

Supporting Information

Conformational Behavior and Stacking Interactions of Contorted Polycyclic Aromatics

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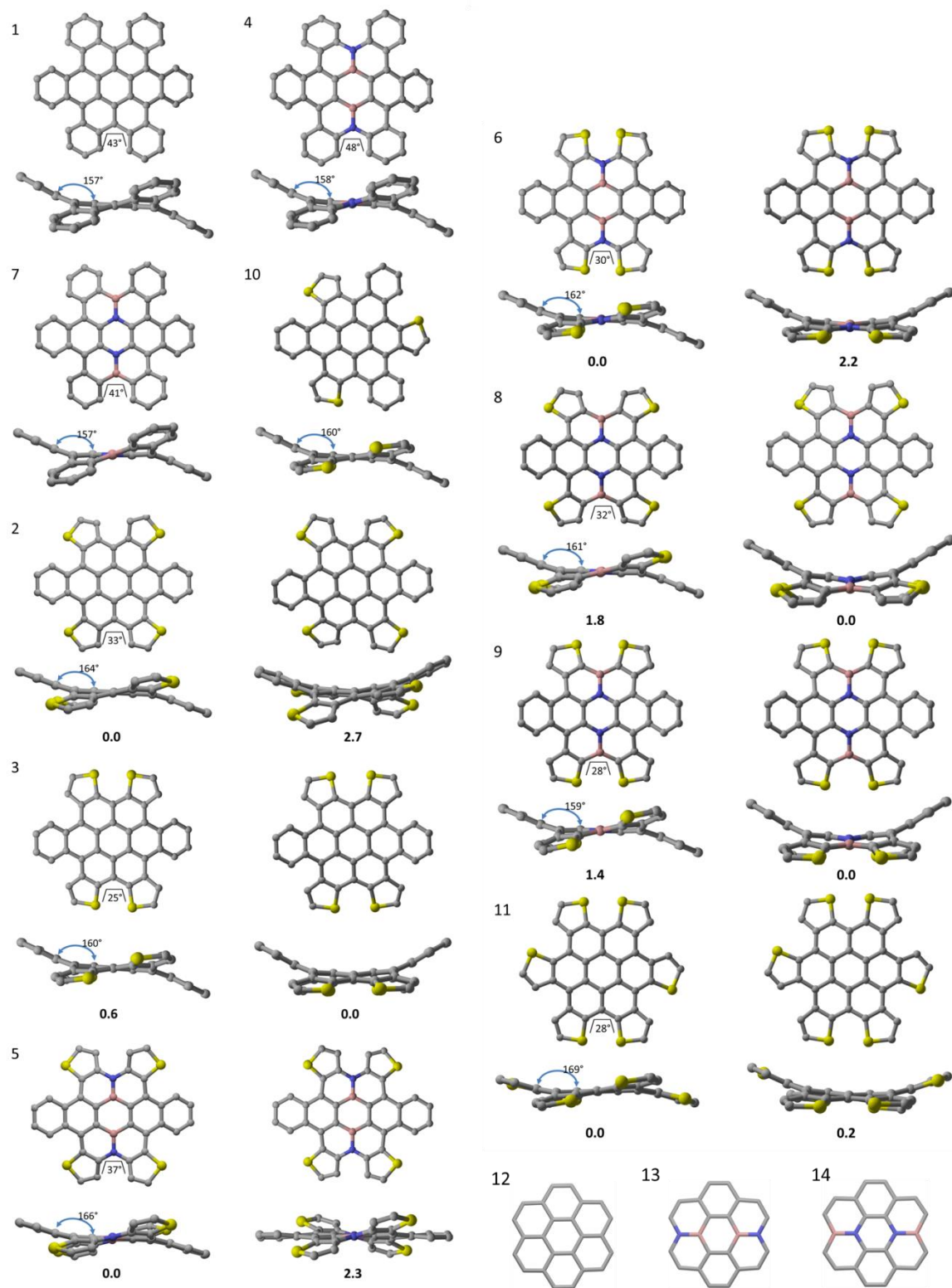
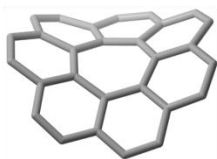
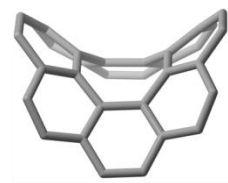


Figure S1. Optimized structures of molecules 1 – 14.

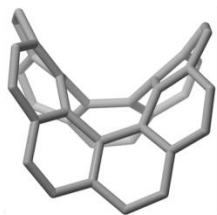
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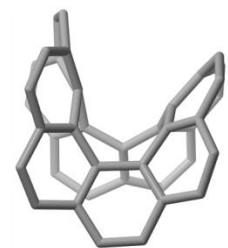


Figure S2. Optimized structures of molecules **15 – 18**.

Table S1. Dispersion corrected B97/TZV(2d,2p) electronic energies for monomers **1-18**.^a

Mol	Conf	d2 ^b	zero ^c	bj ^d	bjm ^e	zero_abc ^f	bj_abc ^g	bjm_abc ^h	zero_tz_abc ⁱ
1	planar	1842.6583	1842.6548	1842.8604	1843.1195	1842.6555	1842.8610	1843.1201	1842.6372
	UD	1842.9100	1842.9046	1843.1058	1843.3660	1842.9048	1843.1059	1843.3661	1842.8862
2	planar	3126.1732	3126.1804	3126.3714	3126.6381	3126.1809	3126.3718	3126.6385	3126.1647
	UD	3126.2160	3126.2230	3126.4095	3126.6720	3126.2232	3126.4098	3126.6722	3126.2071
	TS	3126.2117	3126.2188	3126.4058	3126.6685	3126.2190	3126.4060	3126.6687	3126.2029
3	planar	3126.1579	3126.1634	3126.3555	3126.6246	3126.1639	3126.3560	3126.6251	3126.1478
	S	3126.2192	3126.2234	3126.4111	3126.6748	3126.2236	3126.4113	3126.6750	3126.2075
	UD	3126.2182	3126.2224	3126.4097	3126.6724	3126.2226	3126.4099	3126.6726	3126.2065
4	planar	1849.5420	1849.5381	1849.7348	1849.9903	1849.5387	1849.7354	1849.9909	1849.5201
	UD	1849.7698	1849.7645	1849.9577	1850.2151	1849.7646	1849.9578	1850.2152	1849.7456
5	planar	3133.0253	3133.0324	3133.2147	3133.4779	3133.0329	3133.2152	3133.4783	3133.0163
	UD	3133.0660	3133.0725	3133.2508	3133.5103	3133.0728	3133.2511	3133.5105	3133.0562
	TD	3133.0623	3133.0690	3133.2480	3133.5081	3133.0692	3133.2482	3133.5084	3133.0526
6	planar	3133.0035	3133.0086	3133.1928	3133.4585	3133.0090	3133.1933	3133.4590	3132.9927
	UD	3133.0510	3133.0551	3133.2356	3133.4962	3133.0553	3133.2359	3133.4964	3133.0390
	S	3133.0476	3133.0515	3133.2328	3133.4950	3133.0518	3133.2331	3133.4953	3133.0354
7	planar	1849.5248	1849.5216	1849.7180	1849.9734	1849.5222	1849.7186	1849.9740	1849.5036
	UD	1849.7734	1849.7694	1849.9619	1850.2185	1849.7695	1849.9620	1850.2186	1849.7507
8	planar	3133.0269	3133.0345	3133.2165	3133.4800	3133.0349	3133.2170	3133.4804	3133.0183
	S	3133.0751	3133.0837	3133.2620	3133.5212	3133.0839	3133.2622	3133.5214	3133.0675
	UD	3133.0722	3133.0811	3133.2593	3133.5185	3133.0813	3133.2595	3133.5187	3133.0649
9	planar	3133.0097	3133.0153	3133.1989	3133.4636	3133.0158	3133.1993	3133.4641	3132.9992
	S	3133.0901	3133.0939	3133.2719	3133.5296	3133.0941	3133.2721	3133.5297	3133.0777
	UD	3133.0880	3133.0921	3133.2699	3133.5273	3133.0923	3133.2701	3133.5275	3133.0759
10	planar	2805.3121	2805.3168	2805.5120	2805.7778	2805.3173	2805.5125	2805.7783	2805.3005
	UD	2805.3909	2805.3948	2805.5849	2805.8467	2805.3950	2805.5851	2805.8469	2805.3782
11	planar	3767.8621	3767.8731	3768.0560	3768.3248	3767.8735	3768.0564	3768.3252	3767.8584
	UD	3767.8760	3767.8864	3768.0664	3768.3310	3767.8866	3768.0666	3768.3313	3767.8716
	TS	3767.8756	3767.8859	3768.0663	3768.3315	3767.8862	3768.0665	3768.3318	3767.8713
12	planar	921.4909	921.4914	921.5902	921.7191	921.4915	921.5903	921.7192	921.4834
13	planar	928.3266	928.3269	928.4190	928.5457	928.3269	928.4191	928.5458	928.3185
14	planar	928.3321	928.3330	928.4239	928.5487	928.3330	928.4239	928.5488	928.3243
15	planar	1074.9728	1074.9702	1075.0852	1075.2347	1074.9703	1075.0853	1075.2348	1074.9599
	S	1074.9894	1074.9880	1075.1031	1075.2534	1074.9880	1075.1032	1075.2534	1074.9779
16	planar	1228.2995	1228.2957	1228.4261	1228.5932	1228.2960	1228.4264	1228.5934	1228.2843
	S	1228.4995	1228.4984	1228.6308	1228.8022	1228.4981	1228.6305	1228.8019	1228.4868
17	S	1382.0391	1382.0374	1382.1876	1382.3801	1382.0368	1382.1869	1382.3795	1382.0241
18	S	1535.5978	1535.5949	1535.7634	1535.9770	1535.5937	1535.7622	1535.9759	1535.5795

a: all energies listed are absolute values of the electronic energies. All electronic energies are negative (Hartree)

b: D2 dispersion correction (i.e. “B97-D”)

c: D3 dispersion with default damping

d: D3 dispersion with Becke-Johnson damping

e: D3 dispersion with D3M(BJ), i.e., Becke-Johnson damping with the refitted parameters by Sherrill and coworkers

f: D3 dispersion with three-body correction and default damping

g: D3 dispersion with three-body correction and Becke-Johnson damping

h: three-body interaction considered in the D3 dispersion with D3M(BJ), i.e., Becke-Johnson damping with the refitted parameters by Sherrill and coworkers

i: three-body interaction considered with use of special parameters for calculations with triple-zeta basis sets

Table S2. Dispersion corrected B97/TZV(2d,2p) electronic energies for dimers of **1-18**.^a

Mol	Conf	d2	zero	bj	bjm	zero_tz	zero_abc	bj_abc	bjm_abc	zero_tz_abc
1	UD1	3685.8844	3685.8622	3686.2838	3686.7924	3685.8226	3685.8553	3686.2769	3686.7856	3685.8157
2	UD1	6252.4988	6252.5096	6252.9029	6253.4153	6252.4753	6252.5034	6252.8967	6253.4091	6252.4691
	S2	6252.4982	6252.5065	6252.9022	6253.4154	6252.4718	6252.5001	6252.8958	6253.4090	6252.4654
	S1	6252.4943	6252.5049	6252.9000	6253.4136	6252.4703	6252.4986	6252.8938	6253.4074	6252.4641
	UD2	6252.4936	6252.5057	6252.8949	6253.4068	6252.4725	6252.4998	6252.8891	6253.4010	6252.4666
3	S1	6252.5048	6252.5079	6252.9041	6253.4195	6252.4733	6252.5017	6252.8980	6253.4133	6252.4672
	UD2	6252.5045	6252.5099	6252.9045	6253.4169	6252.4755	6252.5037	6252.8982	6253.4107	6252.4693
	UD1	6252.5039	6252.5077	6252.9039	6253.4178	6252.4730	6252.5016	6252.8977	6253.4116	6252.4668
	S2	6252.5038	6252.5081	6252.9024	6253.4175	6252.4738	6252.5019	6252.8962	6253.4113	6252.4677
4	UD2	3699.6111	3699.5847	3699.9915	3700.4956	3699.5437	3699.5778	3699.9846	3700.4887	3699.5368
	UD1	3699.6098	3699.5842	3699.9911	3700.4951	3699.5433	3699.5773	3699.9843	3700.4883	3699.5364
5	UD2	6266.2057	6266.2110	6266.5889	6267.0965	6266.1753	6266.2049	6266.5828	6267.0904	6266.1692
	UD1	6266.2047	6266.2096	6266.5886	6267.0977	6266.1737	6266.2036	6266.5825	6267.0916	6266.1676
	TD1	6266.1930	6266.1994	6266.5781	6267.0870	6266.1640	6266.1933	6266.5721	6267.0809	6266.1579
	TD2	6266.1916	6266.1976	6266.5769	6267.0863	6266.1619	6266.1916	6266.5708	6267.0802	6266.1559
6	UD2	6266.1749	6266.1759	6266.5578	6267.0674	6266.1407	6266.1698	6266.5517	6267.0613	6266.1346
	UD1	6266.1723	6266.1716	6266.5538	6267.0635	6266.1362	6266.1656	6266.5478	6267.0575	6266.1302
	S1	6266.1648	6266.1645	6266.5484	6267.0610	6266.1294	6266.1584	6266.5423	6267.0548	6266.1233
	S2	6266.1635	6266.1642	6266.5470	6267.0589	6266.1292	6266.1580	6266.5408	6267.0526	6266.1229
7	UD2	3699.6119	3699.5896	3699.9936	3700.4959	3699.5493	3699.5828	3699.9868	3700.4891	3699.5425
	UD1	3699.6114	3699.5886	3699.9930	3700.4954	3699.5483	3699.5818	3699.9861	3700.4885	3699.5414
8	S2	6266.2268	6266.2337	6266.6120	6267.1195	6266.1980	6266.2274	6266.6056	6267.1131	6266.1917
	S1	6266.2198	6266.2292	6266.6073	6267.1159	6266.1938	6266.2230	6266.6011	6267.1097	6266.1876
	UD2	6266.2144	6266.2255	6266.6026	6267.1102	6266.1903	6266.2193	6266.5964	6267.1040	6266.1841
	UD1	6266.2126	6266.2238	6266.6006	6267.1093	6266.1884	6266.2177	6266.5945	6267.1031	6266.1823
9	S2	6266.2489	6266.2489	6266.6238	6267.1289	6266.2137	6266.2427	6266.6176	6267.1227	6266.2075
	S1	6266.2455	6266.2456	6266.6221	6267.1270	6266.2103	6266.2395	6266.6160	6267.1210	6266.2042
	UD2	6266.2448	6266.2474	6266.6229	6267.1262	6266.2124	6266.2412	6266.6168	6267.1200	6266.2062
	UD1	6266.2437	6266.2439	6266.6209	6267.1253	6266.2085	6266.2378	6266.6147	6267.1191	6266.2023
10	UD4	5610.8500	5610.8529	5611.2536	5611.7648	5610.8171	5610.8465	5611.2472	5611.7584	5610.8107
	UD1	5610.8487	5610.8512	5611.2518	5611.7631	5610.8154	5610.8448	5611.2454	5611.7567	5610.8091
	UD5	5610.8476	5610.8535	5611.2547	5611.7669	5610.8177	5610.8473	5611.2485	5611.7607	5610.8115
	UD3	5610.8460	5610.8499	5611.2520	5611.7645	5610.8140	5610.8437	5611.2458	5611.7582	5610.8078
11	UD1	7535.8194	7535.8391	7536.2205	7536.7385	7535.8068	7535.8334	7536.2148	7536.7328	7535.8012
	UD6	7535.8195	7535.8400	7536.2199	7536.7353	7535.8075	7535.8343	7536.2142	7536.7296	7535.8019
	UD2	7535.8186	7535.8391	7536.2192	7536.7346	7535.8066	7535.8334	7536.2135	7536.7290	7535.8009
	UD3	7535.8185	7535.8385	7536.2193	7536.7366	7535.8064	7535.8328	7536.2137	7536.7309	7535.8007
	S1	7535.8179	7535.8375	7536.2196	7536.7388	7535.8053	7535.8318	7536.2139	7536.7331	7535.7996
	S2	7535.8144	7535.8362	7536.2157	7536.7300	7535.8041	7535.8304	7536.2099	7536.7242	7535.7983
12	Conf1	1843.0169	1843.0129	1843.2210	1843.4721	1842.9957	1843.0103	1843.2183	1843.4695	1842.9931
	Conf2	1843.0156	1843.0119	1843.2200	1843.4705	1842.9949	1843.0091	1843.2172	1843.4678	1842.9921
13	Conf1	1856.6939	1856.6848	1856.8805	1857.1286	1856.6666	1856.6820	1856.8777	1857.1258	1856.6638
	Conf2	1856.6936	1856.6843	1856.8799	1857.1283	1856.6659	1856.6815	1856.8771	1857.1255	1856.6631
	Conf3	1856.6925	1856.6845	1856.8791	1857.1275	1856.6664	1856.6820	1856.8766	1857.1249	1856.6638
	Conf4	1856.6901	1856.6824	1856.8770	1857.1250	1856.6644	1856.6798	1856.8744	1857.1223	1856.6618
14	Conf1	1856.7046	1856.6973	1856.8900	1857.1343	1856.6784	1856.6944	1856.8872	1857.1314	1856.6755
	Conf2	1856.7039	1856.6969	1856.8894	1857.1336	1856.6781	1856.6940	1856.8865	1857.1307	1856.6752
	Conf3	1856.7026	1856.6967	1856.8884	1857.1324	1856.6780	1856.6940	1856.8857	1857.1297	1856.6754
	Conf4	1856.7024	1856.6963	1856.8882	1857.1322	1856.6776	1856.6936	1856.8855	1857.1295	1856.6749
15	Conf1	2150.0202	2150.0115	2150.2542	2150.5472	2149.9899	2150.0080	2150.2507	2150.5438	2149.9864
16	Conf1	2457.0361	2457.0288	2457.3035	2457.6400	2457.0049	2457.0249	2457.2996	2457.6361	2457.0010
17	Conf1	2764.1047	2764.0981	2764.4042	2764.7851	2764.0718	2764.0944	2764.4004	2764.7814	2764.0681
18	Conf1	3071.2190	3071.2109	3071.5518	3071.9756	3071.1814	3071.2066	3071.5475	3071.9713	3071.1771

Table S3. Binding energies of stacked dimers **1-18** relative to lowest lying isolated monomers (kcal mol⁻¹).

Mol	Conf	d2	zero	bj	bjm	zero_tz	zero_abc	bj_abc	bjm_abc	zero_tz_abc
1	UD1	-40.4	-33.2	-45.3	-37.9	-31.6	-28.8	-40.8	-33.5	-27.2
2	UD1	-41.9	-39.9	-52.6	-44.8	-38.6	-35.7	-48.4	-40.6	-34.4
	S2	-41.5	-38.0	-52.2	-44.8	-36.5	-33.7	-47.9	-40.5	-32.1
	S1	-39.1	-36.9	-50.8	-43.7	-35.5	-32.7	-46.6	-39.5	-31.3
	UD2	-38.7	-37.5	-47.6	-39.5	-36.9	-33.5	-43.6	-35.5	-32.9
3	S1	-41.7	-38.3	-51.4	-43.9	-36.9	-34.2	-47.3	-39.8	-32.7
	UD2	-41.5	-39.6	-51.6	-42.3	-38.3	-35.4	-47.4	-38.1	-34.1
	UD1	-41.1	-38.2	-51.3	-42.8	-36.7	-34.1	-47.1	-38.7	-32.5
	S2	-41.1	-38.5	-50.3	-42.7	-37.2	-34.3	-46.1	-38.5	-33.1
4	UD2	-44.9	-35.0	-47.8	-41.0	-33.1	-30.5	-43.3	-36.5	-28.6
	UD1	-44.1	-34.7	-47.6	-40.7	-32.8	-30.2	-43.1	-36.3	-28.4
5	UD2	-46.2	-41.4	-54.7	-47.6	-39.8	-37.2	-50.6	-43.5	-35.7
	UD1	-45.6	-40.5	-54.5	-48.4	-38.8	-36.4	-50.4	-44.3	-34.7
	TD1	-38.3	-34.1	-48.0	-41.7	-32.7	-30.0	-43.8	-37.5	-28.6
	TD2	-37.4	-33.0	-47.2	-41.2	-31.4	-28.9	-43.1	-37.1	-27.3
6	UD2	-45.7	-41.3	-54.3	-47.1	-39.7	-37.1	-50.1	-42.9	-35.6
	UD1	-44.1	-38.6	-51.8	-44.7	-36.9	-34.4	-47.7	-40.5	-32.8
	S1	-39.4	-34.1	-48.4	-43.0	-32.6	-30.0	-44.3	-38.9	-28.5
	S2	-38.6	-33.9	-47.5	-41.7	-32.5	-29.7	-43.3	-37.5	-28.2
7	UD2	-40.9	-31.9	-43.8	-37.0	-30.2	-27.5	-39.4	-32.5	-25.8
	UD1	-40.5	-31.3	-43.4	-36.6	-29.6	-26.9	-39.0	-32.2	-25.1
8	S2	-48.1	-41.7	-55.2	-48.4	-39.9	-37.4	-51.0	-44.2	-35.6
	S1	-43.7	-38.8	-52.2	-46.1	-37.2	-34.7	-48.1	-42.0	-33.1
	UD2	-40.3	-36.5	-49.3	-42.6	-35.0	-32.4	-45.2	-38.5	-30.9
	UD1	-39.2	-35.4	-48.0	-42.0	-33.8	-31.3	-44.0	-37.9	-29.7
9	S2	-43.1	-38.3	-50.2	-43.8	-36.8	-34.2	-46.1	-39.7	-32.7
	S1	-41.0	-36.2	-49.1	-42.6	-34.7	-32.2	-45.1	-38.6	-30.6
	UD2	-40.5	-37.4	-49.7	-42.1	-36.0	-33.3	-45.6	-38.0	-31.9
	UD1	-39.8	-35.2	-48.4	-41.5	-33.5	-31.1	-44.3	-37.4	-29.5
10	UD4	-42.8	-39.7	-52.5	-44.8	-38.3	-35.4	-48.3	-40.6	-34.0
	UD1	-42.0	-38.6	-51.4	-43.8	-37.2	-34.3	-47.2	-39.5	-33.0
	UD5	-41.3	-40.1	-53.2	-46.1	-38.7	-35.9	-49.1	-42.0	-34.5
	UD3	-40.3	-37.8	-51.5	-44.6	-36.4	-33.7	-47.4	-40.5	-32.2
11	UD1	-42.3	-41.6	-55.0	-48.0	-40.2	-37.7	-51.1	-43.4	-36.3
	UD6	-42.4	-42.2	-54.7	-45.9	-40.7	-38.3	-50.8	-41.4	-36.8
	UD2	-41.8	-41.6	-54.3	-45.5	-40.1	-37.7	-50.3	-41.0	-36.2
	UD3	-41.7	-41.3	-54.3	-46.8	-40.0	-37.4	-50.4	-42.2	-36.0
	S1	-41.4	-40.6	-54.5	-48.2	-39.2	-36.7	-50.6	-43.6	-35.3
	S2	-39.2	-39.8	-52.1	-42.6	-38.5	-35.8	-48.1	-38.0	-34.5
12	Conf1	-22.0	-18.9	-25.4	-21.3	-18.2	-17.2	-23.7	-19.5	-16.5
	Conf2	-21.2	-18.2	-24.8	-20.3	-17.7	-16.4	-22.9	-18.4	-15.9
13	Conf1	-25.5	-19.5	-26.7	-23.3	-18.6	-17.7	-24.8	-21.5	-16.7
	Conf2	-25.4	-19.2	-26.3	-23.1	-18.2	-17.3	-24.4	-21.3	-16.3
	Conf3	-24.7	-19.3	-25.8	-22.7	-18.5	-17.6	-24.1	-21.0	-16.7
	Conf4	-23.2	-18.0	-24.5	-21.1	-17.2	-16.3	-22.8	-19.3	-15.5
14	Conf1	-25.4	-19.7	-26.5	-23.1	-18.7	-17.8	-24.7	-21.2	-16.9
	Conf2	-24.9	-19.5	-26.1	-22.7	-18.6	-17.6	-24.2	-20.8	-16.7
	Conf3	-24.1	-19.3	-25.5	-22.0	-18.5	-17.5	-23.8	-20.2	-16.8
	Conf4	-24.0	-19.0	-25.4	-21.8	-18.3	-17.3	-23.6	-20.0	-16.5
15	Conf1	-26.0	-22.3	-30.0	-25.4	-21.5	-20.1	-27.8	-23.2	-19.3
16	Conf1	-23.3	-20.2	-26.3	-22.3	-19.3	-18.0	-24.2	-20.2	-17.2
17	Conf1	-16.6	-14.6	-18.2	-15.6	-13.9	-13.1	-16.7	-14.1	-12.4
18	Conf1	-14.7	-13.3	-15.7	-13.5	-12.5	-12.0	-14.5	-12.3	-11.3

