	-1.448042
F	-2.788205	0.319611	-0.088652

6_17

C	0.084281	-1.265149	0.674177
C	1.304792	-0.362601	0.421959
C	1.024588	0.753170	-0.576833
C	-0.336927	1.367814	-0.302837
C	-1.410738	0.348484	-0.689999
C	-1.025243	-1.102837	-0.361775
H	1.611737	0.078669	1.376450
H	0.426393	-2.306910	0.665231

H	1.049101	0.345096	-1.596235
F	-0.458821	-0.986295	1.923920
F	2.353115	-1.141190	-0.064563
F	2.014006	1.723927	-0.481150
H	-1.919888	-1.652458	-0.048069
H	-1.549188	0.392702	-1.778531
F	-2.609544	0.676873	-0.080538
F	-0.532250	-1.678156	-1.542985
F	-0.433212	1.672228	1.051358
H	-0.462324	2.303131	-0.861390

6_18

C	0.248307	-1.401406	0.557590
C	1.357238	-0.425722	0.125742
C	0.823466	0.798743	-0.606225
C	-0.411762	1.347782	0.086794
C	-1.543261	0.310214	0.174766
C	-1.089882	-1.117870	-0.120027
H	1.897735	-0.101884	1.022607
H	0.578991	-2.420657	0.328431
H	0.572566	0.531239	-1.638507
F	0.039961	-1.293224	1.934231
F	2.247645	-1.096056	-0.709521
F	1.808118	1.778883	-0.642956
F	-0.057330	1.711161	1.389993
H	-0.775049	2.243212	-0.430008
F	-0.891832	-1.284104	-1.491858
H	-1.854480	-1.837224	0.195583
H	-1.929184	0.345731	1.199952
F	-2.568252	0.646577	-0.700988

6_19

C	-0.311765	-1.380864	0.245729
C	1.145252	-0.975821	-0.030564
C	1.276258	0.471296	-0.492496
C	0.311764	1.380863	0.245734
C	-1.145252	0.975822	-0.030562
C	-1.276258	-0.471294	-0.492497
H	1.732181	-1.127883	0.881806
H	-0.457225	-2.422421	-0.063647
H	1.055679	0.525590	-1.567988
F	-0.561470	-1.293506	1.613288
F	1.649640	-1.803242	-1.035155
F	2.581811	0.905506	-0.309935
F	0.561468	1.293498	1.613292
H	0.457226	2.422422	-0.063638
H	-1.732183	1.127884	0.881806
F	-1.649638	1.803245	-1.035154
F	-2.581812	-0.905504	-0.309937
H	-1.055680	-0.525585	-1.567989

6_20

C	0.187165	-1.431431	0.286759
C	1.449035	-0.591487	0.546008
C	1.279453	0.880475	0.148991
C	-0.132450	1.315678	0.496596
C	-1.165556	0.610274	-0.384983
C	-0.673392	-0.793550	-0.787623

H	1.655641	-0.643925	1.622317
H	-0.345182	1.056114	1.541953
H	-1.352151	1.214468	-1.280183
H	0.472125	-2.451485	0.005104
F	-0.532075	-1.491994	1.484325
F	2.524908	-1.130737	-0.142374
F	-0.251494	2.693125	0.360545
F	-2.357479	0.517777	0.318251
H	2.021478	1.514594	0.647174
F	1.472749	1.023177	-1.227925
F	-1.752624	-1.603905	-1.091027
H	-0.053310	-0.696505	-1.687010

6_21

C	-1.456913	0.491297	0.206409
C	-1.285673	-1.036012	0.270783
C	0.174352	-1.476601	0.105788
C	1.042320	-0.461503	0.830373
C	1.031362	0.906337	0.120211
C	-0.322100	1.156708	-0.547951
H	-1.644998	-1.357872	1.256362
H	0.629558	-0.324366	1.839134
H	-2.424077	0.737541	-0.245190
F	-1.458137	0.972936	1.525321
F	-2.065381	-1.634938	-0.705519
F	2.339151	-0.923370	0.959238
H	0.333649	-2.486636	0.501312
F	0.502129	-1.500680	-1.246842
F	2.024313	0.951112	-0.845581
H	1.233386	1.704287	0.844446
H	-0.285938	0.746461	-1.564010
F	-0.557815	2.523743	-0.636142

6_22

C	1.134858	0.534778	0.540556
C	-0.043203	1.481402	0.281918
C	-1.301328	0.737087	-0.185122
C	-1.301328	-0.737088	0.185122
C	-0.043202	-1.481402	-0.281917
C	1.134858	-0.534778	-0.540556
H	-0.276289	2.066553	1.178875
H	-1.378933	-0.842077	1.275196
H	-0.276288	-2.066555	-1.178874
H	-1.378932	0.842077	-1.275196
F	0.322035	2.373939	-0.723918
F	-2.424482	1.334944	0.375482
F	-2.424482	-1.334945	-0.375482
F	0.322036	-2.373939	0.723919
F	2.311818	-1.254912	-0.537960
H	1.028907	-0.062740	-1.527358
H	1.028908	0.062740	1.527358
F	2.311818	1.254912	0.537959