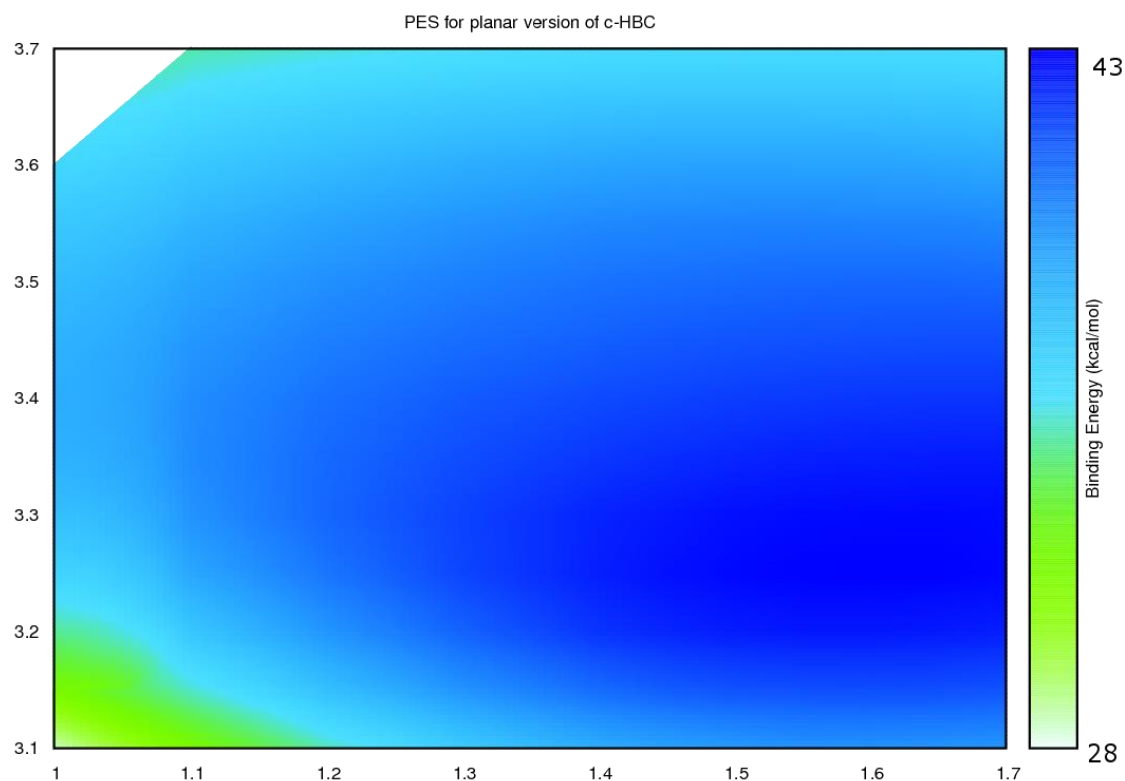


Figure S3. Interaction energies of a hypothetical planar c-HBC (**1**) with respect to displacement distance and stacking distance. The minimum energy structure is at a displacement distance of 1.5-1.7 Å and stacking distance of 3.25 Å.

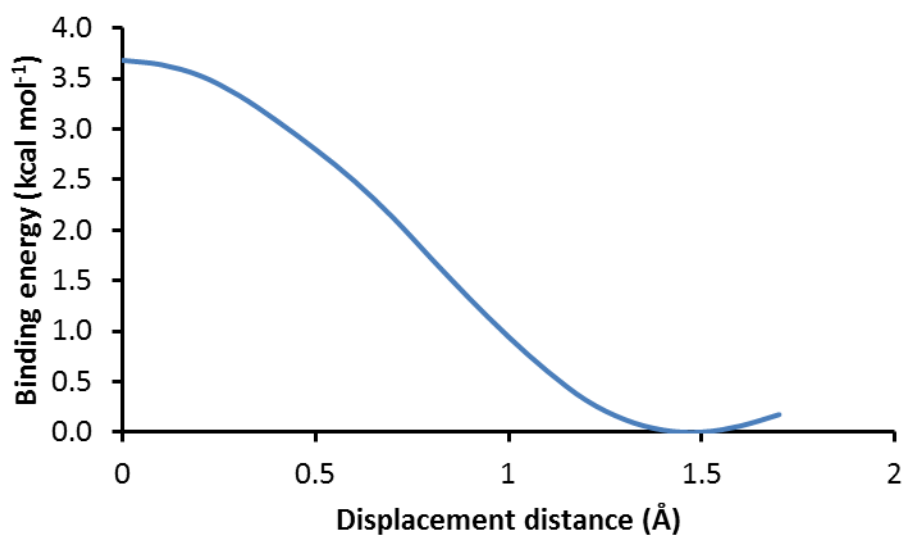


Figure S4. Binding energy in coronene dimer as a function of displacement distance at a stacking distance of 3.62 Å.

Optimized Cartesian Coordinates

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molecule1_conf1

C	1.2069840	0.4225960	3.5252910
C	2.4491590	0.4223150	2.8080160
C	2.4668130	0.0000290	1.4241660
C	3.6564440	-0.4224090	0.7171660
C	3.6564440	-0.4224090	-0.7171660
C	2.4668130	0.0000290	-1.4241660
C	2.4491590	0.4223150	-2.8080160
C	1.2069840	0.4225960	-3.5252910
C	0.0000000	0.0000000	-2.8485250
C	-1.2069840	-0.4225960	-3.5252910
C	-2.4491590	-0.4223150	-2.8080160
C	-2.4668130	-0.0000290	-1.4241660
C	-3.6564440	0.4224090	-0.7171660
C	-3.6564440	0.4224090	0.7171660
C	-2.4668130	-0.0000290	1.4241660
C	-2.4491590	-0.4223150	2.8080160
C	-1.2069840	-0.4225960	3.5252910
C	0.0000000	0.0000000	2.8485250
C	0.0000000	0.0000000	1.4391330
C	1.2462330	0.0003250	0.7195440
C	1.2462330	0.0003250	-0.7195440
C	0.0000000	0.0000000	-1.4391330
C	-1.2462330	-0.0003250	-0.7195440
C	-1.2462330	-0.0003250	0.7195440
C	-1.1822920	-0.9716800	4.8325920
C	-2.3234710	-1.4758090	5.4311270
C	-3.5413930	-1.4755120	4.7278610
C	-3.5935750	-0.9714080	3.4402480
C	3.5935750	0.9714080	3.4402480
C	3.5413930	1.4755120	4.7278610
C	2.3234710	1.4758090	5.4311270
C	1.1822920	0.9716800	4.8325920
C	4.7763100	-0.9712820	-1.3921080
C	5.8651390	-1.4757600	-0.7031980

C	5.8651390	-1.4757600	0.7031980
C	4.7763100	-0.9712820	1.3921080
C	1.1822920	0.9716800	-4.8325920
C	2.3234710	1.4758090	-5.4311270
C	3.5413930	1.4755120	-4.7278610
C	3.5935750	0.9714080	-3.4402480
C	-3.5935750	-0.9714080	-3.4402480
C	-3.5413930	-1.4755120	-4.7278610
C	-2.3234710	-1.4758090	-5.4311270
C	-1.1822920	-0.9716800	-4.8325920
C	-4.7763100	0.9712820	1.3921080
C	-5.8651390	1.4757600	0.7031980
C	-5.8651390	1.4757600	-0.7031980
C	-4.7763100	0.9712820	-1.3921080
H	-0.2332390	-1.0540380	5.3498670
H	-2.2649130	-1.9121740	6.4253030
H	-4.4319150	-1.9114300	5.1741890
H	-4.5160760	-1.0541200	2.8768960
H	4.5160760	1.0541200	2.8768960
H	4.4319150	1.9114300	5.1741890
H	2.2649130	1.9121740	6.4253030
H	0.2332390	1.0540380	5.3498670
H	4.7497270	-1.0532820	-2.4727160
H	6.6968990	-1.9118880	-1.2511220
H	6.6968990	-1.9118880	1.2511220
H	4.7497270	-1.0532820	2.4727160
H	0.2332390	1.0540380	-5.3498670
H	2.2649130	1.9121740	-6.4253030
H	4.4319150	1.9114300	-5.1741890
H	4.5160760	1.0541200	-2.8768960
H	-4.5160760	-1.0541200	-2.8768960
H	-4.4319150	-1.9114300	-5.1741890
H	-2.2649130	-1.9121740	-6.4253030
H	-0.2332390	-1.0540380	-5.3498670
H	-4.7497270	1.0532820	2.4727160
H	-6.6968990	1.9118880	1.2511220
H	-6.6968990	1.9118880	-1.2511220
H	-4.7497270	1.0532820	-2.4727160

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molecule2_conf1

C	0.0150710	1.2538640	0.7211690
C	0.0150710	1.2538640	-0.7211690
C	0.0000000	0.0000000	-1.4319050
C	-0.0150710	-1.2538640	-0.7211690
C	-0.0150710	-1.2538640	0.7211690
C	0.0000000	0.0000000	1.4319050
C	0.0170280	2.4893800	1.4297960
C	0.3326430	3.7092920	0.7149580
C	0.3326430	3.7092920	-0.7149580
C	0.0170280	2.4893800	-1.4297960
C	0.0000000	0.0000000	2.8524200
C	-0.3029660	1.2173250	3.5354180
C	-0.2832460	2.4334060	2.8247540
C	-0.0170280	-2.4893800	1.4297960
C	0.2832460	-2.4334060	2.8247540
C	0.3029660	-1.2173250	3.5354180
C	-0.0170280	-2.4893800	-1.4297960
C	-0.3326430	-3.7092920	-0.7149580
C	-0.3326430	-3.7092920	0.7149580
C	0.0000000	0.0000000	-2.8524200
C	0.3029660	-1.2173250	-3.5354180
C	0.2832460	-2.4334060	-2.8247540
C	-0.2832460	2.4334060	-2.8247540
C	-0.3029660	1.2173250	-3.5354180
C	0.7418590	4.8883420	1.3855990
C	1.1065850	6.0345360	0.7017910
C	1.1065850	6.0345360	-0.7017910
C	0.7418590	4.8883420	-1.3855990
C	-0.7418590	-4.8883420	-1.3855990
C	-1.1065850	-6.0345360	-0.7017910
C	-1.1065850	-6.0345360	0.7017910
C	-0.7418590	-4.8883420	1.3855990
C	-0.7534550	1.3771120	4.8870990
C	-1.0704830	2.6681950	5.1901560
S	-0.8166620	3.7399980	3.8616260
S	0.8166620	-3.7399980	3.8616260

C	1.0704830	-2.6681950	5.1901560
C	0.7534550	-1.3771120	4.8870990
S	-0.8166620	3.7399980	-3.8616260
C	-1.0704830	2.6681950	-5.1901560
C	-0.7534550	1.3771120	-4.8870990
C	0.7534550	-1.3771120	-4.8870990
C	1.0704830	-2.6681950	-5.1901560
S	0.8166620	-3.7399980	-3.8616260
H	0.8327750	4.8848330	2.4648580
H	1.4289950	6.9137620	1.2540020
H	1.4289950	6.9137620	-1.2540020
H	0.8327750	4.8848330	-2.4648580
H	-0.8327750	-4.8848330	-2.4648580
H	-1.4289950	-6.9137620	-1.2540020
H	-1.4289950	-6.9137620	1.2540020
H	-0.8327750	-4.8848330	2.4648580
H	-0.8988820	0.5568000	5.5782300
H	-1.4608660	3.0548720	6.1237050
H	1.4608660	-3.0548720	6.1237050
H	0.8988820	-0.5568000	5.5782300
H	-1.4608660	3.0548720	-6.1237050
H	-0.8988820	0.5568000	-5.5782300
H	0.8988820	-0.5568000	-5.5782300
H	1.4608660	-3.0548720	-6.1237050

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molecule2_conf2

C	0.7872240	1.1937050	-0.0835340
C	-0.6487900	1.2883400	-0.1705450
C	-1.4254800	0.0929500	0.0174120
C	-0.7872240	-1.1937050	-0.0835340
C	0.6487900	-1.2883400	-0.1705450
C	1.4254800	-0.0929500	0.0174120
C	1.5629130	2.3806030	-0.0478840
C	0.9715820	3.6097860	-0.5304420
C	-0.4469380	3.6910970	-0.7050040
C	-1.2765020	2.5557730	-0.3327180
C	2.8202220	-0.1817010	0.2778010

C	3.4961380	1.0121530	0.7026130	H	0.6144770	-6.8005060	-2.1425010
C	2.8819410	2.2626620	0.4804160	H	2.0259340	-4.9186410	-1.5401010
C	1.2765020	-2.5557730	-0.3327180	H	5.3114250	0.3112010	1.7999420
C	2.6909040	-2.6043300	-0.1479440	H	5.8848580	2.7981060	2.2991960
C	3.4604170	-1.4532050	0.1508990	H	6.1104190	-3.5563190	0.1359520
C	-1.5629130	-2.3806030	-0.0478840	H	5.6389620	-1.0083890	0.3610080
C	-0.9715820	-3.6097860	-0.5304420	H	-6.1104190	3.5563190	0.1359520
C	0.4469380	-3.6910970	-0.7050040	H	-5.6389620	1.0083890	0.3610080
C	-2.8202220	0.1817010	0.2778010	H	-5.3114250	-0.3112010	1.7999420
C	-3.4961380	-1.0121530	0.7026130	H	-5.8848580	-2.7981060	2.2991960
C	-2.8819410	-2.2626620	0.4804160				
C	-2.6909040	2.6043300	-0.1479440				
C	-3.4604170	1.4532050	0.1508990	60			
C	1.7706850	4.7042280	-0.9403700	molecule3_conf1			
C	1.2199180	5.8506590	-1.4859940	C	-1.2476150	0.0360410	0.7224270
C	-0.1679800	5.9272060	-1.6736140	C	-1.2476150	0.0360410	-0.7224270
C	-0.9715820	4.8620330	-1.3024600	C	0.0000000	0.0000000	-1.4381780
C	-1.7706850	-4.7042280	-0.9403700	C	1.2476150	-0.0360410	-0.7224270
C	-1.2199180	-5.8506590	-1.4859940	C	1.2476150	-0.0360410	0.7224270
C	0.1679800	-5.9272060	-1.6736140	C	0.0000000	0.0000000	1.4381780
C	0.9715820	-4.8620330	-1.3024600	C	-2.4797380	0.0893710	1.4232510
C	4.7225580	1.1415780	1.4359360	C	-3.7027680	-0.2224680	0.7153260
C	5.0338020	2.4358540	1.7355030	C	-3.7027680	-0.2224680	-0.7153260
S	3.8642630	3.5521570	1.1383000	C	-2.4797380	0.0893710	-1.4232510
S	3.7271350	-4.0182190	-0.1795530	C	0.0000000	0.0000000	2.8688560
C	5.1398780	-3.0759350	0.1107290	C	-1.2256220	0.3078450	3.5212330
C	4.8614780	-1.7501070	0.2488790	C	-2.4456250	0.3993050	2.8231580
S	-3.7271350	4.0182190	-0.1795530	C	2.4797380	-0.0893710	1.4232510
C	-5.1398780	3.0759350	0.1107290	C	2.4456250	-0.3993050	2.8231580
C	-4.8614780	1.7501070	0.2488790	C	1.2256220	-0.3078450	3.5212330
C	-4.7225580	-1.1415780	1.4359360	C	2.4797380	-0.0893710	-1.4232510
C	-5.0338020	-2.4358540	1.7355030	C	3.7027680	0.2224680	-0.7153260
S	-3.8642630	-3.5521570	1.1383000	C	3.7027680	0.2224680	0.7153260
H	2.8500960	4.6241720	-0.8871630	C	0.0000000	0.0000000	-2.8688560
H	1.8668990	6.6642260	-1.8043800	C	1.2256220	-0.3078450	-3.5212330
H	-0.6144770	6.8005060	-2.1425010	C	2.4456250	-0.3993050	-2.8231580
H	-2.0259340	4.9186410	-1.5401010	C	-2.4456250	0.3993050	-2.8231580
H	-2.8500960	-4.6241720	-0.8871630	C	-1.2256220	0.3078450	-3.5212330
H	-1.8668990	-6.6642260	-1.8043800	C	-4.8684200	-0.6675270	1.3895270

C	-6.0036200	-1.0599210	0.7026960
C	-6.0036200	-1.0599210	-0.7026960
C	-4.8684200	-0.6675270	-1.3895270
C	4.8684200	0.6675270	-1.3895270
C	6.0036200	1.0599210	-0.7026960
C	6.0036200	1.0599210	0.7026960
C	4.8684200	0.6675270	1.3895270
S	-1.4308260	0.7423790	5.1985290
C	-3.1022560	1.0998250	4.9533810
C	-3.5026470	0.8798330	3.6679300
C	3.5026470	-0.8798330	3.6679300
C	3.1022560	-1.0998250	4.9533810
S	1.4308260	-0.7423790	5.1985290
C	-3.5026470	0.8798330	-3.6679300
C	-3.1022560	1.0998250	-4.9533810
S	-1.4308260	0.7423790	-5.1985290
S	1.4308260	-0.7423790	-5.1985290
C	3.1022560	-1.0998250	-4.9533810
C	3.5026470	-0.8798330	-3.6679300
H	-4.8492670	-0.7755730	2.4666190
H	-4.8492670	-0.7755730	-2.4666190
H	4.8492670	0.7755730	-2.4666190
H	4.8492670	0.7755730	2.4666190
H	-3.6951250	1.4787660	5.7768470
H	-4.5033720	1.1031310	3.3207150
H	4.5033720	-1.1031310	3.3207150
H	3.6951250	-1.4787660	5.7768470
H	-4.5033720	1.1031310	-3.3207150
H	-3.6951250	1.4787660	-5.7768470
H	3.6951250	-1.4787660	-5.7768470
H	4.5033720	-1.1031310	-3.3207150
H	-6.8718710	-1.4158850	1.2519890
H	-6.8718710	-1.4158850	-1.2519890
H	6.8718710	1.4158850	1.2519890
H	6.8718710	1.4158850	-1.2519890

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molecule3_conf2

C	1.2381230	0.7222580	0.1132600
C	1.2381230	-0.7222580	0.1132600
C	0.0000000	-1.4364200	-0.0303050
C	-1.2381230	-0.7222580	0.1132600
C	-1.2381230	0.7222580	0.1132600
C	0.0000000	1.4364200	-0.0303050
C	2.4671550	1.4208520	0.1926110
C	3.6274130	0.7154640	0.6976860
C	3.6274130	-0.7154640	0.6976860
C	2.4671550	-1.4208520	0.1926110
C	0.0000000	2.8496750	-0.2594310
C	1.2672610	3.4837710	-0.4034770
C	2.4847510	2.7993230	-0.1942380
C	-2.4671550	1.4208520	0.1926110
C	-2.4847510	2.7993230	-0.1942380
C	-1.2672610	3.4837710	-0.4034770
C	-2.4671550	-1.4208520	0.1926110
C	-3.6274130	-0.7154640	0.6976860
C	-3.6274130	0.7154640	0.6976860
C	0.0000000	-2.8496750	-0.2594310
C	-1.2672610	-3.4837710	-0.4034770
C	-2.4847510	-2.7993230	-0.1942380
C	2.4847510	-2.7993230	-0.1942380
C	1.2672610	-3.4837710	-0.4034770
C	4.7075650	1.3903550	1.3184030
C	5.7674290	0.7025210	1.8844500
C	5.7674290	-0.7025210	1.8844500
C	4.7075650	-1.3903550	1.3184030
C	-4.7075650	-1.3903550	1.3184030
C	-5.7674290	-0.7025210	1.8844500
C	-5.7674290	0.7025210	1.8844500
C	-4.7075650	1.3903550	1.3184030
S	1.5619280	5.1292970	-0.9046320
C	3.2705810	4.8861750	-0.8933950
C	3.6168890	3.6250890	-0.5075200
C	-3.6168890	3.6250890	-0.5075200
C	-3.2705810	4.8861750	-0.8933950
S	-1.5619280	5.1292970	-0.9046320
C	3.6168890	-3.6250890	-0.5075200

C	3.2705810	-4.8861750	-0.8933950
S	1.5619280	-5.1292970	-0.9046320
S	-1.5619280	-5.1292970	-0.9046320
C	-3.2705810	-4.8861750	-0.8933950
C	-3.6168890	-3.6250890	-0.5075200
H	4.6702520	2.4680350	1.4202250
H	4.6702520	-2.4680350	1.4202250
H	-4.6702520	-2.4680350	1.4202250
H	-4.6702520	2.4680350	1.4202250
H	3.9278810	5.6917520	-1.1968960
H	4.6421820	3.2789670	-0.4984210
H	-4.6421820	3.2789670	-0.4984210
H	-3.9278810	5.6917520	-1.1968960
H	4.6421820	-3.2789670	-0.4984210
H	3.9278810	-5.6917520	-1.1968960
H	-3.9278810	-5.6917520	-1.1968960
H	-4.6421820	-3.2789670	-0.4984210
H	6.5696300	1.2513940	2.3717390
H	6.5696300	-1.2513940	2.3717390
H	-6.5696300	1.2513940	2.3717390
H	-6.5696300	-1.2513940	2.3717390

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molecule4_conf1

C	-2.4442860	0.3930710	2.8526540
C	-1.1840900	0.4235020	3.5503790
C	1.1840900	-0.4235020	3.5503790
C	2.4442860	-0.3930710	2.8526540
C	2.5265380	-0.0002000	1.4400870
C	3.7245530	0.3987770	0.7249130
C	3.7245530	0.3987770	-0.7249130
C	2.5265380	-0.0002000	-1.4400870
C	2.4442860	-0.3930710	-2.8526540
C	1.1840900	-0.4235020	-3.5503790
C	-1.1840900	0.4235020	-3.5503790
C	-2.4442860	0.3930710	-2.8526540
C	-2.5265380	0.0002000	-1.4400870
C	-3.7245530	-0.3987770	-0.7249130

C	-3.7245530	-0.3987770	0.7249130
C	-2.5265380	0.0002000	1.4400870
C	-1.3384830	0.0393360	0.7129730
C	1.3384830	-0.0393360	0.7129730
C	1.3384830	-0.0393360	-0.7129730
C	-1.3384830	0.0393360	-0.7129730
C	-4.8548710	-0.9346010	1.3930630
C	-5.9483310	-1.4272480	0.7033060
C	-5.9483310	-1.4272480	-0.7033060
C	-4.8548710	-0.9346010	-1.3930630
C	-1.1228390	1.0058190	4.8299300
C	-2.2552800	1.5092570	5.4571350
C	-3.4894300	1.4732730	4.7990020
C	-3.5641360	0.9424300	3.5188040
C	3.5641360	-0.9424300	3.5188040
C	3.4894300	-1.4732730	4.7990020
C	2.2552800	-1.5092570	5.4571350
C	1.1228390	-1.0058190	4.8299300
C	4.8548710	0.9346010	-1.3930630
C	5.9483310	1.4272480	-0.7033060
C	5.9483310	1.4272480	0.7033060
C	4.8548710	0.9346010	1.3930630
C	1.1228390	-1.0058190	-4.8299300
C	2.2552800	-1.5092570	-5.4571350
C	3.4894300	-1.4732730	-4.7990020
C	3.5641360	-0.9424300	-3.5188040
C	-3.5641360	0.9424300	-3.5188040
C	-3.4894300	1.4732730	-4.7990020
C	-2.2552800	1.5092570	-5.4571350
C	-1.1228390	1.0058190	-4.8299300
H	-4.8325370	-1.0173520	2.4739190
H	-6.7868700	-1.8514730	1.2504310
H	-6.7868700	-1.8514730	-1.2504310
H	-4.8325370	-1.0173520	-2.4739190
H	-0.1601050	1.0985770	5.3185550
H	-2.1653380	1.9633790	6.4408030
H	-4.3765830	1.8963830	5.2630990
H	-4.5024580	1.0081130	2.9803370
H	4.5024580	-1.0081130	2.9803370

H	4.3765830	-1.8963830	5.2630990	C	-0.2820370	-1.2029860	-3.5528990
H	2.1653380	-1.9633790	6.4408030	C	-0.2258030	-2.4336100	-2.8620230
H	0.1601050	-1.0985770	5.3185550	C	0.2258030	2.4336100	-2.8620230
H	4.8325370	1.0173520	-2.4739190	C	0.2820370	1.2029860	-3.5528990
H	6.7868700	1.8514730	-1.2504310	C	-0.6825020	4.9797990	1.3875970
H	6.7868700	1.8514730	1.2504310	C	-1.0096160	6.1364180	0.7021120
H	4.8325370	1.0173520	2.4739190	C	-1.0096160	6.1364180	-0.7021120
H	0.1601050	-1.0985770	-5.3185550	C	-0.6825020	4.9797990	-1.3875970
H	2.1653380	-1.9633790	-6.4408030	C	0.6825020	-4.9797990	-1.3875970
H	4.3765830	-1.8963830	-5.2630990	C	1.0096160	-6.1364180	-0.7021120
H	4.5024580	-1.0081130	-2.9803370	C	1.0096160	-6.1364180	0.7021120
H	-4.5024580	1.0081130	-2.9803370	C	0.6825020	-4.9797990	1.3875970
H	-4.3765830	1.8963830	-5.2630990	C	0.7691280	1.3272990	4.8879890
H	-2.1653380	1.9633790	-6.4408030	C	1.0620460	2.6205310	5.2224780
H	-0.1601050	1.0985770	-5.3185550	S	0.7634430	3.7105680	3.9295210
B	0.0000000	0.0000000	1.4529100	S	-0.7634430	-3.7105680	3.9295210
B	0.0000000	0.0000000	-1.4529100	C	-1.0620460	-2.6205310	5.2224780
N	0.0000000	0.0000000	2.8931980	C	-0.7691280	-1.3272990	4.8879890
N	0.0000000	0.0000000	-2.8931980	S	0.7634430	3.7105680	-3.9295210
				C	1.0620460	2.6205310	-5.2224780
				C	0.7691280	1.3272990	-4.8879890
				C	-0.7691280	-1.3272990	-4.8879890
				C	-1.0620460	-2.6205310	-5.2224780
				S	-0.7634430	-3.7105680	-3.9295210
				H	-0.7653690	4.9832240	2.4680660
				H	-1.2981180	7.0284040	1.2528100
				H	-1.2981180	7.0284040	-1.2528100
				H	-0.7653690	4.9832240	-2.4680660
				H	0.7653690	-4.9832240	-2.4680660
				H	1.2981180	-7.0284040	-1.2528100
				H	1.2981180	-7.0284040	1.2528100
				H	0.7653690	-4.9832240	2.4680660
				H	0.9449160	0.4898260	5.5499600
				H	1.4531680	2.9885670	6.1626380
				H	-1.4531680	-2.9885670	6.1626380
				H	-0.9449160	-0.4898260	5.5499600
				H	1.4531680	2.9885670	-6.1626380
				H	0.9449160	0.4898260	-5.5499600
				H	-0.9449160	-0.4898260	-5.5499600

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molecule5_conf1

C	-0.0059130	1.3519330	0.7151340
C	-0.0059130	1.3519330	-0.7151340
C	0.0059130	-1.3519330	-0.7151340
C	0.0059130	-1.3519330	0.7151340
C	-0.0370480	2.5550230	1.4428570
C	-0.3157410	3.7841450	0.7224260
C	-0.3157410	3.7841450	-0.7224260
C	-0.0370480	2.5550230	-1.4428570
C	0.2820370	1.2029860	3.5528990
C	0.2258030	2.4336100	2.8620230
C	0.0370480	-2.5550230	1.4428570
C	-0.2258030	-2.4336100	2.8620230
C	-0.2820370	-1.2029860	3.5528990
C	0.0370480	-2.5550230	-1.4428570
C	0.3157410	-3.7841450	-0.7224260
C	0.3157410	-3.7841450	0.7224260

H	-1.4531680	-2.9885670	-6.1626380
N	0.0000000	0.0000000	2.8924440
N	0.0000000	0.0000000	-2.8924440
B	0.0000000	0.0000000	1.4419160
B	0.0000000	0.0000000	-1.4419160

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molecule5_conf2

C	1.3553370	0.0570640	0.7132990
C	1.3553370	-0.0570640	-0.7132990
C	-1.3553370	0.0570640	-0.7132990
C	-1.3553370	-0.0570640	0.7132990
C	2.5576750	0.1185370	1.4439590
C	3.8117680	0.0091070	0.7219990
C	3.8117680	-0.0091070	-0.7219990
C	2.5576750	-0.1185370	-1.4439590
C	1.1798260	0.3580240	3.5484610
C	2.4150440	0.3769200	2.8646930
C	-2.5576750	-0.1185370	1.4439590
C	-2.4150440	-0.3769200	2.8646930
C	-1.1798260	-0.3580240	3.5484610
C	-2.5576750	0.1185370	-1.4439590
C	-3.8117680	0.0091070	-0.7219990
C	-3.8117680	-0.0091070	0.7219990
C	-1.1798260	0.3580240	-3.5484610
C	-2.4150440	0.3769200	-2.8646930
C	2.4150440	-0.3769200	-2.8646930
C	1.1798260	-0.3580240	-3.5484610
C	5.0626590	-0.0926840	1.3814580
C	6.2649510	-0.0742210	0.6984830
C	6.2649510	0.0742210	-0.6984830
C	5.0626590	0.0926840	-1.3814580
C	-5.0626590	-0.0926840	-1.3814580
C	-6.2649510	-0.0742210	-0.6984830
C	-6.2649510	0.0742210	0.6984830
C	-5.0626590	0.0926840	1.3814580
C	1.2587710	0.8623260	4.8805120
C	2.5263480	1.2402840	5.2246250

S	3.6439310	1.0046940	3.9432390
S	-3.6439310	-1.0046940	3.9432390
C	-2.5263480	-1.2402840	5.2246250
C	-1.2587710	-0.8623260	4.8805120
S	3.6439310	-1.0046940	-3.9432390
C	2.5263480	-1.2402840	-5.2246250
C	1.2587710	-0.8623260	-4.8805120
C	-1.2587710	0.8623260	-4.8805120
C	-2.5263480	1.2402840	-5.2246250
S	-3.6439310	1.0046940	-3.9432390
H	5.0876020	-0.2170350	2.4572300
H	7.2005750	-0.1601270	1.2455190
H	7.2005750	0.1601270	-1.2455190
H	5.0876020	0.2170350	-2.4572300
H	-5.0876020	-0.2170350	-2.4572300
H	-7.2005750	-0.1601270	-1.2455190
H	-7.2005750	0.1601270	1.2455190
H	-5.0876020	0.2170350	2.4572300
H	0.4043120	0.9876640	5.5320750
H	2.8601340	1.6597820	6.1653510
H	-2.8601340	-1.6597820	6.1653510
H	-0.4043120	-0.9876640	5.5320750
H	2.8601340	-1.6597820	-6.1653510
H	0.4043120	-0.9876640	-5.5320750
H	-0.4043120	0.9876640	-5.5320750
H	-2.8601340	1.6597820	-6.1653510
N	0.0000000	0.0000000	2.8850430
N	0.0000000	0.0000000	-2.8850430
B	0.0000000	0.0000000	1.4355800
B	0.0000000	0.0000000	-1.4355800

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molecule6_conf1

C	-1.3434680	0.0552150	0.7161670
C	-1.3434680	0.0552150	-0.7161670
C	1.3434680	-0.0552150	-0.7161670
C	1.3434680	-0.0552150	0.7161670
C	-2.5435400	0.0704860	1.4385320

C	-3.7733250	-0.2131580	0.7228800	H	-3.6219570	1.4747880	5.8418050
C	-3.7733250	-0.2131580	-0.7228800	H	-4.4872660	1.0343640	3.4129430
C	-2.5435400	0.0704860	-1.4385320	H	4.4872660	-1.0343640	3.4129430
C	-1.2088830	0.2876750	3.5423830	H	3.6219570	-1.4747880	5.8418050
C	-2.4444230	0.3465710	2.8635220	H	-4.4872660	1.0343640	-3.4129430
C	2.5435400	-0.0704860	1.4385320	H	-3.6219570	1.4747880	-5.8418050
C	2.4444230	-0.3465710	2.8635220	H	3.6219570	-1.4747880	-5.8418050
C	1.2088830	-0.2876750	3.5423830	H	4.4872660	-1.0343640	-3.4129430
C	2.5435400	-0.0704860	-1.4385320	H	-6.9704490	-1.3387720	1.2510380
C	3.7733250	0.2131580	-0.7228800	H	-6.9704490	-1.3387720	-1.2510380
C	3.7733250	0.2131580	0.7228800	H	6.9704490	1.3387720	1.2510380
C	1.2088830	-0.2876750	-3.5423830	H	6.9704490	1.3387720	-1.2510380
C	2.4444230	-0.3465710	-2.8635220	N	0.0000000	0.0000000	2.9120310
C	-2.4444230	0.3465710	-2.8635220	N	0.0000000	0.0000000	-2.9120310
C	-1.2088830	0.2876750	-3.5423830	B	0.0000000	0.0000000	1.4463530
C	-4.9513860	-0.6327480	1.3909690	B	0.0000000	0.0000000	-1.4463530
C	-6.0930200	-1.0039650	0.7028420				
C	-6.0930200	-1.0039650	-0.7028420				
C	-4.9513860	-0.6327480	-1.3909690	60			
C	4.9513860	0.6327480	-1.3909690	molecule6_conf2			
C	6.0930200	1.0039650	-0.7028420	C	-1.3343510	0.7166210	0.0083270
C	6.0930200	1.0039650	0.7028420	C	-1.3343510	-0.7166210	0.0083270
C	4.9513860	0.6327480	1.3909690	C	1.3343510	-0.7166210	0.0083270
S	-1.3621310	0.7849530	5.2060010	C	1.3343510	0.7166210	0.0083270
C	-3.0473090	1.0998050	5.0045460	C	-2.5286930	1.4361580	0.1325230
C	-3.4736800	0.8352110	3.7364280	C	-3.7038170	0.7225160	0.6009990
C	3.4736800	-0.8352110	3.7364280	C	-3.7038170	-0.7225160	0.6009990
C	3.0473090	-1.0998050	5.0045460	C	-2.5286930	-1.4361580	0.1325230
S	1.3621310	-0.7849530	5.2060010	C	-1.2467110	3.5370120	-0.3390700
C	-3.4736800	0.8352110	-3.7364280	C	-2.4743500	2.8531450	-0.1787240
C	-3.0473090	1.0998050	-5.0045460	C	2.5286930	1.4361580	0.1325230
S	-1.3621310	0.7849530	-5.2060010	C	2.4743500	2.8531450	-0.1787240
S	1.3621310	-0.7849530	-5.2060010	C	1.2467110	3.5370120	-0.3390700
C	3.0473090	-1.0998050	-5.0045460	C	2.5286930	-1.4361580	0.1325230
C	3.4736800	-0.8352110	-3.7364280	C	3.7038170	-0.7225160	0.6009990
H	-4.9377150	-0.7368500	2.4687690	C	3.7038170	0.7225160	0.6009990
H	-4.9377150	-0.7368500	-2.4687690	C	1.2467110	-3.5370120	-0.3390700
H	4.9377150	0.7368500	-2.4687690	C	2.4743500	-2.8531450	-0.1787240
H	4.9377150	0.7368500	2.4687690	C	-2.4743500	-2.8531450	-0.1787240

C	-1.2467110	-3.5370120	-0.3390700
C	-4.7987190	1.3902530	1.2050560
C	-5.8673820	0.7025250	1.7531360
C	-5.8673820	-0.7025250	1.7531360
C	-4.7987190	-1.3902530	1.2050560
C	4.7987190	-1.3902530	1.2050560
C	5.8673820	-0.7025250	1.7531360
C	5.8673820	0.7025250	1.7531360
C	4.7987190	1.3902530	1.2050560
S	-1.5060330	5.2081340	-0.7697890
C	-3.2162810	4.9943020	-0.7949050
C	-3.5779330	3.7190020	-0.4771950
C	3.5779330	3.7190020	-0.4771950
C	3.2162810	4.9943020	-0.7949050
S	1.5060330	5.2081340	-0.7697890
C	-3.5779330	-3.7190020	-0.4771950
C	-3.2162810	-4.9943020	-0.7949050
S	-1.5060330	-5.2081340	-0.7697890
S	1.5060330	-5.2081340	-0.7697890
C	3.2162810	-4.9943020	-0.7949050
C	3.5779330	-3.7190020	-0.4771950
H	-4.7670190	2.4674940	1.3110470
H	-4.7670190	-2.4674940	1.3110470
H	4.7670190	-2.4674940	1.3110470
H	4.7670190	2.4674940	1.3110470
H	-3.8522460	5.8281320	-1.0631820
H	-4.6068720	3.3853410	-0.5069030
H	4.6068720	3.3853410	-0.5069030
H	3.8522460	5.8281320	-1.0631820
H	-4.6068720	-3.3853410	-0.5069030
H	-3.8522460	-5.8281320	-1.0631820
H	3.8522460	-5.8281320	-1.0631820
H	4.6068720	-3.3853410	-0.5069030
H	-6.6788710	1.2512910	2.2251570
H	-6.6788710	-1.2512910	2.2251570
H	6.6788710	1.2512910	2.2251570
H	6.6788710	-1.2512910	2.2251570
N	0.0000000	2.9184710	-0.2375460
N	0.0000000	-2.9184710	-0.2375460

B	0.0000000	1.4519590	-0.1115790
B	0.0000000	-1.4519590	-0.1115790
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molecule7_conf1			
C	0.4308580	2.4962770	2.7988980
C	0.4248030	1.3067100	3.5760390
C	-0.4248030	-1.3067100	3.5760390
C	-0.4308580	-2.4962770	2.7988980
C	0.0344540	-2.4432200	1.4180660
C	0.4840240	-3.6200820	0.7137220
C	0.4840240	-3.6200820	-0.7137220
C	0.0344540	-2.4432200	-1.4180660
C	-0.4308580	-2.4962770	-2.7988980
C	-0.4248030	-1.3067100	-3.5760390
C	0.4248030	1.3067100	-3.5760390
C	0.4308580	2.4962770	-2.7988980
C	-0.0344540	2.4432200	-1.4180660
C	-0.4840240	3.6200820	-0.7137220
C	-0.4840240	3.6200820	0.7137220
C	-0.0344540	2.4432200	1.4180660
C	-0.0466490	1.2206200	0.7172140
C	0.0466490	-1.2206200	0.7172140
C	0.0466490	-1.2206200	-0.7172140
C	-0.0466490	1.2206200	-0.7172140
C	-1.0409530	4.7351960	1.3924200
C	-1.5588360	5.8165200	0.7038040
C	-1.5588360	5.8165200	-0.7038040
C	-1.0409530	4.7351960	-1.3924200
C	0.9482200	1.3434660	4.8872830
C	1.4683520	2.5125920	5.4279780
C	1.5040010	3.6769690	4.6436700
C	1.0021350	3.6690980	3.3496150
C	-1.0021350	-3.6690980	3.3496150
C	-1.5040010	-3.6769690	4.6436700
C	-1.4683520	-2.5125920	5.4279780
C	-0.9482200	-1.3434660	4.8872830
C	1.0409530	-4.7351960	-1.3924200

C	1.5588360	-5.8165200	-0.7038040
C	1.5588360	-5.8165200	0.7038040
C	1.0409530	-4.7351960	1.3924200
C	-0.9482200	-1.3434660	-4.8872830
C	-1.4683520	-2.5125920	-5.4279780
C	-1.5040010	-3.6769690	-4.6436700
C	-1.0021350	-3.6690980	-3.3496150
C	1.0021350	3.6690980	-3.3496150
C	1.5040010	3.6769690	-4.6436700
C	1.4683520	2.5125920	-5.4279780
C	0.9482200	1.3434660	-4.8872830
H	-1.1121030	4.7099920	2.4739020
H	-2.0036120	6.6435650	1.2518370
H	-2.0036120	6.6435650	-1.2518370
H	-1.1121030	4.7099920	-2.4739020
H	0.9846600	0.4254730	5.4663300
H	1.8771170	2.5186120	6.4356620
H	1.9528010	4.5858890	5.0383180
H	1.0912040	4.5616950	2.7401370
H	-1.0912040	-4.5616950	2.7401370
H	-1.9528010	-4.5858890	5.0383180
H	-1.8771170	-2.5186120	6.4356620
H	-0.9846600	-0.4254730	5.4663300
H	1.1121030	-4.7099920	-2.4739020
H	2.0036120	-6.6435650	-1.2518370
H	2.0036120	-6.6435650	1.2518370
H	1.1121030	-4.7099920	2.4739020
H	-0.9846600	-0.4254730	-5.4663300
H	-1.8771170	-2.5186120	-6.4356620
H	-1.9528010	-4.5858890	-5.0383180
H	-1.0912040	-4.5616950	-2.7401370
H	1.0912040	4.5616950	-2.7401370
H	1.9528010	4.5858890	-5.0383180
H	1.8771170	2.5186120	-6.4356620
H	0.9846600	0.4254730	-5.4663300
N	0.0000000	0.0000000	1.4206750
N	0.0000000	0.0000000	-1.4206750
B	0.0000000	0.0000000	2.8904150
B	0.0000000	0.0000000	-2.8904150

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molecule8_conf1

C	-1.2067420	0.7166110	0.1327980
C	-1.2067420	-0.7166110	0.1327980
C	1.2067420	-0.7166110	0.1327980
C	1.2067420	0.7166110	0.1327980
C	-2.4259860	1.4218120	0.2554190
C	-3.5493320	0.7135020	0.8320760
C	-3.5493320	-0.7135020	0.8320760
C	-2.4259860	-1.4218120	0.2554190
C	-1.3680570	3.4884200	-0.6565250
C	-2.4943820	2.7758070	-0.2211360
C	2.4259860	1.4218120	0.2554190
C	2.4943820	2.7758070	-0.2211360
C	1.3680570	3.4884200	-0.6565250
C	2.4259860	-1.4218120	0.2554190
C	3.5493320	-0.7135020	0.8320760
C	3.5493320	0.7135020	0.8320760
C	1.3680570	-3.4884200	-0.6565250
C	2.4943820	-2.7758070	-0.2211360
C	-2.4943820	-2.7758070	-0.2211360
C	-1.3680570	-3.4884200	-0.6565250
C	-4.6129700	1.3883750	1.4778270
C	-5.6553230	0.7017740	2.0768900
C	-5.6553230	-0.7017740	2.0768900
C	-4.6129700	-1.3883750	1.4778270
C	4.6129700	-1.3883750	1.4778270
C	5.6553230	-0.7017740	2.0768900
C	5.6553230	0.7017740	2.0768900
C	4.6129700	1.3883750	1.4778270
C	-1.7208360	4.7624010	-1.2012350
C	-3.0673860	4.9995570	-1.2043630
S	-3.9576420	3.6913270	-0.5218990
S	3.9576420	3.6913270	-0.5218990
C	3.0673860	4.9995570	-1.2043630
C	1.7208360	4.7624010	-1.2012350
S	-3.9576420	-3.6913270	-0.5218990

C	-3.0673860	-4.9995570	-1.2043630
C	-1.7208360	-4.7624010	-1.2012350
C	1.7208360	-4.7624010	-1.2012350
C	3.0673860	-4.9995570	-1.2043630
S	3.9576420	-3.6913270	-0.5218990
H	-4.5834860	2.4677090	1.5676730
H	-6.4442880	1.2529800	2.5822670
H	-6.4442880	-1.2529800	2.5822670
H	-4.5834860	-2.4677090	1.5676730
H	4.5834860	-2.4677090	1.5676730
H	6.4442880	-1.2529800	2.5822670
H	6.4442880	1.2529800	2.5822670
H	4.5834860	2.4677090	1.5676730
H	-1.0114340	5.4785720	-1.5957470
H	-3.5924920	5.8750110	-1.5674140
H	3.5924920	5.8750110	-1.5674140
H	1.0114340	5.4785720	-1.5957470
H	-3.5924920	-5.8750110	-1.5674140
H	-1.0114340	-5.4785720	-1.5957470
H	1.0114340	-5.4785720	-1.5957470
H	3.5924920	-5.8750110	-1.5674140
B	0.0000000	2.8299410	-0.4906890
B	0.0000000	-2.8299410	-0.4906890
N	0.0000000	-1.4052710	-0.1029090
N	0.0000000	1.4052710	-0.1029090

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molecule8_conf2

C	-0.0368060	1.2267850	0.7176720
C	-0.0368060	1.2267850	-0.7176720
C	0.0368060	-1.2267850	-0.7176720
C	0.0368060	-1.2267850	0.7176720
C	-0.0257050	2.4605030	1.4226600
C	-0.3984050	3.6624380	0.7124040
C	-0.3984050	3.6624380	-0.7124040
C	-0.0257050	2.4605030	-1.4226600
C	0.3312250	1.3075790	3.5914220
C	0.3256920	2.4681220	2.8196410

C	0.0257050	-2.4605030	1.4226600
C	-0.3256920	-2.4681220	2.8196410
C	-0.3312250	-1.3075790	3.5914220
C	0.0257050	-2.4605030	-1.4226600
C	0.3984050	-3.6624380	-0.7124040
C	0.3984050	-3.6624380	0.7124040
C	-0.3312250	-1.3075790	-3.5914220
C	-0.3256920	-2.4681220	-2.8196410
C	0.3256920	2.4681220	-2.8196410
C	0.3312250	1.3075790	-3.5914220
C	-0.8672810	4.8185870	1.3868180
C	-1.2885240	5.9435900	0.7022580
C	-1.2885240	5.9435900	-0.7022580
C	-0.8672810	4.8185870	-1.3868180
C	0.8672810	-4.8185870	-1.3868180
C	1.2885240	-5.9435900	-0.7022580
C	1.2885240	-5.9435900	0.7022580
C	0.8672810	-4.8185870	1.3868180
C	0.7874030	1.5330320	4.9264770
C	1.1513890	2.8320390	5.1523580
S	0.9219940	3.8229750	3.7570800
S	-0.9219940	-3.8229750	3.7570800
C	-1.1513890	-2.8320390	5.1523580
C	-0.7874030	-1.5330320	4.9264770
S	0.9219940	3.8229750	-3.7570800
C	1.1513890	2.8320390	-5.1523580
C	0.7874030	1.5330320	-4.9264770
C	-0.7874030	-1.5330320	-4.9264770
C	-1.1513890	-2.8320390	-5.1523580
S	-0.9219940	-3.8229750	-3.7570800
H	-0.9614050	4.8061840	2.4654040
H	-1.6602770	6.8032620	1.2541380
H	-1.6602770	6.8032620	-1.2541380
H	-0.9614050	4.8061840	-2.4654040
H	0.9614050	-4.8061840	-2.4654040
H	1.6602770	-6.8032620	-1.2541380
H	1.6602770	-6.8032620	1.2541380
H	0.9614050	-4.8061840	2.4654040
H	0.8767630	0.7509900	5.6728670

H	1.5475160	3.2715010	6.0602040
H	-1.5475160	-3.2715010	6.0602040
H	-0.8767630	-0.7509900	5.6728670
H	1.5475160	3.2715010	-6.0602040
H	0.8767630	0.7509900	-5.6728670
H	-0.8767630	-0.7509900	-5.6728670
H	-1.5475160	-3.2715010	-6.0602040
B	0.0000000	0.0000000	2.8967690
B	0.0000000	0.0000000	-2.8967690
N	0.0000000	0.0000000	-1.4185440
N	0.0000000	0.0000000	1.4185440

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molecule9_conf1

C	1.2119550	0.7185110	0.1578740
C	1.2119550	-0.7185110	0.1578740
C	-1.2119550	-0.7185110	0.1578740
C	-1.2119550	0.7185110	0.1578740
C	2.4355760	1.4165080	0.2541590
C	3.5660000	0.7129870	0.8156460
C	3.5660000	-0.7129870	0.8156460
C	2.4355760	-1.4165080	0.2541590
C	1.3653700	3.5058030	-0.4817250
C	2.5322130	2.7860690	-0.1975400
C	-2.4355760	1.4165080	0.2541590
C	-2.5322130	2.7860690	-0.1975400
C	-1.3653700	3.5058030	-0.4817250
C	-2.4355760	-1.4165080	0.2541590
C	-3.5660000	-0.7129870	0.8156460
C	-3.5660000	0.7129870	0.8156460
C	-1.3653700	-3.5058030	-0.4817250
C	-2.5322130	-2.7860690	-0.1975400
C	2.5322130	-2.7860690	-0.1975400
C	1.3653700	-3.5058030	-0.4817250
C	4.6223380	1.3913780	1.4740370
C	5.6562210	0.7029980	2.0839740
C	5.6562210	-0.7029980	2.0839740
C	4.6223380	-1.3913780	1.4740370

C	-4.6223380	-1.3913780	1.4740370
C	-5.6562210	-0.7029980	2.0839740
C	-5.6562210	0.7029980	2.0839740
C	-4.6223380	1.3913780	1.4740370
S	1.7436010	5.0872550	-1.0693710
C	3.4378990	4.7861420	-0.9866880
C	3.7177850	3.5332690	-0.5135740
C	-3.7177850	3.5332690	-0.5135740
C	-3.4378990	4.7861420	-0.9866880
S	-1.7436010	5.0872550	-1.0693710
C	3.7177850	-3.5332690	-0.5135740
C	3.4378990	-4.7861420	-0.9866880
S	1.7436010	-5.0872550	-1.0693710
S	-1.7436010	-5.0872550	-1.0693710
C	-3.4378990	-4.7861420	-0.9866880
C	-3.7177850	-3.5332690	-0.5135740
H	4.5828780	2.4702630	1.5648470
H	4.5828780	-2.4702630	1.5648470
H	-4.5828780	-2.4702630	1.5648470
H	-4.5828780	2.4702630	1.5648470
H	4.1447520	5.5406680	-1.3105420
H	4.7265980	3.1476230	-0.4404160
H	-4.7265980	3.1476230	-0.4404160
H	-4.1447520	5.5406680	-1.3105420
H	4.7265980	-3.1476230	-0.4404160
H	4.1447520	-5.5406680	-1.3105420
H	-4.1447520	-5.5406680	-1.3105420
H	-4.7265980	-3.1476230	-0.4404160
H	6.4380050	1.2516300	2.6035320
H	6.4380050	-1.2516300	2.6035320
H	-6.4380050	1.2516300	2.6035320
H	-6.4380050	-1.2516300	2.6035320
N	0.0000000	1.4147070	-0.0348270
N	0.0000000	-1.4147070	-0.0348270
B	0.0000000	2.8647700	-0.3290290
B	0.0000000	-2.8647700	-0.3290290

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molecule9_conf2				C	3.2440860	-1.2066790	-4.8768590
C	-1.2239890	0.0016290	0.7189760	C	3.5864190	-0.9424720	-3.5780580
C	-1.2239890	0.0016290	-0.7189760	H	-4.7958460	-0.8677170	2.4690180
C	1.2239890	-0.0016290	-0.7189760	H	-4.7958460	-0.8677170	-2.4690180
C	1.2239890	-0.0016290	0.7189760	H	4.7958460	0.8677170	-2.4690180
C	-2.4545160	0.0559390	1.4164200	H	4.7958460	0.8677170	2.4690180
C	-3.6626380	-0.2996010	0.7123620	H	-3.8769860	1.6201350	5.6530170
C	-3.6626380	-0.2996010	-0.7123620	H	-4.5691570	1.1517620	3.1740110
C	-2.4545160	0.0559390	-1.4164200	H	4.5691570	-1.1517620	3.1740110
C	-1.3171590	0.3347900	3.5731690	H	3.8769860	-1.6201350	5.6530170
C	-2.4871360	0.4191940	2.8170180	H	-4.5691570	1.1517620	-3.1740110
C	2.4545160	-0.0559390	1.4164200	H	-3.8769860	1.6201350	-5.6530170
C	2.4871360	-0.4191940	2.8170180	H	3.8769860	-1.6201350	-5.6530170
C	1.3171590	-0.3347900	3.5731690	H	4.5691570	-1.1517620	-3.1740110
C	2.4545160	-0.0559390	-1.4164200	H	-6.7967030	-1.5768320	1.2523410
C	3.6626380	0.2996010	-0.7123620	H	-6.7967030	-1.5768320	-1.2523410
C	3.6626380	0.2996010	0.7123620	H	6.7967030	1.5768320	1.2523410
C	1.3171590	-0.3347900	-3.5731690	H	6.7967030	1.5768320	-1.2523410
C	2.4871360	-0.4191940	-2.8170180	N	0.0000000	0.0000000	1.4253290
C	-2.4871360	0.4191940	-2.8170180	N	0.0000000	0.0000000	-1.4253290
C	-1.3171590	0.3347900	-3.5731690	B	0.0000000	0.0000000	2.9088070
C	-4.8168930	-0.7713820	1.3905620	B	0.0000000	0.0000000	-2.9088070
C	-5.9385610	-1.1969080	0.7032990				
C	-5.9385610	-1.1969080	-0.7032990				
C	-4.8168930	-0.7713820	-1.3905620	63			
C	4.8168930	0.7713820	-1.3905620	molecule11_conf1			
C	5.9385610	1.1969080	-0.7032990	C	-2.4612510	2.8656290	-0.3647360
C	5.9385610	1.1969080	0.7032990	C	-1.2185450	3.5699060	-0.3581090
C	4.8168930	0.7713820	1.3905620	C	0.0000000	2.8549540	-0.0402380
S	-1.5924700	0.8381290	5.2044600	C	1.2121800	3.5077700	0.3414860
C	-3.2440860	1.2066790	4.8768590	C	2.4305420	2.7933660	0.2966430
C	-3.5864190	0.9424720	3.5780580	C	2.4884280	1.4177720	-0.0614660
C	3.5864190	-0.9424720	3.5780580	C	3.7123340	0.6986910	-0.3647360
C	3.2440860	-1.2066790	4.8768590	C	3.7009020	-0.7296620	-0.3581090
S	1.5924700	-0.8381290	5.2044600	C	2.4724630	-1.4274770	-0.0402380
C	-3.5864190	0.9424720	-3.5780580	C	2.4317280	-2.8036630	0.3414860
C	-3.2440860	1.2066790	-4.8768590	C	1.2038540	-3.5015940	0.2966430
S	-1.5924700	0.8381290	-5.2044600	C	-0.0163870	-2.8639280	-0.0614660
S	1.5924700	-0.8381290	-5.2044600	C	-1.2510820	-3.5643210	-0.3647360

C	-2.4823560	-2.8402440	-0.3581090	H	4.9033400	2.4404770	-0.8546050
C	-2.4724630	-1.4274770	-0.0402380	H	-4.5801330	-2.9386430	-0.8744240
C	-3.6439080	-0.7041060	0.3414860	H	-4.5702940	-5.3135890	-1.4841500
C	-3.6343970	0.7082290	0.2966430	H	-2.4187830	-6.5935210	-1.4599940
C	-2.4720400	1.4461550	-0.0614660	H	-0.3381550	-5.4666550	-0.8546050
C	-1.2476790	0.7219430	-0.1121780	H	4.4884310	-3.2389540	1.0842110
C	0.0046520	1.4396630	-0.1084870	H	3.6672780	-5.6400530	1.7087210
C	1.2490600	0.7195500	-0.1121780	H	0.5608010	5.5065720	1.0842110
C	1.2444590	-0.7238600	-0.1084870	H	3.0507900	5.9959830	1.7087210
C	-0.0013810	-1.4414930	-0.1121780	H	-5.0492320	-2.2676190	1.0842110
C	-1.2491100	-0.7158030	-0.1084870	H	-6.7180690	-0.3559300	1.7087210
C	-1.2039610	4.9220880	-0.7792380				
C	-2.3641920	5.5815070	-1.1489590				
C	-3.5888220	4.8948510	-1.1380450				
C	-3.6260670	3.5602150	-0.7690100	54			
C	4.8646340	-1.4183830	-0.7792380	molecule11_conf1			
C	6.0158230	-0.7433040	-1.1489590	C	-1.0130040	1.0306050	-0.0077000
C	6.0334760	0.6605850	-1.1380450	C	0.3819450	1.3907060	0.0039760
C	4.8962700	1.3601590	-0.7690100	C	1.3934710	0.3622250	0.0079280
C	-3.6606730	-3.5037050	-0.7792380	C	1.0130040	-1.0306050	0.0077000
C	-3.6516310	-4.8382040	-1.1489590	C	-0.3819450	-1.3907060	-0.0039760
C	-2.4446540	-5.5554360	-1.1380450	C	-1.3934710	-0.3622250	-0.0079280
C	-1.2702030	-4.9203730	-0.7690100	C	-0.7667320	-2.7715160	-0.0101770
C	3.4867860	-3.6043320	0.8970210	C	-2.1415170	-3.0776620	-0.2170260
C	3.0790120	-4.8569270	1.2459760	C	-3.1354580	-2.0834440	-0.2517320
S	1.4089640	-5.1310900	0.9047680	C	-2.7728040	-0.7200540	-0.0097310
C	1.3780490	4.8218110	0.8970210	C	-3.7486620	0.2950010	0.2456040
C	2.6667160	5.0949660	1.2459760	C	-3.3658640	1.6485970	0.2029300
S	3.7391720	3.7857430	0.9047680	C	-2.0176160	2.0498360	-0.0219500
C	-4.8648360	-1.2174800	0.8970210	C	-1.6197220	3.4128480	-0.2166360
C	-5.7457280	-0.2380390	1.2459760	C	-0.2535810	3.7456100	-0.1752080
S	-5.1481360	1.3453460	0.9047680	C	0.7667320	2.7715160	0.0101770
H	-0.2548720	5.4358330	-0.8744240	C	2.1415170	3.0776620	0.2170260
H	-2.3165560	6.6147850	-1.4841500	C	3.1354580	2.0834440	0.2517320
H	-4.5007660	5.3914880	-1.4599940	C	2.7728040	0.7200540	0.0097310
H	-4.5651850	3.0261780	-0.8546050	C	3.7486620	-0.2950010	-0.2456040
H	4.8350060	-2.4971910	-0.8744240	C	3.3658640	-1.6485970	-0.2029300
H	6.8868500	-1.3011960	-1.4841500	C	2.0176160	-2.0498360	0.0219500
H	6.9195480	1.2020330	-1.4599940	C	1.6197220	-3.4128480	0.2166360
				C	0.2535810	-3.7456100	0.1752080

C	-5.1162490	0.1333630	0.6507920
C	-5.7485250	1.3191980	0.8797270
S	-4.7177270	2.6771690	0.6195330
S	-2.8243850	-4.6472790	-0.5641300
C	-4.3937510	-3.9706870	-0.8038490
C	-4.4162320	-2.6203130	-0.6134390
C	2.4379830	-4.5582530	0.4935420
C	1.7178630	-5.7079040	0.6360240
S	0.0232790	-5.4543760	0.4449600
C	5.1162490	-0.1333630	-0.6507920
C	5.7485250	-1.3191980	-0.8797270
S	4.7177270	-2.6771690	-0.6195330
S	2.8243850	4.6472790	0.5641300
C	4.3937510	3.9706870	0.8038490
C	4.4162320	2.6203130	0.6134390
C	-2.4379830	4.5582530	-0.4935420
C	-1.7178630	5.7079040	-0.6360240
S	-0.0232790	5.4543760	-0.4449600
H	-5.5902430	-0.8210010	0.8354400
H	-6.7667310	1.4741290	1.2151190
H	-5.2140540	-4.6131550	-1.0996920
H	-5.3018580	-2.0250720	-0.7904470
H	3.5112420	-4.5348020	0.6302090
H	2.0903310	-6.6988970	0.8642930
H	5.5902430	0.8210010	-0.8354400
H	6.7667310	-1.4741290	-1.2151190
H	5.2140540	4.6131550	1.0996920
H	5.3018580	2.0250720	0.7904470
H	-3.5112420	4.5348020	-0.6302090
H	-2.0903310	6.6988970	-0.8642930

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molecule12_conf2

C	-1.0375090	1.0022330	0.0342860
C	0.3422890	1.4005820	-0.0681330
C	1.3776650	0.4008930	0.0204180
C	1.0375090	-1.0022330	0.0342860
C	-0.3422890	-1.4005820	-0.0681330

C	-1.3776650	-0.4008930	0.0204180
C	-0.6878110	-2.7856750	-0.2056670
C	-2.0668970	-3.1137070	-0.3494940
C	-3.0867200	-2.1520260	-0.2203550
C	-2.7432660	-0.7977040	0.0855680
C	-3.7205840	0.1753570	0.4688100
C	-3.3785890	1.5406920	0.4576560
C	-2.0668970	1.9918320	0.1259200
C	-1.7251130	3.3682240	-0.0764180
C	-0.3739100	3.7332500	-0.2365900
C	0.6878110	2.7856750	-0.2056670
C	2.0668970	3.1137070	-0.3494940
C	3.0867200	2.1520260	-0.2203550
C	2.7432660	0.7977040	0.0855680
C	3.7205840	-0.1753570	0.4688100
C	3.3785890	-1.5406920	0.4576560
C	2.0668970	-1.9918320	0.1259200
C	1.7251130	-3.3682240	-0.0764180
C	0.3739100	-3.7332500	-0.2365900
C	-5.0442890	-0.0468020	0.9769080
C	-5.6868950	1.1073160	1.3139630
S	-4.7182870	2.5057750	1.0336510
S	-2.7412070	-4.6723680	-0.7578750
C	-4.3421070	-4.0313220	-0.8047170
C	-4.3807660	-2.7008350	-0.5085210
C	2.5976770	-4.5021610	-0.1842360
C	1.9321810	-5.6735110	-0.3942490
S	0.2246940	-5.4559940	-0.4758820
C	5.0442890	0.0468020	0.9769080
C	5.6868950	-1.1073160	1.3139630
S	4.7182870	-2.5057750	1.0336510
S	2.7412070	4.6723680	-0.7578750
C	4.3421070	4.0313220	-0.8047170
C	4.3807660	2.7008350	-0.5085210
C	-2.5976770	4.5021610	-0.1842360
C	-1.9321810	5.6735110	-0.3942490
S	-0.2246940	5.4559940	-0.4758820
H	-5.4750330	-1.0228400	1.1547550
H	-6.6763920	1.2156920	1.7409740

H	-5.1691130	-4.6762740	-1.0753450
H	-5.2935690	-2.1229220	-0.5588020
H	3.6781400	-4.4602110	-0.1495120
H	2.3548410	-6.6624820	-0.5212640
H	5.4750330	1.0228400	1.1547550
H	6.6763920	-1.2156920	1.7409740
H	5.1691130	4.6762740	-1.0753450
H	5.2935690	2.1229220	-0.5588020
H	-3.6781400	4.4602110	-0.1495120
H	-2.3548410	6.6624820	-0.5212640

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molecule12_conf1

C	0.0000000	1.2482100	3.5383410
C	0.0000000	0.0000000	2.8528280
C	0.0000000	0.0000000	1.4268930
C	0.0000000	1.2357090	0.7134760
C	0.0000000	2.4705300	1.4264570
C	0.0000000	2.4400580	2.8502430
C	0.0000000	-1.2357090	0.7134760
C	0.0000000	1.2357090	-0.7134760
C	0.0000000	0.0000000	-1.4268930
C	0.0000000	-1.2357090	-0.7134760
C	0.0000000	0.0000000	-2.8528280
C	0.0000000	1.2482100	-3.5383410
C	0.0000000	2.4400580	-2.8502430
C	0.0000000	2.4705300	-1.4264570
C	0.0000000	3.6882930	-0.6881170
C	0.0000000	3.6882930	0.6881170
H	0.0000000	4.6282660	1.2363170
H	0.0000000	4.6282660	-1.2363170
H	0.0000000	1.2432190	4.6264810
H	0.0000000	3.3847520	3.3902900
H	0.0000000	1.2432190	-4.6264810
H	0.0000000	3.3847520	-3.3902900
C	0.0000000	-1.2482100	3.5383410
C	0.0000000	-2.4400580	2.8502430
C	0.0000000	-2.4705300	1.4264570

H	0.0000000	-1.2432190	4.6264810
H	0.0000000	-3.3847520	3.3902900
C	0.0000000	-3.6882930	0.6881170
C	0.0000000	-3.6882930	-0.6881170
C	0.0000000	-2.4705300	-1.4264570
H	0.0000000	-4.6282660	1.2363170
H	0.0000000	-4.6282660	-1.2363170
C	0.0000000	-1.2482100	-3.5383410
H	0.0000000	-1.2432190	-4.6264810
C	0.0000000	-2.4400580	-2.8502430
H	0.0000000	-3.3847520	-3.3902900

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molecule13_conf1

C	0.0000000	1.2276510	3.5442080
C	0.0000000	2.4298800	2.8816610
C	0.0000000	2.5389840	1.4382580
C	0.0000000	3.7585360	0.6954020
C	0.0000000	3.7585360	-0.6954020
C	0.0000000	2.5389840	-1.4382580
C	0.0000000	2.4298800	-2.8816610
C	0.0000000	1.2276510	-3.5442080
N	0.0000000	0.0000000	-2.8814410
C	0.0000000	-1.2276510	-3.5442080
C	0.0000000	-2.4298800	-2.8816610
C	0.0000000	-2.5389840	-1.4382580
C	0.0000000	-3.7585360	-0.6954020
C	0.0000000	-3.7585360	0.6954020
C	0.0000000	-2.5389840	1.4382580
C	0.0000000	-2.4298800	2.8816610
C	0.0000000	-1.2276510	3.5442080
N	0.0000000	0.0000000	2.8814410
B	0.0000000	0.0000000	1.4302980
C	0.0000000	1.3341650	0.7060970
C	0.0000000	1.3341650	-0.7060970
B	0.0000000	0.0000000	-1.4302980
C	0.0000000	-1.3341650	-0.7060970
C	0.0000000	-1.3341650	0.7060970

H	0.0000000	1.1810360	4.6309700
H	0.0000000	3.3328370	3.4879090
H	0.0000000	4.7102100	1.2257700
H	0.0000000	4.7102100	-1.2257700
H	0.0000000	3.3328370	-3.4879090
H	0.0000000	1.1810360	-4.6309700
H	0.0000000	-1.1810360	-4.6309700
H	0.0000000	-3.3328370	-3.4879090
H	0.0000000	-4.7102100	-1.2257700
H	0.0000000	-4.7102100	1.2257700
H	0.0000000	-3.3328370	3.4879090
H	0.0000000	-1.1810360	4.6309700

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molecule14_conf1

C	0.0000000	1.3576350	3.6056830
C	0.0000000	2.4894560	2.8505690
C	0.0000000	2.4454350	1.4156720
C	0.0000000	3.6589650	0.6849740
C	0.0000000	3.6589650	-0.6849740
C	0.0000000	2.4454350	-1.4156720
C	0.0000000	2.4894560	-2.8505690
C	0.0000000	1.3576350	-3.6056830
B	0.0000000	0.0000000	-2.9104490
C	0.0000000	-1.3576350	-3.6056830
C	0.0000000	-2.4894560	-2.8505690
C	0.0000000	-2.4454350	-1.4156720
C	0.0000000	-3.6589650	-0.6849740
C	0.0000000	-3.6589650	0.6849740
C	0.0000000	-2.4454350	1.4156720
C	0.0000000	-2.4894560	2.8505690
C	0.0000000	-1.3576350	3.6056830
B	0.0000000	0.0000000	2.9104490
N	0.0000000	0.0000000	1.4274440
C	0.0000000	1.2081760	0.7105490
C	0.0000000	1.2081760	-0.7105490
N	0.0000000	0.0000000	-1.4274440
C	0.0000000	-1.2081760	-0.7105490

C	0.0000000	-1.2081760	0.7105490
H	0.0000000	1.4487680	4.6914460
H	0.0000000	3.4840730	3.2995210
H	0.0000000	4.5919210	1.2432680
H	0.0000000	4.5919210	-1.2432680
H	0.0000000	3.4840730	-3.2995210
H	0.0000000	1.4487680	-4.6914460
H	0.0000000	-1.4487680	-4.6914460
H	0.0000000	-3.4840730	-3.2995210
H	0.0000000	-4.5919210	-1.2432680
H	0.0000000	-4.5919210	1.2432680
H	0.0000000	-3.4840730	3.2995210
H	0.0000000	-1.4487680	4.6914460

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molecule15_conf1

C	0.7268630	1.4849910	0.1611710
C	-0.7280130	1.4850450	0.1570180
C	-1.5982590	0.3733810	-0.2336790
C	-1.2971060	-1.0410820	-0.0542210
C	0.0007970	-1.6358820	0.2588270
C	1.2973860	-1.0403760	-0.0592110
C	1.5983760	0.3748460	-0.2313020
C	1.3805470	2.7327570	0.4650030
C	2.9293080	0.7186700	-0.6596050
C	2.4074210	-1.9536110	-0.1713850
C	0.0022550	-2.9936340	0.7355560
C	-2.4082620	-1.9541260	-0.1566450
C	-2.9283770	0.7147450	-0.6661100
C	-1.3828870	2.7341350	0.4530500
C	3.6364040	-1.5702390	-0.7698680
C	3.8725400	-0.2663150	-1.0597660
C	3.4490540	2.0376930	-0.5448240
C	2.7355600	2.9828780	0.1156960
C	0.6753650	3.8359420	1.0148950
C	-0.6812330	3.8371160	1.0077460
C	-2.7353060	2.9840310	0.0938660
C	-3.4469340	2.0352690	-0.5635290

C	-3.6385980	-1.5740550	-0.7545050
C	-3.8730240	-0.2727060	-1.0570030
C	-1.1953640	-3.7429230	0.9009530
C	-2.3522930	-3.2701570	0.3745960
C	1.2003670	-3.7447230	0.8889450
C	2.3534110	-3.2721190	0.3539840
H	4.8236030	0.0607950	-1.4733200
H	4.4602590	2.2302790	-0.8953790
H	3.1528290	3.9641230	0.3296030
H	1.2424400	4.7059450	1.3378870
H	-1.2501400	4.7082020	1.3245690
H	-3.1526220	3.9669120	0.3000390
H	-4.4566670	2.2263840	-0.9190880
H	-4.3954690	-2.3391980	-0.9116930
H	-4.8239020	0.0517530	-1.4730470
H	-1.1310880	-4.7407510	1.3282850
H	-3.2557560	-3.8752870	0.3521080
H	3.2559800	-3.8781900	0.3226840
H	4.3919810	-2.3349150	-0.9353160
H	1.1385730	-4.7433580	1.3147700

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molecule16_conf1

C	-1.3165480	-1.1318080	0.4204730
C	-1.7457550	0.0157900	-0.3906450
C	-1.1318080	1.3165480	-0.4204730
C	0.0157900	1.7457550	0.3906450
C	1.3165480	1.1318080	0.4204730
C	1.7457550	-0.0157900	-0.3906450
C	1.1318080	-1.3165480	-0.4204730
C	-0.0157900	-1.7457550	0.3906450
C	-2.3706810	-1.8574480	1.0701910
C	-3.7264890	-1.7457550	0.6346180
C	-4.0056720	-1.0368580	-0.4932220
C	-3.0412130	-0.1105950	-0.9951750
C	-1.8574480	2.3706810	-1.0701910
C	-1.7457550	3.7264890	-0.6346180
C	-1.0368580	4.0056720	0.4932220

C	-0.1105950	3.0412130	0.9951750
C	2.3706810	1.8574480	1.0701910
C	3.7264890	1.7457550	0.6346180
C	4.0056720	1.0368580	-0.4932220
C	3.0412130	0.1105950	-0.9951750
C	1.8574480	-2.3706810	-1.0701910
C	1.7457550	-3.7264890	-0.6346180
C	1.0368580	-4.0056720	0.4932220
C	0.1105950	-3.0412130	0.9951750
C	2.0774930	2.9085070	1.9792260
C	2.9085070	-2.0774930	-1.9792260
C	-2.0774930	-2.9085070	1.9792260
C	-2.9085070	2.0774930	-1.9792260
C	-0.8481990	-3.5000330	1.9366940
C	3.5000330	-0.8481990	-1.9366940
C	0.8481990	3.5000330	1.9366940
C	-3.5000330	0.8481990	-1.9366940
H	-4.4842060	-2.3459870	1.1328390
H	-4.9925680	-1.0575310	-0.9497140
H	-2.3459870	4.4842060	-1.1328390
H	-1.0575310	4.9925680	0.9497140
H	4.4842060	2.3459870	1.1328390
H	4.9925680	1.0575310	-0.9497140
H	2.3459870	-4.4842060	-1.1328390
H	1.0575310	-4.9925680	0.9497140
H	2.8873040	3.3329500	2.5685140
H	3.3329500	-2.8873040	-2.5685140
H	-2.8873040	-3.3329500	2.5685140
H	-3.3329500	2.8873040	-2.5685140
H	-0.6430830	-4.4138140	2.4900930
H	4.4138140	-0.6430830	-2.4900930
H	0.6430830	4.4138140	2.4900930
H	-4.4138140	0.6430830	-2.4900930

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molecule17_conf1

C	0.0000000	0.0000000	1.9130730
C	0.6576060	1.1371490	1.2919510

C	-0.6576060	-1.1371490	1.2919510	H	1.1138700	0.4949740	5.1303040
C	0.0000000	-1.8831580	0.2453540	H	-2.9917640	-3.5312550	2.1807100
C	0.9537590	-1.4002610	-0.7482070	H	-1.5327180	-4.9239560	0.7184680
C	0.6101740	-0.4019480	-1.7227750	H	3.2416760	-0.8481590	-3.8951350
C	-0.6101740	0.4019480	-1.7227750	H	3.9263040	-2.4667950	-2.1359750
C	-0.9537590	1.4002610	-0.7482070	H	2.9190160	-4.2468890	-0.8470950
C	0.0000000	1.8831580	0.2453540	H	0.7797100	-5.2299020	-0.0044780
C	1.3370440	-0.4144710	-2.9554300	H	-2.7895400	-1.8934070	3.9164310
C	0.6753800	-0.1045490	-4.1831770	H	-1.1138700	-0.4949740	5.1303040
C	-0.6753800	0.1045490	-4.1831770	H	2.9917640	3.5312550	2.1807100
C	-1.3370440	0.4144710	-2.9554300	H	1.5327180	4.9239560	0.7184680
C	-2.0638210	2.2596790	-1.0418740	H	-3.9263040	2.4667950	-2.1359750
C	-2.0601800	3.6215220	-0.6147400	H	-3.2416760	0.8481590	-3.8951350
C	-0.8945130	4.1571950	-0.1434730				
C	0.1697220	3.3016310	0.2732110				
C	1.6686570	1.8137060	2.0574740	60			
C	1.9689210	1.4104980	3.3909850	molecule18_conf1			
C	1.0573160	0.6373350	4.0532050	C	-1.0144750	0.8184820	-1.3677960
C	0.0000000	0.0000000	3.3412760	C	-0.6282950	1.7854640	-0.3667980
C	-1.6686570	-1.8137060	2.0574740	C	0.6282950	1.7854640	0.3667980
C	-2.1373240	-3.0994680	1.6646500	C	1.0144750	0.8184820	1.3677960
C	-1.3399470	-3.8622180	0.8574070	C	0.0000000	0.0000000	2.0000900
C	-0.1697220	-3.3016310	0.2732110	C	-1.0144750	-0.8184820	1.3677960
C	2.6334460	-0.9974090	-3.0054880	C	-0.6282950	-1.7854640	0.3667980
C	3.0095090	-1.8894940	-2.0382940	C	0.0000000	0.0000000	-2.0000900
C	2.0638210	-2.2596790	-1.0418740	C	1.0144750	-0.8184820	-1.3677960
C	2.0601800	-3.6215220	-0.6147400	C	0.6282950	-1.7854640	-0.3667980
C	0.8945130	-4.1571950	-0.1434730	C	-1.3627360	3.0070510	-0.3369150
C	-1.9689210	-1.4104980	3.3909850	C	-0.6814490	4.2341470	-0.0674540
C	-1.0573160	-0.6373350	4.0532050	C	0.6814490	4.2341470	0.0674540
C	2.1373240	3.0994680	1.6646500	C	1.3627360	3.0070510	0.3369150
C	1.3399470	3.8622180	0.8574070	C	0.0000000	0.0000000	-3.4235490
C	-3.0095090	1.8894940	-2.0382940	C	-1.2249530	0.2229730	-4.1210110
C	-2.6334460	0.9974090	-3.0054880	C	-2.3541180	0.5915400	-3.4398830
H	1.2376840	-0.1815640	-5.1109480	C	-2.2257050	1.0506650	-2.0951790
H	-1.2376840	0.1815640	-5.1109480	C	1.3627360	-3.0070510	-0.3369150
H	-2.9190160	4.2468890	-0.8470950	C	2.7072620	-3.0259310	-0.8117600
H	-0.7797100	5.2299020	-0.0044780	C	3.1557330	-2.0277660	-1.6336230
H	2.7895400	1.8934070	3.9164310	C	2.2257050	-1.0506650	-2.0951790

C	-2.2257050	-1.0506650	2.0951790
C	-3.1557330	-2.0277660	1.6336230
C	-2.7072620	-3.0259310	0.8117600
C	-1.3627360	-3.0070510	0.3369150
C	2.2257050	1.0506650	2.0951790
C	2.3541180	0.5915400	3.4398830
C	1.2249530	0.2229730	4.1210110
C	0.0000000	0.0000000	3.4235490
C	1.2249530	-0.2229730	-4.1210110
C	2.3541180	-0.5915400	-3.4398830
C	-3.1557330	2.0277660	-1.6336230
C	-2.7072620	3.0259310	-0.8117600
C	2.7072620	3.0259310	0.8117600
C	3.1557330	2.0277660	1.6336230
C	-2.3541180	-0.5915400	3.4398830
C	-1.2249530	-0.2229730	4.1210110
C	-0.6814490	-4.2341470	0.0674540
C	0.6814490	-4.2341470	-0.0674540
H	-1.2456310	5.1631110	-0.1096470
H	1.2456310	5.1631110	0.1096470
H	-1.2386960	0.0866080	-5.2002540
H	-3.3003690	0.7350510	-3.9567130
H	3.3172000	-3.9059720	-0.6186070
H	4.1351940	-2.0892020	-2.1028110
H	-4.1351940	-2.0892020	2.1028110
H	-3.3172000	-3.9059720	0.6186070
H	3.3003690	0.7350510	3.9567130
H	1.2386960	0.0866080	5.2002540
H	1.2386960	-0.0866080	-5.2002540
H	3.3003690	-0.7350510	-3.9567130
H	-4.1351940	2.0892020	-2.1028110
H	-3.3172000	3.9059720	-0.6186070
H	3.3172000	3.9059720	0.6186070
H	4.1351940	2.0892020	2.1028110
H	-3.3003690	-0.7350510	3.9567130
H	-1.2386960	-0.0866080	5.2002540
H	-1.2456310	-5.1631110	0.1096470
H	1.2456310	-5.1631110	-0.1096470

Stacking dimer Geometry for molecule 1-18

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C	1.5345880	1.2195280	3.5447190
C	1.5343270	2.4589830	2.8293820
C	1.8833300	2.4660390	1.4252220
C	2.3509110	3.6364980	0.7168110
C	2.3509110	3.6364980	-0.7168110
C	1.8833300	2.4660390	-1.4252220
C	1.5343270	2.4589830	-2.8293820
C	1.5345880	1.2195280	-3.5447190
C	1.8848160	0.0004990	-2.8489400
C	2.3527560	-1.1981620	-3.5081910
C	2.3521310	-2.4394960	-2.7912920
C	1.8845760	-2.4678940	-1.4235080
C	1.5327260	-3.6794860	-0.7156520
C	1.5327260	-3.6794860	0.7156520
C	1.8845760	-2.4678940	1.4235080
C	2.3521310	-2.4394960	2.7912920
C	2.3527560	-1.1981620	3.5081910
C	1.8848160	0.0004990	2.8489400
C	1.8124970	-0.0010360	1.4403830
C	1.8110910	1.2470430	0.7197160
C	1.8110910	1.2470430	-0.7197160
C	1.8124970	-0.0010360	-1.4403830
C	1.8132380	-1.2471970	-0.7205720
C	1.8132380	-1.2471970	0.7205720
C	2.9690750	-1.1597160	4.7859100
C	3.5220970	-2.2867260	5.3650420
C	3.5203430	-3.5044450	4.6624010
C	2.9669290	-3.5659280	3.3969650
C	1.0920300	3.6230240	3.5043650
C	0.6588540	3.5897580	4.8168410
C	0.6590290	2.3734610	5.5188810
C	1.0923500	1.2207890	4.8904360
C	2.9661170	4.7243810	-1.3889370
C	3.5173590	5.7905170	-0.7028890

C	3.5173590	5.7905170	0.7028890	C	-2.3521310	2.4394960	2.7912920
C	2.9661170	4.7243810	1.3889370	C	-1.8845760	2.4678940	1.4235080
C	1.0923500	1.2207890	-4.8904360	C	-1.5327260	3.6794860	0.7156520
C	0.6590290	2.3734610	-5.5188810	C	-1.5327260	3.6794860	-0.7156520
C	0.6588540	3.5897580	-4.8168410	C	-1.8845760	2.4678940	-1.4235080
C	1.0920300	3.6230240	-3.5043650	C	-2.3521310	2.4394960	-2.7912920
C	2.9669290	-3.5659280	-3.3969650	C	-2.3527560	1.1981620	-3.5081910
C	3.5203430	-3.5044450	-4.6624010	C	-1.8848160	-0.0004990	-2.8489400
C	3.5220970	-2.2867260	-5.3650420	C	-1.5345880	-1.2195280	-3.5447190
C	2.9690750	-1.1597160	-4.7859100	C	-1.5343270	-2.4589830	-2.8293820
C	1.0896030	-4.8453300	1.3866250	C	-1.8833300	-2.4660390	-1.4252220
C	0.6530010	-5.9643230	0.7021070	C	-2.3509110	-3.6364980	-0.7168110
C	0.6530010	-5.9643230	-0.7021070	C	-2.3509110	-3.6364980	0.7168110
C	1.0896030	-4.8453300	-1.3866250	C	-1.8833300	-2.4660390	1.4252220
H	3.0727850	-0.2078340	5.2924480	C	-1.5343270	-2.4589830	2.8293820
H	4.0060940	-2.2133800	6.3360450	C	-1.5345880	-1.2195280	3.5447190
H	4.0025560	-4.3829370	5.0845930	C	-1.8848160	-0.0004990	2.8489400
H	3.0691260	-4.4810040	2.8262300	C	-1.8124970	0.0010360	1.4403830
H	1.0353170	4.5521710	2.9550980	C	-1.8132380	1.2471970	0.7205720
H	0.2854420	4.4958050	5.2874910	C	-1.8132380	1.2471970	-0.7205720
H	0.2856000	2.3276050	6.5388230	C	-1.8124970	0.0010360	-1.4403830
H	1.0342650	0.2795330	5.4184720	C	-1.8110910	-1.2470430	-0.7197160
H	3.0701980	4.6869600	-2.4664900	C	-1.8110910	-1.2470430	0.7197160
H	3.9990380	6.5958730	-1.2523170	C	-1.0923500	-1.2207890	4.8904360
H	3.9990380	6.5958730	1.2523170	C	-0.6590290	-2.3734610	5.5188810
H	3.0701980	4.6869600	2.4664900	C	-0.6588540	-3.5897580	4.8168410
H	1.0342650	0.2795330	-5.4184720	C	-1.0920300	-3.6230240	3.5043650
H	0.2856000	2.3276050	-6.5388230	C	-2.9669290	3.5659280	3.3969650
H	0.2854420	4.4958050	-5.2874910	C	-3.5203430	3.5044450	4.6624010
H	1.0353170	4.5521710	-2.9550980	C	-3.5220970	2.2867260	5.3650420
H	3.0691260	-4.4810040	-2.8262300	C	-2.9690750	1.1597160	4.7859100
H	4.0025560	-4.3829370	-5.0845930	C	-1.0896030	4.8453300	-1.3866250
H	4.0060940	-2.2133800	-6.3360450	C	-0.6530010	5.9643230	-0.7021070
H	3.0727850	-0.2078340	-5.2924480	C	-0.6530010	5.9643230	0.7021070
H	1.0354430	-4.8339460	2.4660480	C	-1.0896030	4.8453300	1.3866250
H	0.2780020	-6.8240840	1.2516700	C	-2.9690750	1.1597160	-4.7859100
H	0.2780020	-6.8240840	-1.2516700	C	-3.5220970	2.2867260	-5.3650420
H	1.0354430	-4.8339460	-2.4660480	C	-3.5203430	3.5044450	-4.6624010
C	-2.3527560	1.1981620	3.5081910	C	-2.9669290	3.5659280	-3.3969650

C	-1.0920300	-3.6230240	-3.5043650
C	-0.6588540	-3.5897580	-4.8168410
C	-0.6590290	-2.3734610	-5.5188810
C	-1.0923500	-1.2207890	-4.8904360
C	-2.9661170	-4.7243810	1.3889370
C	-3.5173590	-5.7905170	0.7028890
C	-3.5173590	-5.7905170	-0.7028890
C	-2.9661170	-4.7243810	-1.3889370
H	-1.0342650	-0.2795330	5.4184720
H	-0.2856000	-2.3276050	6.5388230
H	-0.2854420	-4.4958050	5.2874910
H	-1.0353170	-4.5521710	2.9550980
H	-3.0691260	4.4810040	2.8262300
H	-4.0025560	4.3829370	5.0845930
H	-4.0060940	2.2133800	6.3360450
H	-3.0727850	0.2078340	5.2924480
H	-1.0354430	4.8339460	-2.4660480
H	-0.2780020	6.8240840	-1.2516700
H	-0.2780020	6.8240840	1.2516700
H	-1.0354430	4.8339460	2.4660480
H	-3.0727850	0.2078340	-5.2924480
H	-4.0060940	2.2133800	-6.3360450
H	-4.0025560	4.3829370	-5.0845930
H	-3.0691260	4.4810040	-2.8262300
H	-1.0353170	-4.5521710	-2.9550980
H	-0.2854420	-4.4958050	-5.2874910
H	-0.2856000	-2.3276050	-6.5388230
H	-1.0342650	-0.2795330	-5.4184720
H	-3.0701980	-4.6869600	2.4664900
H	-3.9990380	-6.5958730	1.2523170
H	-3.9990380	-6.5958730	-1.2523170
H	-3.0701980	-4.6869600	-2.4664900

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C	-1.7294180	1.3591260	0.7204600
C	-1.7294180	1.3591260	-0.7204600
C	-1.7604490	0.1079480	-1.4313720

C	-1.7950290	-1.1461920	-0.7212870
C	-1.7950290	-1.1461920	0.7212870
C	-1.7604490	0.1079480	1.4313720
C	-1.7439860	2.5945700	1.4262270
C	-1.4323670	3.8144260	0.7138580
C	-1.4323670	3.8144260	-0.7138580
C	-1.7439860	2.5945700	-1.4262270
C	-1.7912450	0.1129460	2.8508690
C	-2.1053580	1.3315860	3.5260050
C	-2.0746710	2.5436190	2.8121430
C	-1.8547400	-2.3794670	1.4310210
C	-1.5954710	-2.3280720	2.8341950
C	-1.5477140	-1.1109970	3.5412130
C	-1.8547400	-2.3794670	-1.4310210
C	-2.2145140	-3.5859090	-0.7145890
C	-2.2145140	-3.5859090	0.7145890
C	-1.7912450	0.1129460	-2.8508690
C	-1.5477140	-1.1109970	-3.5412130
C	-1.5954710	-2.3280720	-2.8341950
C	-2.0746710	2.5436190	-2.8121430
C	-2.1053580	1.3315860	-3.5260050
C	-1.0332560	4.9940820	1.3849530
C	-0.6546700	6.1347370	0.7009870
C	-0.6546700	6.1347370	-0.7009870
C	-1.0332560	4.9940820	-1.3849530
C	-2.6810910	-4.7444230	-1.3829600
C	-3.1057780	-5.8698650	-0.7014000
C	-3.1057780	-5.8698650	0.7014000
C	-2.6810910	-4.7444230	1.3829600
C	-2.6052790	1.4950500	4.8600080
C	-2.9494270	2.7833600	5.1428780
S	-2.6658850	3.8499250	3.8163700
S	-1.1888780	-3.6487110	3.9060650
C	-0.9311510	-2.5848660	5.2360630
C	-1.1678030	-1.2834550	4.9105930
S	-2.6658850	3.8499250	-3.8163700
C	-2.9494270	2.7833600	-5.1428780
C	-2.6052790	1.4950500	-4.8600080
C	-1.1678030	-1.2834550	-4.9105930

C	-0.9311510	-2.5848660	-5.2360630	C	2.0746710	-2.5436190	-2.8121430
S	-1.1888780	-3.6487110	-3.9060650	C	1.5954710	2.3280720	-2.8341950
H	-0.9518950	4.9910680	2.4636340	C	1.5477140	1.1109970	-3.5412130
H	-0.3190620	7.0086650	1.2529820	C	2.6810910	4.7444230	1.3829600
H	-0.3190620	7.0086650	-1.2529820	C	3.1057780	5.8698650	0.7014000
H	-0.9518950	4.9910680	-2.4636340	C	3.1057780	5.8698650	-0.7014000
H	-2.7699360	-4.7394580	-2.4618470	C	2.6810910	4.7444230	-1.3829600
H	-3.4719940	-6.7308920	-1.2551820	C	1.0332560	-4.9940820	-1.3849530
H	-3.4719940	-6.7308920	1.2551820	C	0.6546700	-6.1347370	-0.7009870
H	-2.7699360	-4.7394580	2.4618470	C	0.6546700	-6.1347370	0.7009870
H	-2.7690310	0.6787070	5.5512690	C	1.0332560	-4.9940820	1.3849530
H	-3.3800990	3.1689960	6.0590360	C	1.1678030	1.2834550	4.9105930
H	-0.5904330	-2.9836230	6.1832750	C	0.9311510	2.5848660	5.2360630
H	-1.0156090	-0.4648770	5.5999140	S	1.1888780	3.6487110	3.9060650
H	-3.3800990	3.1689960	-6.0590360	S	2.6658850	-3.8499250	3.8163700
H	-2.7690310	0.6787070	-5.5512690	C	2.9494270	-2.7833600	5.1428780
H	-1.0156090	-0.4648770	-5.5999140	C	2.6052790	-1.4950500	4.8600080
H	-0.5904330	-2.9836230	-6.1832750	S	1.1888780	3.6487110	-3.9060650
C	1.7950290	1.1461920	0.7212870	C	0.9311510	2.5848660	-5.2360630
C	1.7950290	1.1461920	-0.7212870	C	1.1678030	1.2834550	-4.9105930
C	1.7604490	-0.1079480	-1.4313720	C	2.6052790	-1.4950500	-4.8600080
C	1.7294180	-1.3591260	-0.7204600	C	2.9494270	-2.7833600	-5.1428780
C	1.7294180	-1.3591260	0.7204600	S	2.6658850	-3.8499250	-3.8163700
C	1.7604490	-0.1079480	1.4313720	H	2.7699360	4.7394580	2.4618470
C	1.8547400	2.3794670	1.4310210	H	3.4719940	6.7308920	1.2551820
C	2.2145140	3.5859090	0.7145890	H	3.4719940	6.7308920	-1.2551820
C	2.2145140	3.5859090	-0.7145890	H	2.7699360	4.7394580	-2.4618470
C	1.8547400	2.3794670	-1.4310210	H	0.9518950	-4.9910680	-2.4636340
C	1.7912450	-0.1129460	2.8508690	H	0.3190620	-7.0086650	-1.2529820
C	1.5477140	1.1109970	3.5412130	H	0.3190620	-7.0086650	1.2529820
C	1.5954710	2.3280720	2.8341950	H	0.9518950	-4.9910680	2.4636340
C	1.7439860	-2.5945700	1.4262270	H	1.0156090	0.4648770	5.5999140
C	2.0746710	-2.5436190	2.8121430	H	0.5904330	2.9836230	6.1832750
C	2.1053580	-1.3315860	3.5260050	H	3.3800990	-3.1689960	6.0590360
C	1.7439860	-2.5945700	-1.4262270	H	2.7690310	-0.6787070	5.5512690
C	1.4323670	-3.8144260	-0.7138580	H	0.5904330	2.9836230	-6.1832750
C	1.4323670	-3.8144260	0.7138580	H	1.0156090	0.4648770	-5.5999140
C	1.7912450	-0.1129460	-2.8508690	H	2.7690310	-0.6787070	-5.5512690
C	2.1053580	-1.3315860	-3.5260050	H	3.3800990	-3.1689960	-6.0590360

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C	-1.9849290	0.0023810	1.4464630
C	-1.9849290	1.2514830	0.7252940
C	-2.0000000	1.2400660	-0.7159520
C	-2.0150710	-0.0023810	-1.4464630
C	-2.0150710	-1.2514830	-0.7252940
C	-2.0000000	-1.2400660	0.7159520
C	-1.9829720	0.0064500	2.8707640
C	-1.6673570	1.2354740	3.5698200
C	-1.6673570	2.4738180	2.8548620
C	-1.9829720	2.4829300	1.4409680
C	-2.0000000	-2.4702680	1.4262100
C	-2.3029660	-2.4530990	2.8219430
C	-2.2832460	-1.2296060	3.5197680
C	-2.0170280	-2.4829300	-1.4409680
C	-1.7167540	-3.6630120	-0.6950140
C	-1.6970340	-3.6704240	0.7134750
C	-2.0170280	-0.0064500	-2.8707640
C	-2.3326430	-1.2354740	-3.5698200
C	-2.3326430	-2.4738180	-2.8548620
C	-2.0000000	2.4702680	-1.4262100
C	-1.6970340	2.4530990	-2.8219430
C	-1.7167540	1.2296060	-3.5197680
C	-2.2832460	3.6630120	0.6950140
C	-2.3029660	3.6704240	-0.7134750
C	-1.2581410	1.2442070	4.9262280
C	-0.8934150	2.4094990	5.5769570
C	-0.8934150	3.6250370	4.8751660
C	-1.2581410	3.6441350	3.5406290
C	-2.7418590	-1.2442070	-4.9262280
C	-3.1065850	-2.4094990	-5.5769570
C	-3.1065850	-3.6250370	-4.8751660
C	-2.7418590	-3.6441350	-3.5406290
C	-2.7534550	-3.5437960	3.6361630
C	-3.0704830	-3.1607100	4.9058030
S	-2.8166620	-1.4742670	5.1697460

S	-1.1833380	-5.2142650	-1.3081200
C	-0.9295170	-5.8289040	0.2843530
C	-1.2465450	-4.9209080	1.2509350
S	-2.8166620	5.2142650	1.3081200
C	-3.0704830	5.8289040	-0.2843530
C	-2.7534550	4.9209080	-1.2509350
C	-1.2465450	3.5437960	-3.6361630
C	-0.9295170	3.1607100	-4.9058030
S	-1.1833380	1.4742670	-5.1697460
H	-1.1672250	0.3077870	5.4628180
H	-0.5710050	2.3708830	6.6144950
H	-0.5710050	4.5428790	5.3604930
H	-1.1672250	4.5770460	2.9979610
H	-2.8327750	-0.3077870	-5.4628180
H	-3.4289950	-2.3708830	-6.6144950
H	-3.4289950	-4.5428780	-5.3604930
H	-2.8327750	-4.5770460	-2.9979610
H	-2.8988820	-4.5524890	3.2713180
H	-3.4608660	-3.7758480	5.7074490
H	-0.5391340	-6.8307200	0.4162560
H	-1.1011180	-5.1092890	2.3069120
H	-3.4608660	6.8307200	-0.4162560
H	-2.8988820	5.1092890	-2.3069120
H	-1.1011180	4.5524890	-3.2713180
H	-0.5391340	3.7758480	-5.7074490
C	1.9849290	-0.0023810	1.4464630
C	1.9849290	-1.2514830	0.7252940
C	2.0000000	-1.2400660	-0.7159520
C	2.0150710	0.0023810	-1.4464630
C	2.0150710	1.2514830	-0.7252940
C	2.0000000	1.2400660	0.7159520
C	1.9829720	-0.0064500	2.8707640
C	1.6673570	-1.2354740	3.5698200
C	1.9829720	-2.4738180	2.8548620
C	2.0000000	2.4702680	1.4409680
C	2.3029660	2.4530990	2.8219430
C	2.2832460	1.2296060	3.5197680
C	2.0170280	2.4829300	-1.4409680

C	1.7167540	3.6630120	-0.6950140	H	3.4608660	3.7758480	5.7074490
C	1.6970340	3.6704240	0.7134750	H	0.5391340	6.8307200	0.4162560
C	2.0170280	0.0064500	-2.8707640	H	1.1011180	5.1092890	2.3069120
C	2.3326430	1.2354740	-3.5698200	H	3.4608660	-6.8307200	-0.4162560
C	2.3326430	2.4738180	-2.8548620	H	2.8988820	-5.1092890	-2.3069120
C	2.0000000	-2.4702680	-1.4262100	H	1.1011180	-4.5524890	-3.2713180
C	1.6970340	-2.4530990	-2.8219430	H	0.5391340	-3.7758480	-5.7074490
C	1.7167540	-1.2296060	-3.5197680				
C	2.2832460	-3.6630120	0.6950140				
C	2.3029660	-3.6704240	-0.7134750	120			
C	1.2581410	-1.2442070	4.9262280	molecule2_S1			
C	0.8934150	-2.4094990	5.5769570	C	-1.1484280	0.8543580	-1.7983450
C	0.8934150	-3.6250370	4.8751660	C	-1.3235370	-0.5715720	-1.8998840
C	1.2581410	-3.6441350	3.5406290	C	-0.1753360	-1.4148280	-1.7054830
C	2.7418590	1.2442070	-4.9262280	C	1.1484280	-0.8543580	-1.7983450
C	3.1065850	2.4094990	-5.5769570	C	1.3235370	0.5715720	-1.8998840
C	3.1065850	3.6250370	-4.8751660	C	0.1753360	1.4148280	-1.7054830
C	2.7418590	3.6441350	-3.5406290	C	-2.2863170	1.7023810	-1.7990230
C	2.7534550	3.5437960	3.6361630	C	-3.5384660	1.1812840	-2.3022130
C	3.0704830	3.1607100	4.9058030	C	-3.6921830	-0.2267290	-2.5067050
S	2.8166620	1.4742670	5.1697460	C	-2.6142950	-1.1268160	-2.1320290
S	1.1833380	5.2142650	-1.3081200	C	0.3455130	2.8070560	-1.4894360
C	0.9295170	5.8289040	0.2843530	C	-0.8044020	3.5694610	-1.1005610
C	1.2465450	4.9209080	1.2509350	C	-2.0894580	3.0309490	-1.3189500
S	2.8166620	-5.2142650	1.3081200	C	2.6142950	1.1268160	-2.1320290
C	3.0704830	-5.8289040	-0.2843530	C	2.7336910	2.5459190	-2.0279150
C	2.7534550	-4.9209080	-1.2509350	C	1.6399240	3.3779710	-1.6886940
C	1.2465450	-3.5437960	-3.6361630	C	2.2863170	-1.7023810	-1.7990230
C	0.9295170	-3.1607100	-4.9058030	C	3.5384660	-1.1812840	-2.3022130
S	1.1833380	-1.4742670	-5.1697460	C	3.6921830	0.2267290	-2.5067050
H	1.1672250	-0.3077870	5.4628180	C	-0.3455130	-2.8070560	-1.4894360
H	0.5710050	-2.3708830	6.6144950	C	0.8044020	-3.5694610	-1.1005610
H	0.5710050	-4.5428790	5.3604930	C	2.0894580	-3.0309490	-1.3189500
H	1.1672250	-4.5770460	2.9979610	C	-2.7336910	-2.5459190	-2.0279150
H	2.8327750	0.3077870	-5.4628180	C	-1.6399240	-3.3779710	-1.6886940
H	3.4289950	2.3708830	-6.6144950	C	-4.5848050	2.0419920	-2.7127820
H	3.4289950	4.5428780	-5.3604930	C	-5.7502800	1.5673750	-3.2854720
H	2.8327750	4.5770460	-2.9979610	C	-5.8964430	0.1904540	-3.5040840
H	2.8988820	4.5524890	3.2713180	C	-4.8801800	-0.6722580	-3.1334800

C	4.5848050	-2.0419920	-2.7127820	C	-3.6799960	0.6709610	1.3086630
C	5.7502800	-1.5673750	-3.2854720	C	-3.6461250	-0.7476090	1.1326780
C	5.8964430	-0.1904540	-3.5040840	C	-2.4411140	-1.4794690	1.4813310
C	4.8801800	0.6722580	-3.1334800	C	-0.0473090	2.8160980	2.1166070
C	-0.8583780	4.8441140	-0.4503680	C	-1.2891620	3.3804680	2.5612450
C	-2.1295580	5.2720470	-0.2125420	C	-2.4848920	2.6697850	2.3306240
S	-3.3120460	4.1569210	-0.7763030	C	2.4411140	1.4794690	1.4813310
S	4.1708770	3.5264740	-2.2491480	C	2.3749550	2.8897720	1.6855590
C	3.3120460	4.9866790	-1.9476590	C	1.1692360	3.5564460	2.0105340
C	1.9967430	4.7679180	-1.6799360	C	2.4974920	-1.3593140	1.7740170
S	-4.1708770	-3.5264740	-2.2491480	C	3.6799960	-0.6709610	1.3086630
C	-3.3120460	-4.9866790	-1.9476590	C	3.6461250	0.7476090	1.1326780
C	-1.9967430	-4.7679180	-1.6799360	C	0.0473090	-2.8160980	2.1166070
C	0.8583780	-4.8441140	-0.4503680	C	1.2891620	-3.3804680	2.5612450
C	2.1295580	-5.2720470	-0.2125420	C	2.4848920	-2.6697850	2.3306240
S	3.3120460	-4.1569210	-0.7763030	C	-2.3749550	-2.8897720	1.6855590
H	-4.4527640	3.1139750	-2.6360280	C	-1.1692360	-3.5564460	2.0105340
H	-6.5227910	2.2647030	-3.6001970	C	-4.8463950	1.3745810	0.9290420
H	-6.7841340	-0.2019250	-3.9941010	C	-5.9503790	0.7314890	0.3989840
H	-4.9937560	-1.7156750	-3.3931480	C	-5.9157470	-0.6569450	0.2157430
H	4.4527640	-3.1139750	-2.6360280	C	-4.7842420	-1.3689390	0.5728640
H	6.5227910	-2.2647030	-3.6001970	C	4.8463950	-1.3745810	0.9290420
H	6.7841340	0.2019250	-3.9941010	C	5.9503790	-0.7314890	0.3989840
H	4.9937560	1.7156750	-3.3931480	C	5.9157470	0.6569450	0.2157430
H	0.0057020	5.3764490	-0.0830130	C	4.7842420	1.3689390	0.5728640
H	-2.4416080	6.1700910	0.3052440	C	-1.5166790	4.5731060	3.3248060
H	3.8282970	5.9368240	-2.0081990	C	-2.8303860	4.7672950	3.6380360
H	1.3007980	5.5804670	-1.5362700	S	-3.8480100	3.5209260	3.0210220
H	-3.8282970	-5.9368240	-2.0081990	S	3.7026240	4.0319380	1.6767320
H	-1.3007980	-5.5804670	-1.5362700	C	2.6587970	5.3560510	2.0182540
H	-0.0057020	-5.3764490	-0.0830130	C	1.3597840	4.9710720	2.1573800
H	2.4416080	-6.1700910	0.3052440	S	-3.7026240	-4.0319380	1.6767320
C	-1.2515150	0.6869280	1.7130490	C	-2.6587970	-5.3560510	2.0182540
C	-1.2291290	-0.7516230	1.6255580	C	-1.3597840	-4.9710720	2.1573800
C	0.0238610	-1.4267490	1.8199630	C	1.5166790	-4.5731060	3.3248060
C	1.2515150	-0.6869280	1.7130490	C	2.8303860	-4.7672950	3.6380360
C	1.2291290	0.7516230	1.6255580	S	3.8480100	-3.5209260	3.0210220
C	-0.0238610	1.4267490	1.8199630	H	-4.8556870	2.4553760	0.9849140
C	-2.4974920	1.3593140	1.7740170	H	-6.8145290	1.3097280	0.0836630

H	-6.7523380	-1.1743700	-0.2457760	C	0.98248200	3.61108100
H	-4.7589030	-2.4231550	0.3369330	2.02641500		
H	4.8556870	-2.4553760	0.9849140	C	-0.39011300	3.71311600
H	6.8145290	-1.3097280	0.0836630	1.70921300		
H	6.7523380	1.1743700	-0.2457760	C	2.83516600	-0.24244300
H	4.7589030	2.4231550	0.3369330	1.73260200		
H	-0.7372930	5.2197350	3.7031170	C	3.55575600	0.86014000
H	-3.2576030	5.5689110	4.2282520	2.26156900		
H	3.0624840	6.3596800	2.0729640	C	2.95750800	2.10937800
H	0.5630630	5.6843250	2.3085270	2.51181300		
H	-3.0624840	-6.3596800	2.0729640	C	1.21627800	-2.57662400
H	-0.5630630	-5.6843250	2.3085270	1.48357800		
H	0.7372930	-5.2197350	3.7031170	C	2.61615000	-2.63469500
H	3.2576030	-5.5689110	4.2282520	1.10674500		
				C	3.43126200	-1.47228400
120				1.26334700		
molecule2_S2				C	-1.59781200	-2.32382400
C	-0.60912400	1.30136500		2.10536500		
1.62620200				C	-0.98248200	-3.61108100
C	-1.42449800	0.11559900		2.02641500		
1.69977300				C	0.39011300	-3.71311600
C	-0.81162100	-1.17892700		1.70921300		
1.81186000				C	-3.55575600	-0.86014000
C	0.60912400	-1.30136500		2.26156900		
1.62620200				C	-2.95750800	-2.10937800
C	1.42449800	-0.11559900		2.51181300		
1.69977300				C	-3.20000100	3.78072900
C	0.81162100	1.17892700		0.52416200		
1.81186000				C	-4.52784200	3.81451400
C	-1.21627800	2.57662400		0.13769400		
1.48357800				C	-5.33277500	2.68053600
C	-2.61615000	2.63469500		0.31217100		
1.10674500				C	-4.78333500	1.53414900
C	-3.43126200	1.47228400		0.85640300		
1.26334700				C	3.20000100	-3.78072900
C	-2.83516600	0.24244300		0.52416200		
1.73260200				C	4.52784200	-3.81451400
C	1.59781200	2.32382400		0.13769400		
2.10536500						

C	5.33277500	-2.68053600		H	4.92943900	-4.70656000	-
0.31217100				0.33511100			
C	4.78333500	-1.53414900		H	6.36691800	-2.68068800	-
0.85640300				0.02010000			
C	1.58876100	4.90066900		H	5.39171500	-0.64081000	
2.19783700				0.90723600			
C	0.70685600	5.92977100		H	2.64620600	5.06708700	
2.08991400				2.33578600			
S	-0.88991800	5.39189600		H	0.91064800	6.99056200	
1.73734600				2.16396700			
S	5.18364900	0.81936200		H	5.85416300	2.84592000	
2.90026500				4.09660500			
C	5.03695000	2.41512800		H	3.54490600	3.94141500	
3.53187200				3.64649700			
C	3.82712400	2.97493400		H	-5.85416300	-2.84592000	
3.25482200				4.09660500			
S	-5.18364900	-0.81936200		H	-3.54490600	-3.94141500	
2.90026500				3.64649700			
C	-5.03695000	-2.41512800		H	-2.64620600	-5.06708700	
3.53187200				2.33578600			
C	-3.82712400	-2.97493400		H	-0.91064800	-6.99056200	
3.25482200				2.16396700			
C	-1.58876100	-4.90066900		C	1.42449800	0.11559900	-
2.19783700				1.69977300			
C	-0.70685600	-5.92977100		C	0.60912400	1.30136500	-
2.08991400				1.62620200			
S	0.88991800	-5.39189600		C	-0.81162100	1.17892700	-
1.73734600				1.81186000			
H	-2.57985400	4.63630800		C	-1.42449800	-0.11559900	-
0.29539700				1.69977300			
H	-4.92943900	4.70656000	-	C	-0.60912400	-1.30136500	-
0.33511100				1.62620200			
H	-6.36691800	2.68068800	-	C	0.81162100	-1.17892700	-
0.02010000				1.81186000			
H	-5.39171500	0.64081000		C	2.83516600	0.24244300	-
0.90723600				1.73260200			
H	2.57985400	-4.63630800		C	3.43126200	1.47228400	-
0.29539700				1.26334700			

C	2.61615000	2.63469500	-
1.10674500			
C	1.21627800	2.57662400	-
1.48357800			
C	1.59781200	-2.32382400	-
2.10536500			
C	2.95750800	-2.10937800	-
2.51181300			
C	3.55575600	-0.86014000	-
2.26156900			
C	-1.21627800	-2.57662400	-
1.48357800			
C	-0.39011300	-3.71311600	-
1.70921300			
C	0.98248200	-3.61108100	-
2.02641500			
C	-2.83516600	-0.24244300	-
1.73260200			
C	-3.43126200	-1.47228400	-
1.26334700			
C	-2.61615000	-2.63469500	-
1.10674500			
C	-1.59781200	2.32382400	-
2.10536500			
C	-2.95750800	2.10937800	-
2.51181300			
C	-3.55575600	0.86014000	-
2.26156900			
C	0.39011300	3.71311600	-
1.70921300			
C	-0.98248200	3.61108100	-
2.02641500			
C	4.78333500	1.53414900	-
0.85640300			
C	5.33277500	2.68053600	-
0.31217100			
C	4.52784200	3.81451400	-
0.13769400			

C	3.20000100	3.78072900	-
0.52416200			
C	-4.78333500	-1.53414900	-
0.85640300			
C	-5.33277500	-2.68053600	-
0.31217100			
C	-4.52784200	-3.81451400	-
0.13769400			
C	-3.20000100	-3.78072900	-
0.52416200			
C	3.82712400	-2.97493400	-
3.25482200			
C	5.03695000	-2.41512800	-
3.53187200			
S	5.18364900	-0.81936200	-
2.90026500			
S	-0.88991800	-5.39189600	-
1.73734600			
C	0.70685600	-5.92977100	-
2.08991400			
C	1.58876100	-4.90066900	-
2.19783700			
S	0.88991800	5.39189600	-
1.73734600			
C	-0.70685600	5.92977100	-
2.08991400			
C	-1.58876100	4.90066900	-
2.19783700			
C	-3.82712400	2.97493400	-
3.25482200			
C	-5.03695000	2.41512800	-
3.53187200			
S	-5.18364900	0.81936200	-
2.90026500			
H	5.39171500	0.64081000	-
0.90723600			
H	6.36691800	2.68068800	
0.02010000			

H	4.92943900	4.70656000		C	-2.0131860	3.4936620	1.0136350
0.33511100				C	-1.9844410	3.4991760	-0.4156150
H	2.57985400	4.63630800	-	C	-1.6302350	2.2859020	-1.1224120
0.29539700				C	-1.9586130	-0.2029090	3.1522510
H	-5.39171500	-0.64081000	-	C	-1.7113110	1.0205340	3.8317880
0.90723600				C	-1.5137490	2.2313730	3.1429710
H	-6.36691800	-2.68068800		C	-1.9776690	-2.6812130	1.6991300
0.02010000				C	-2.4110350	-2.6375150	3.0640940
H	-4.92943900	-4.70656000		C	-2.3474640	-1.4210650	3.7702540
0.33511100				C	-1.7196000	-2.6736090	-1.1304590
H	-2.57985400	-4.63630800	-	C	-1.4770160	-3.8969460	-0.4024840
0.29539700				C	-1.6410990	-3.9116670	1.0160030
H	3.54490600	-3.94141500	-	C	-1.6475180	-0.1964470	-2.5742480
3.64649700				C	-1.9059890	-1.4297650	-3.2338520
H	5.85416300	-2.84592000	-	C	-1.9716960	-2.6514370	-2.5394100
4.09660500				C	-1.3401440	2.2626530	-2.5262300
H	0.91064800	-6.99056200	-	C	-1.4043770	1.0418390	-3.2261070
2.16396700				C	-2.5052840	4.6432190	1.6828100
H	2.64620600	-5.06708700	-	C	-2.9172980	5.7699260	0.9960210
2.33578600				C	-2.8941340	5.7741720	-0.4078350
H	-0.91064800	6.99056200	-	C	-2.4577510	4.6531860	-1.0895880
2.16396700				C	-0.9659200	-5.0533540	-1.0403470
H	-2.64620600	5.06708700	-	C	-0.6757540	-6.2066060	-0.3370930
2.33578600				C	-0.8719340	-6.2374070	1.0531080
H	-3.54490600	3.94141500	-	C	-1.3298380	-5.1091020	1.7088310
3.64649700				S	-1.5121920	1.2440140	5.5495140
H	-5.85416300	2.84592000	-	C	-1.0736190	2.8978760	5.3357540
4.09660500				C	-1.1087850	3.2834540	4.0284330
				C	-2.9928780	-3.6795500	3.8625920
				C	-3.3029410	-3.2764400	5.1282350
				S	-2.9194360	-1.6165300	5.4068820
120				C	-0.9482290	3.3396210	-3.3883450
molecule3_UD1				C	-0.7773220	2.9562000	-4.6845550
C	-1.7238860	1.0429140	1.0176450	C	-1.0752900	1.2758350	-4.9205300
C	-1.6644170	1.0500160	-0.4255120	S	-2.3251330	-1.6458130	-4.9126210
C	-1.6616460	-0.1970650	-1.1433950	C	-2.6329130	-3.3265220	-4.6742720
C	-1.7144510	-1.4437700	-0.4286710	C	-2.4087250	-3.7226530	-3.3889300
C	-1.8213230	-1.4489090	1.0114220	H	-2.6358450	4.6173020	2.7566080
C	-1.8221480	-0.2040770	1.7279270	H	-2.5566680	4.6367650	-2.1664500
C	-1.7094610	2.2713730	1.7240310				

H	-0.7261460	-5.0086370	-2.0949000	C	0.6757540	6.2066060	0.3370930
H	-1.3686320	-5.1227560	2.7892590	C	0.8719340	6.2374070	-1.0531080
H	-0.7771720	3.4887730	6.1932000	C	1.3298380	5.1091020	-1.7088310
H	-0.8054870	4.2686550	3.7008290	C	2.5052840	-4.6432190	-1.6828100
H	-3.2306020	-4.6687270	3.4932370	C	2.9172980	-5.7699260	-0.9960210
H	-3.7708870	-3.8579360	5.9131960	C	2.8941340	-5.7741720	0.4078350
H	-0.7411090	4.3421740	-3.0450830	C	2.4577510	-4.6531860	1.0895880
H	-0.4481060	3.5637400	-5.5181350	S	2.3251330	1.6458130	4.9126210
H	-2.9858650	-3.9292840	-5.5021180	C	2.6329130	3.3265220	4.6742720
H	-2.5995660	-4.7307180	-3.0440200	C	2.4087250	3.7226530	3.3889300
H	-3.3086630	6.6242510	1.5434090	C	0.9482290	-3.3396210	3.3883450
H	-3.2669410	6.6319690	-0.9624820	C	0.7773220	-2.9562000	4.6845550
H	-0.6106120	-7.1249180	1.6242990	S	1.0752900	-1.2758350	4.9205300
H	-0.2474030	-7.0624730	-0.8513840	C	2.9928780	3.6795500	-3.8625920
C	1.7144510	1.4437700	0.4286710	C	3.3029410	3.2764400	-5.1282350
C	1.8213230	1.4489090	-1.0114220	S	2.9194360	1.6165300	-5.4068820
C	1.8221480	0.2040770	-1.7279270	S	1.5121920	-1.2440140	-5.5495140
C	1.7238860	-1.0429140	-1.0176450	C	1.0736190	-2.8978760	-5.3357540
C	1.6644170	-1.0500160	0.4255120	C	1.1087850	-3.2834540	-4.0284330
C	1.6616460	0.1970650	1.1433950	H	0.7261460	5.0086370	2.0949000
C	1.7196000	2.6736090	1.1304590	H	1.3686320	5.1227560	-2.7892590
C	1.4770160	3.8969460	0.4024840	H	2.6358450	-4.6173020	-2.7566080
C	1.6410990	3.9116670	-1.0160030	H	2.5566680	-4.6367650	2.1664500
C	1.9776690	2.6812130	-1.6991300	H	2.9858650	3.9292840	5.5021180
C	1.6475180	0.1964470	2.5742480	H	2.5995660	4.7307180	3.0440200
C	1.9059890	1.4297650	3.2338520	H	0.7411090	-4.3421740	3.0450830
C	1.9716960	2.6514370	2.5394100	H	0.4481060	-3.5637400	5.5181350
C	1.6302350	-2.2859020	1.1224120	H	3.2306020	4.6687270	-3.4932370
C	1.3401440	-2.2626530	2.5262300	H	3.7708870	3.8579360	-5.9131960
C	1.4043770	-1.0418390	3.2261070	H	0.7771720	-3.4887730	-6.1932000
C	1.7094610	-2.2713730	-1.7240310	H	0.8054870	-4.2686550	-3.7008290
C	2.0131860	-3.4936620	-1.0136350	H	0.2474030	7.0624730	0.8513840
C	1.9844410	-3.4991760	0.4156150	H	0.6106120	7.1249180	-1.6242990
C	1.9586130	0.2029090	-3.1522510	H	3.2669410	-6.6319690	0.9624820
C	1.7113110	-1.0205340	-3.8317880	H	3.3086630	-6.6242510	-1.5434090
C	1.5137490	-2.2313730	-3.1429710				
C	2.4110350	2.6375150	-3.0640940				
C	2.3474640	1.4210650	-3.7702540				
C	0.9659200	5.0533540	1.0403470				

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C	-1.2593970	0.7354380	-1.7260930	C	2.8223920	5.1658170	-0.9297210
C	0.0008370	1.4400500	-1.7411540	S	3.8364560	3.8224370	-1.3028430
C	1.2344540	0.7002490	-1.7813900	S	5.1702780	1.2701410	-2.7224070
C	1.2205490	-0.7372380	-1.7856830	C	5.7751180	-0.3205400	-3.0133960
C	-0.0398740	-1.4424420	-1.7862740	C	4.8701100	-1.2910150	-2.7001680
C	-1.2719260	-0.7029990	-1.7623120	H	-4.5452310	3.0274150	-2.5637230
C	-2.4743360	1.4676590	-1.6947030	H	-0.2326880	5.4069300	-2.6623620
C	-2.4532120	2.8772690	-2.0218290	H	4.4933620	-3.0393300	-0.9943360
C	-1.2039210	3.5727330	-2.0457940	H	0.2040420	-5.4610620	-1.1077480
C	0.0117430	2.8574510	-1.7286930	H	-6.9109130	0.3761690	-0.4745530
C	-2.5180080	-1.4016870	-1.8073710	H	-5.1567650	2.2813750	-0.7459490
C	-3.6931050	-0.6545230	-1.5308330	H	-0.6931350	-5.5226950	-2.9726560
C	-3.6855040	0.7489170	-1.4214820	H	-3.2120840	-5.9850310	-3.4711390
C	-0.0501870	-2.8583670	-1.8671870	H	0.7187920	5.5780260	-0.8211330
C	-1.2800000	-3.5053340	-2.2194090	H	3.2638500	6.0951840	-0.5934850
C	-2.4838270	-2.7807480	-2.1484450	H	6.7660790	-0.4495220	-3.4312030
C	2.4330280	-1.4695950	-1.8453110	H	5.0588220	-2.3422290	-2.8747790
C	2.4105510	-2.8846230	-1.5500400	H	-4.4721320	5.3683220	-3.2383430
C	1.1648790	-3.5841390	-1.5746770	H	-2.2785760	6.5785370	-3.2986670
C	2.4801760	1.3984250	-1.8529740	H	2.2490460	-6.6457440	-0.4820350
C	3.6381520	0.6408300	-2.1747940	H	4.4248450	-5.4105710	-0.4130080
C	3.6312030	-0.7664080	-2.1977170	C	0.0391940	-1.4407960	1.7869010
C	1.2584280	3.5197550	-1.4807660	C	-1.2208910	-0.7350080	1.7866300
C	2.4593240	2.7966580	-1.6037090	C	-1.2341390	0.7024710	1.7819970
C	-3.6106540	3.5642210	-2.4697860	C	-0.0002170	1.4417260	1.7409660
C	-3.5656880	4.8826910	-2.8845700	C	1.2596860	0.7365250	1.7259630
C	-2.3360380	5.5618240	-2.9169830	C	1.2715650	-0.7019100	1.7626520
C	-1.1829250	4.9068690	-2.5269320	C	0.0488860	-2.8567200	1.8677620
C	3.5670250	-3.5819540	-1.1244880	C	-1.1665380	-3.5818780	1.5751470
C	3.5242630	-4.9177750	-0.7694590	C	-2.4119300	-2.8817970	1.5510870
C	2.3027860	-5.6088530	-0.8049530	C	-2.4336780	-1.4668200	1.8466990
C	1.1509740	-4.9465990	-1.1886190	C	2.5173200	-1.4011550	1.8077440
S	-5.2739610	-1.3008570	-1.1840800	C	2.4825380	-2.7800850	2.1493120
C	-5.8925690	0.2676400	-0.8254820	C	1.2784090	-3.5041970	2.2201480
C	-4.9598010	1.2472380	-0.9902000	C	2.4749550	1.4681640	1.6940450
C	-1.4883710	-4.8217310	-2.7545870	C	3.6857840	0.7487970	1.4210250
C	-2.7957530	-5.0822130	-3.0413340	C	3.6927320	-0.6546130	1.5307910
S	-3.8321780	-3.7494250	-2.6834940	C	-0.0105120	2.8591330	1.7275080
C	1.4990640	4.8707280	-1.0634890	C	1.2056010	3.5741450	2.0435270

C	2.4545270	2.8780150	2.0200490	H	-4.4276090	-5.4064380	0.4135600
C	-2.4795160	1.4012280	1.8537480	H	4.4751610	5.3693350	3.2331320
C	-2.4581420	2.7993220	1.6036370	H	2.2823180	6.5809610	3.2922120
C	-1.2569930	3.5217940	1.4794750				
C	-3.6313780	-0.7630180	2.1995480				
C	-3.6376820	0.6442380	2.1763500	120			
C	-1.1532740	-4.9441200	1.1883140	molecule3_S1			
C	-2.3054840	-5.6057450	0.8047270	C	-0.7981550	0.6079560	-1.7612750
C	-3.5267000	-4.9141660	0.7699340	C	0.6349430	0.4122910	-1.7887500
C	-3.5687970	-3.5784740	1.1255190	C	1.1742690	-0.9163820	-1.6902490
C	1.1855290	4.9089540	2.5228690	C	0.3116740	-2.0010700	-1.3155510
C	2.3391040	5.5636950	2.9119030	C	-1.1197500	-1.8131930	-1.3094650
C	3.5683560	4.8837940	2.8801620	C	-1.6698650	-0.5312210	-1.6501000
C	3.6124710	3.5648150	2.4669200	C	-1.3295730	1.9089360	-1.9482150
S	3.8303910	-3.7490600	2.6850880	C	-0.4535540	3.0488680	-1.7784360
C	2.7933600	-5.0813270	3.0431100	C	0.9615410	2.8549770	-1.8158050
C	1.4861760	-4.8205120	2.7558160	C	1.4885210	1.5219210	-2.0134410
C	4.9603050	1.2464440	0.9896100	C	-3.0776230	-0.3897390	-1.8704320
C	5.8925320	0.2663410	0.8248340	C	-3.5558130	0.9007470	-2.2297760
S	5.2732090	-1.3017980	1.1838520	C	-2.7151070	2.0317550	-2.2945850
C	-4.8703480	-1.2869320	2.7025820	C	-1.9656560	-2.9252350	-1.0696640
C	-5.7747160	-0.3159660	3.0161310	C	-3.3358370	-2.8269390	-1.4666600
S	-5.1692590	1.2743760	2.7245720	C	-3.8672140	-1.5736780	-1.8336230
S	-3.8350200	3.8255600	1.3031530	C	0.8449770	-3.2843370	-1.0498310
C	-2.8205920	5.1682030	0.9284170	C	0.0080890	-4.2579310	-0.3863480
C	-1.4973020	4.8726590	1.0615980	C	-1.4096910	-4.0919920	-0.4184750
H	-0.2066120	-5.4589620	1.1065810	C	2.5592910	-1.1603240	-1.9631580
H	-4.4949040	-3.0354140	0.9956400	C	3.0065500	-2.5113170	-1.9176060
H	0.2356620	5.4098520	2.6577090	C	2.1820830	-3.5635650	-1.4703880
H	4.5467850	3.0275860	2.5611300	C	2.8374060	1.2654170	-2.4248350
H	3.2092440	-5.9841290	3.4733830	C	3.3462790	-0.0499150	-2.3759950
H	0.6906530	-5.5211350	2.9738630	C	-0.9455560	4.3396740	-1.4670040
H	5.1578060	2.2804610	0.7452590	C	-0.1020620	5.4092580	-1.2347130
H	6.9109090	0.3743400	0.4738340	C	1.2877990	5.2194490	-1.2749200
H	-5.0595000	-2.3380060	2.8775320	C	1.7989710	3.9639770	-1.5434760
H	-6.7655260	-0.4444060	3.4344630	C	0.5507710	-5.3113670	0.3865730
H	-3.2618680	6.0975670	0.5919210	C	-0.2542230	-6.2036200	1.0703090
H	-0.7171570	5.5797250	0.8180770	C	-1.6493720	-6.0599840	1.0168540
H	-2.2522660	-6.6425010	0.4812830	C	-2.2067660	-5.0181960	0.2973370

S	-5.1748900	1.2984260	-2.7425830	C	-3.1130980	2.2846030	1.3024730
C	-4.7212660	2.9207880	-3.1036700	C	-2.3148630	3.4443740	1.3922760
C	-3.4092540	3.1692920	-2.8311130	C	-1.3858130	-1.5470460	2.2309690
C	-4.2909620	-3.8826860	-1.6518180	C	-2.7881180	-1.4598540	1.9581030
C	-5.5043630	-3.4381490	-2.0855680	C	-3.3588270	-0.2143850	1.6145340
S	-5.5406290	-1.7286550	-2.3079470	C	1.4439950	-1.8290460	2.0914510
C	3.7823750	2.1703590	-3.0174940	C	0.6669750	-2.8314550	2.7909010
C	4.9623980	1.5749430	-3.3495270	C	-0.7549960	-2.6893480	2.8630270
S	4.9830680	-0.1062880	-2.9751080	C	3.0673160	0.4235430	1.3187750
S	4.5424780	-3.1272330	-2.4721320	C	3.5826420	-0.9015340	1.3159310
C	4.0707840	-4.7546060	-2.1532300	C	2.8024360	-2.0176940	1.6866970
C	2.8135050	-4.8420370	-1.6340440	C	3.2661510	2.8955890	1.1889320
H	-2.0053850	4.4764500	-1.3118480	C	3.8131140	1.6035550	1.0409170
H	2.8635810	3.8105730	-1.4482960	C	-0.6294720	5.6359000	2.6301450
H	1.6248940	-5.3791810	0.5011380	C	0.1781870	6.6737640	3.0627300
H	-3.2757430	-4.8657660	0.3516920	C	1.5752720	6.5351930	3.0154470
H	-5.4514710	3.6020670	-3.5228450	C	2.1325410	5.3619800	2.5362560
H	-2.9427140	4.1167760	-3.0630130	C	1.2827900	-3.8564910	3.5502660
H	-4.0682340	-4.9342780	-1.5292350	C	0.5452930	-4.7347940	4.3239550
H	-6.3820100	-4.0280130	-2.3203400	C	-0.8500920	-4.5969740	4.3940320
H	3.5768620	3.2076300	-3.2434560	C	-1.4769410	-3.5835190	3.6906250
H	5.8262710	2.0315360	-3.8166530	S	-4.7443160	2.6863640	0.8383320
H	4.7477240	-5.5654180	-2.3934100	C	-4.3567550	4.3613620	0.7189720
H	2.3315620	-5.7888780	-1.4289920	C	-3.0562410	4.6207670	1.0355800
H	-0.5164540	6.3758790	-0.9596170	C	-3.7641650	-2.5098880	1.9190970
H	1.9608590	6.0373720	-1.0308620	C	-5.0128750	-2.0749000	1.5912020
H	-2.2916280	-6.7298240	1.5832810	S	-5.0667720	-0.3743650	1.3144000
H	0.1953450	-6.9775630	1.6865480	C	4.1938590	3.9094870	0.7730030
C	-0.3465870	2.0326040	1.6914230	C	5.3919360	3.4057560	0.3607420
C	1.0873850	1.8917630	1.6384280	S	5.4524780	1.6855640	0.4544000
C	1.6714710	0.5814380	1.5800340	S	5.1955880	-1.3918510	0.8764220
C	0.8542970	-0.5598940	1.8790350	C	4.8163550	-3.0564360	1.1197990
C	-0.5795280	-0.4190200	1.9425970	C	3.5332590	-3.2428540	1.5370440
C	-1.1782680	0.8621350	1.6946610	H	-1.6988500	5.7129190	2.7817660
C	-0.9245450	3.3243530	1.7106160	H	3.2036280	5.2252800	2.6158960
C	-0.0893140	4.4435740	2.0888150	H	2.3634040	-3.9080810	3.5925700
C	1.3337570	4.3028760	2.0400660	H	-2.5361610	-3.4246180	3.8459840
C	1.9059730	3.0454940	1.6100920	H	-5.1129310	5.0641790	0.3918430
C	-2.5937770	0.9816940	1.5443120	H	-2.6231940	5.6080990	0.9502170

H	-3.5328030	-3.5536820	2.0697090
H	-5.9091820	-2.6674140	1.4586990
H	3.9579330	4.9637730	0.7199090
H	6.2454100	3.9523510	-0.0210380
H	5.5592150	-3.8125170	0.9008720
H	3.1046960	-4.2241750	1.6837080
H	-0.2712700	7.5669910	3.4900650
H	2.2188500	7.3199020	3.4060000
H	-1.4354720	-5.2487720	5.0381880
H	1.0534800	-5.4937110	4.9142200

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C	-1.3167800	-0.5685130	1.6870560
C	-0.1534240	-1.4210700	1.7417810
C	1.1543070	-0.8446650	1.8682150
C	1.3176500	0.5692010	1.6865950
C	0.1542870	1.4217560	1.7414280
C	-1.1533870	0.8453640	1.8683920
C	-2.6061300	-1.1414810	1.5777520
C	-2.7079560	-2.5223070	1.1523310
C	-1.5670410	-3.3759400	1.2800040
C	-0.3230500	-2.8244650	1.7665550
C	-2.2820090	1.6705780	2.1657400
C	-3.5537730	1.0385840	2.2141940
C	-3.7379870	-0.3307720	1.9189010
C	0.3238680	2.8251670	1.7656940
C	-0.7496910	3.6183620	2.2829770
C	-2.0173420	3.0342160	2.4807140
C	2.6069620	1.1421540	1.5769390
C	2.7086750	2.5229180	1.1511610
C	1.5677160	3.3765200	1.2786900
C	2.2830000	-1.6698720	2.1653370
C	3.5547620	-1.0378550	2.2134000
C	3.7388920	0.3315030	1.9180000
C	0.7506140	-3.6175360	2.2837850
C	2.0184050	-3.0334340	2.4807280
C	-3.8676570	-3.0414270	0.5313280
C	-3.9437290	-4.3581840	0.1151400

C	-2.8322330	-5.2034470	0.2620240
C	-1.6631410	-4.7076390	0.8092000
C	3.8682470	3.0419900	0.5299120
C	3.9442200	4.3586770	0.1134980
C	2.8326790	5.2039000	0.2602010
C	1.6636230	4.7081150	0.8074460
S	-5.0603990	1.7853890	2.6795780
C	-5.9092660	0.2905360	2.5324070
C	-5.1009820	-0.7326010	2.1360940
C	-0.7012730	4.9640060	2.7793190
C	-1.8851120	5.3803610	3.3126620
S	-3.1058240	4.1648630	3.2402460
C	0.7022640	-4.9629370	2.7807880
C	1.8863280	-5.3792340	3.3136780
S	3.1071290	-4.1638790	3.2402160
S	5.0614970	-1.7846150	2.6785240
C	5.9102450	-0.2897030	2.5314390
C	5.1018880	0.7333970	2.1352080
H	-4.6852830	-2.3742330	0.2944380
H	-0.7788520	-5.3316400	0.8098090
H	4.6858450	2.3748250	0.2928980
H	0.7791950	5.3319490	0.8076310
H	-6.9644860	0.2460750	2.7723190
H	-5.4601860	-1.7494590	2.0573410
H	0.1935190	5.5724470	2.7958040
H	-2.1056860	6.3344450	3.7755410
H	-0.1925680	-5.5713030	2.7980270
H	2.1070130	-6.3331840	3.7767770
H	6.9654420	-0.2451840	2.7714420
H	5.4610720	1.7502610	2.0564980
H	-4.8406380	-4.7142550	-0.3837860
H	-2.8637610	-6.2219130	-0.1157570
H	2.8641890	6.2222990	-0.1177650
H	4.8410990	4.7146860	-0.3855390
C	-1.3176670	0.5684290	-1.6867680
C	-0.1543630	1.4210440	-1.7416280
C	1.1533520	0.8447350	-1.8684200
C	1.3167870	-0.5691420	-1.6868990
C	0.1534720	-1.4217940	-1.7414760

C	-1.1542440	-0.8454490	-1.8681600	H	-4.6860930	2.3740620	-0.2936650
C	-2.6070220	1.1413720	-1.5773150	H	-0.7794520	5.3312260	-0.8081320
C	-2.7088180	2.5221770	-1.1517400	H	4.6854210	-2.3744530	-0.2941120
C	-1.5678970	3.3758130	-1.2792760	H	0.7791790	-5.3323130	-0.8086340
C	-0.3240090	2.8244350	-1.7661200	H	-6.9654010	-0.2463080	-2.7717570
C	-2.2828730	-1.6707130	-2.1653160	H	-5.4611080	1.7492790	-2.0570160
C	-3.5546600	-1.0387510	-2.2136630	H	0.1927050	-5.5723970	-2.7963170
C	-3.7388890	0.3306230	-1.9183880	H	-2.1067430	-6.3344750	-3.7753870
C	0.3231530	-2.8252070	-1.7658970	H	-0.1938050	5.5715990	-2.7965940
C	-0.7504840	-3.6184270	-2.2830030	H	2.1054120	6.3336520	-3.7761660
C	-2.0182060	-3.0343270	-2.4803710	H	6.9643120	0.2453680	-2.7729530
C	2.6061360	-1.1420310	-1.5775610	H	5.4601630	-1.7500730	-2.0576430
C	2.7080290	-2.5227850	-1.1518470	H	-4.8414210	4.7139840	0.3847130
C	1.5671410	-3.3765110	-1.2792370	H	-2.8643770	6.2214760	0.1173270
C	2.2819560	1.6699750	-2.1658040	H	2.8642450	-6.2221880	0.1167970
C	3.5537300	1.0379980	-2.2142290	H	4.8409930	-4.7142960	0.3844940
C	3.7379500	-0.3313600	-1.9188970				
C	0.7495070	3.6176230	-2.2834440				
C	2.0172150	3.0335620	-2.4809720	144			
C	-3.8684850	3.0412510	-0.5306130	molecule4_UD1			
C	-3.9445000	4.3579420	-0.1142180	C	-1.1381540	3.0377890	2.8688150
C	-2.8329340	5.2031590	-0.2608670	C	-1.2080270	1.7834690	3.5631130
C	-1.6638600	4.7073870	-0.8080800	C	-2.3174980	-0.4638770	3.5295300
C	3.8678030	-3.0417120	-0.5308320	C	-2.4856810	-1.7124050	2.8312830
C	3.9439910	-4.3583750	-0.1143820	C	-2.0535720	-1.8759060	1.4388490
C	2.8325530	-5.2037470	-0.2610410	C	-1.9522740	-3.1340870	0.7226300
C	1.6633760	-4.7081490	-0.8081970	C	-1.9522740	-3.1340870	-0.7226300
S	-5.0613260	-1.7856090	-2.6788780	C	-2.0535720	-1.8759060	-1.4388490
C	-5.9101800	-0.2907460	-2.5318460	C	-2.4856810	-1.7124050	-2.8312830
C	-5.1018880	0.7324250	-2.1356520	C	-2.3174980	-0.4638770	-3.5295300
C	-0.7021330	-4.9640390	-2.7794370	C	-1.2080270	1.7834690	-3.5631130
C	-1.8861050	-5.3804230	-3.3124730	C	-1.1381540	3.0377890	-2.8688150
S	-3.1068920	-4.1650370	-3.2395120	C	-1.4549930	3.1323010	-1.4385290
C	0.7010080	4.9631850	-2.7799890	C	-1.8118990	4.3396210	-0.7241930
C	1.8848720	5.3795830	-3.3132430	C	-1.8118990	4.3396210	0.7241930
S	3.1056450	4.1641410	-3.2406670	C	-1.4549930	3.1323010	1.4385290
S	5.0603450	1.7847830	-2.6796750	C	-1.4115110	1.9422670	0.7124670
C	5.9091610	0.2898840	-2.5327490	C	-1.7856470	-0.7143990	0.7144540
C	5.1009000	-0.7332280	-2.1363260	C	-1.7856470	-0.7143990	-0.7144540

C	-1.4115110	1.9422670	-0.7124670	H	-1.3168100	-6.4625520	1.2510440
C	-2.3140800	5.4871260	1.3910660	H	-1.6533830	-4.3630120	2.4639540
C	-2.7577760	6.6013310	0.7034100	H	-2.8827970	0.6720320	-5.2708160
C	-2.7577760	6.6013310	-0.7034100	H	-4.1119460	-1.1390690	-6.3621060
C	-2.3140800	5.4871260	-1.3910660	H	-4.4121680	-3.3291880	-5.1751120
C	-0.6989830	1.6939690	4.8701850	H	-3.4996390	-3.6096400	-2.9265360
C	-0.1577840	2.7913170	5.5238180	H	-0.4633450	5.0689480	-3.0485440
C	-0.1099970	4.0273820	4.8727800	H	0.3342210	4.8924850	-5.3581990
C	-0.5873100	4.1312330	3.5744200	H	0.2539590	2.6725230	-6.5224060
C	-3.2649020	-2.7044190	3.4719800	H	-0.7123750	0.7332990	-5.3659540
C	-3.8146740	-2.5356450	4.7337240	B	-1.5690830	0.6090940	1.4522330
C	-3.6465970	-1.3156860	5.3953700	B	-1.5690830	0.6090940	-1.4522330
C	-2.9302940	-0.2950910	4.7860910	N	-1.6767510	0.6255650	2.8904170
C	-1.7337230	-4.3650050	-1.3865000	N	-1.6767510	0.6255650	-2.8904170
C	-1.5244560	-5.5473170	-0.7019690	C	2.4856810	1.7124050	2.8312830
C	-1.5244560	-5.5473170	0.7019690	C	2.3174980	0.4638770	3.5295300
C	-1.7337230	-4.3650050	1.3865000	C	1.2080270	-1.7834690	3.5631130
C	-2.9302940	-0.2950910	-4.7860910	C	1.1381540	-3.0377890	2.8688150
C	-3.6465970	-1.3156860	-5.3953700	C	1.4549930	-3.1323010	1.4385290
C	-3.8146740	-2.5356450	-4.7337240	C	1.8118990	-4.3396210	0.7241930
C	-3.2649020	-2.7044190	-3.4719800	C	1.8118990	-4.3396210	-0.7241930
C	-0.5873100	4.1312330	-3.5744200	C	1.4549930	-3.1323010	-1.4385290
C	-0.1099970	4.0273820	-4.8727800	C	1.1381540	-3.0377890	-2.8688150
C	-0.1577840	2.7913170	-5.5238180	C	1.2080270	-1.7834690	-3.5631130
C	-0.6989830	1.6939690	-4.8701850	C	2.3174980	0.4638770	-3.5295300
H	-2.4145680	5.4654140	2.4698060	C	2.4856810	1.7124050	-2.8312830
H	-3.1525020	7.4538130	1.2512920	C	2.0535720	1.8759060	-1.4388490
H	-3.1525020	7.4538130	-1.2512920	C	1.9522740	3.1340870	-0.7226300
H	-2.4145680	5.4654140	-2.4698060	C	1.9522740	3.1340870	0.7226300
H	-0.7123750	0.7332990	5.3659540	C	2.0535720	1.8759060	1.4388490
H	0.2539590	2.6725230	6.5224060	C	1.7856470	0.7143990	0.7144540
H	0.3342210	4.8924850	5.3581990	C	1.4115110	-1.9422670	0.7124670
H	-0.4633450	5.0689480	3.0485440	C	1.4115110	-1.9422670	-0.7124670
H	-3.4996390	-3.6096400	2.9265360	C	1.7856470	0.7143990	-0.7144540
H	-4.4121680	-3.3291880	5.1751120	C	1.7337230	4.3650050	1.3865000
H	-4.1119460	-1.1390690	6.3621060	C	1.5244560	5.5473170	0.7019690
H	-2.8827970	0.6720320	5.2708160	C	1.5244560	5.5473170	-0.7019690
H	-1.6533830	-4.3630120	-2.4639540	C	1.7337230	4.3650050	-1.3865000
H	-1.3168100	-6.4625520	-1.2510440	C	2.9302940	0.2950910	4.7860910

C	3.6465970	1.3156860	5.3953700	H	3.4996390	3.6096400	-2.9265360
C	3.8146740	2.5356450	4.7337240	H	4.4121680	3.3291880	-5.1751120
C	3.2649020	2.7044190	3.4719800	H	4.1119460	1.1390690	-6.3621060
C	0.5873100	-4.1312330	3.5744200	H	2.8827970	-0.6720320	-5.2708160
C	0.1099970	-4.0273820	4.8727800	B	1.5690830	-0.6090940	1.4522330
C	0.1577840	-2.7913170	5.5238180	B	1.5690830	-0.6090940	-1.4522330
C	0.6989830	-1.6939690	4.8701850	N	1.6767510	-0.6255650	2.8904170
C	2.3140800	-5.4871260	-1.3910660	N	1.6767510	-0.6255650	-2.8904170
C	2.7577760	-6.6013310	-0.7034100				
C	2.7577760	-6.6013310	0.7034100	144			
C	2.3140800	-5.4871260	1.3910660	molecule4_UD2			
C	0.6989830	-1.6939690	-4.8701850	C	0.8634630	-3.5779050	-1.6074850
C	0.1577840	-2.7913170	-5.5238180	C	2.0981790	-2.8457110	-1.6226770
C	0.1099970	-4.0273820	-4.8727800	C	3.1920410	-0.7753800	-2.5100670
C	0.5873100	-4.1312330	-3.5744200	C	3.2297640	0.6635680	-2.4940500
C	3.2649020	2.7044190	-3.4719800	C	2.1207460	1.4513280	-1.9467910
C	3.8146740	2.5356450	-4.7337240	C	2.1444010	2.8769150	-1.6783360
C	3.6465970	1.3156860	-5.3953700	C	0.9013580	3.6111490	-1.6139690
C	2.9302940	0.2950910	-4.7860910	C	-0.3553080	2.9043290	-1.7885650
H	1.6533830	4.3630120	2.4639540	C	-1.6392440	3.5063990	-2.1628060
H	1.3168100	6.4625520	1.2510440	C	-2.8737480	2.7703600	-2.0618710
H	1.3168100	6.4625520	-1.2510440	C	-4.0406480	0.7636440	-1.1128630
H	1.6533830	4.3630120	-2.4639540	C	-4.0715080	-0.6714110	-1.1488790
H	2.8827970	-0.6720320	5.2708160	C	-2.8955570	-1.4463260	-1.5638290
H	4.1119460	1.1390690	6.3621060	C	-2.9094780	-2.7986720	-2.0796950
H	4.4121680	3.3291880	5.1751120	C	-1.6649620	-3.5290300	-2.2047790
H	3.4996390	3.6096400	2.9265360	C	-0.4242310	-2.9002240	-1.8011090
H	0.4633450	-5.0689480	3.0485440	C	-0.4385250	-1.5206050	-1.5903950
H	-0.3342210	-4.8924850	5.3581990	C	0.9077430	0.7939250	-1.7449360
H	-0.2539590	-2.6725230	6.5224060	C	-0.3210980	1.5166620	-1.6580500
H	0.7123750	-0.7332990	5.3659540	C	-1.6632470	-0.7987740	-1.4781370
H	2.4145680	-5.4654140	-2.4698060	C	-1.6933550	-4.7829620	-2.8683950
H	3.1525020	-7.4538130	-1.2512920	C	-2.8660410	-5.3329910	-3.3514450
H	3.1525020	-7.4538130	1.2512920	C	-4.0752760	-4.6255890	-3.2248900
H	2.4145680	-5.4654140	2.4698060	C	-4.0838850	-3.3819470	-2.6215560
H	0.7123750	-0.7332990	-5.3659540	C	3.2826570	-3.4880310	-1.2271910
H	-0.2539590	-2.6725230	-6.5224060	C	3.3024300	-4.8242700	-0.8558870
H	-0.3342210	-4.8924850	-5.3581990	C	2.1153810	-5.5614850	-0.8704250
H	0.4633450	-5.0689480	-3.0485440	C	0.9308560	-4.9383860	-1.2357490

C	4.2729160	1.2872590	-3.2193130	H	-5.0840050	2.5351180	-0.4982330
C	5.2559570	0.5759590	-3.8896290	B	0.8749050	-0.7356450	-1.6980510
C	5.2000630	-0.8212310	-3.9032420	B	-1.6270570	0.7355420	-1.4942010
C	4.1705120	-1.4754920	-3.2421690	N	2.0984450	-1.4619250	-1.9285600
C	0.9608780	4.9820030	-1.2630830	N	-2.8762690	1.4562230	-1.5341780
C	2.1522490	5.6180050	-0.9661350	C	-3.2243230	0.6958320	2.4932360
C	3.3579660	4.8994820	-1.0136420	C	-3.1980730	-0.7433440	2.5112110
C	3.3424900	3.5631240	-1.3657590	C	-2.1211140	-2.8234300	1.6260740
C	-4.0405730	3.3131220	-2.6334240	C	-0.8922080	-3.5655030	1.6108780
C	-4.0492910	4.5624990	-3.2377220	C	0.4009000	-2.8980830	1.8035050
C	-2.8617300	5.2945080	-3.3338910	C	1.6364830	-3.5365880	2.2079180
C	-1.6888760	4.7536870	-2.8285680	C	2.8867510	-2.8164250	2.0823670
C	-5.2190950	-1.3051870	-0.6227040	C	2.8839550	-1.4645220	1.5651990
C	-6.2841210	-0.6031790	-0.0781900	C	4.0661690	-0.6994310	1.1499260
C	-6.2358140	0.7931890	-0.0431380	C	4.0470370	0.7358340	1.1131360
C	-5.1300770	1.4562440	-0.5565150	C	2.8958090	2.7528330	2.0595280
H	-0.7586840	-5.2960750	-3.0616400	C	1.6671310	3.4988310	2.1588840
H	-2.8414770	-6.2880350	-3.8710270	C	0.3786570	2.9065040	1.7849750
H	-4.9932970	-5.0295150	-3.6453610	C	-0.8722410	3.6232450	1.6092990
H	-5.0027470	-2.8075130	-2.6222910	C	-2.1212660	2.8994930	1.6748660
H	4.1926300	-2.9069270	-1.1827830	C	-2.1090470	1.4739640	1.9449190
H	4.2329320	-5.2767620	-0.5233340	C	-0.9014960	0.8065260	1.7436370
H	2.1067080	-6.6025270	-0.5579040	C	0.4263490	-1.5188590	1.5913890
H	0.0059370	-5.4918920	-1.1556820	C	1.6569510	-0.8071050	1.4784920
H	4.2649370	2.3660610	-3.3125500	C	0.3333060	1.5190470	1.6559300
H	6.0292600	1.1063900	-4.4394100	C	-3.3136140	3.5953720	1.3616900
H	5.9285440	-1.4011350	-4.4646880	C	-3.3178470	4.9312610	1.0074510
H	4.0926170	-2.5517990	-3.3306950	C	-2.1061220	5.6394620	0.9582030
H	0.0346090	5.5269460	-1.1457460	C	-0.9201050	4.9939250	1.2559460
H	2.1470840	6.6612290	-0.6594110	C	-4.1819570	-1.4346470	3.2444830
H	4.2949370	5.3793660	-0.7419620	C	-5.2062190	-0.7713360	3.9047320
H	4.2663270	3.0024350	-1.3521100	C	-5.2510270	0.6262300	3.8891360
H	-4.9466440	2.7204510	-2.6458370	C	-4.2624240	1.3287350	3.2177100
H	-4.9710060	4.9390990	-3.6745630	C	-0.9705540	-4.9255370	1.2400590
H	-2.8401980	6.2533300	-3.8455810	C	-2.1601290	-5.5396730	0.8759240
H	-0.7599520	5.2782010	-3.0145060	C	-3.3413850	-4.7932300	0.8618850
H	-5.2400790	-2.3869780	-0.5964760	C	-3.3108120	-3.4569130	1.2321230
H	-7.1296530	-1.1397500	0.3438680	C	4.0563760	-3.4085380	2.6251300
H	-7.0423120	1.3648270	0.4087140	C	4.0375340	-4.6512780	3.2300210

C	2.8225960	-5.3488150	3.3570600
C	1.6545440	-4.7900240	2.8728970
C	5.1424690	1.4191600	0.5571640
C	6.2428530	0.7468400	0.0442800
C	6.2796440	-0.6498460	0.0798900
C	5.2087600	-1.3428410	0.6245200
C	1.7263500	4.7466540	2.8228180
C	2.9032490	5.2789550	3.3278040
C	4.0849200	4.5372980	3.2334550
C	4.0665330	3.2870580	2.6310560
H	-4.2421440	3.0425450	1.3494450
H	-4.2507960	5.4186400	0.7352730
H	-2.0923210	6.6820500	0.6495700
H	0.0108520	5.5303770	1.1366660
H	-4.1125800	-2.5114350	3.3343540
H	-5.9391560	-1.3446700	4.4671260
H	-6.0200260	1.1636250	4.4381870
H	-4.2458400	2.4075490	3.3096270
H	-0.0499630	-5.4861310	1.1597080
H	-2.1596900	-6.5808740	0.5638470
H	-4.2756680	-5.2386280	0.5303510
H	-4.2160730	-2.8685370	1.1873510
H	4.9798520	-2.8415700	2.6253310
H	4.9521310	-5.0620760	3.6513060
H	2.7902580	-6.3030090	3.8777730
H	0.7156920	-5.2954250	3.0661710
H	5.1057870	2.4984010	0.4989650
H	7.0542130	1.3117350	-0.4073430
H	7.1208750	-1.1935810	-0.3415950
H	5.2210010	-2.4248030	0.5988970
H	0.8015010	5.2787560	3.0075000
H	2.8891050	6.2387410	3.8379430
H	5.0094340	4.9071430	3.6701470
H	4.9678490	2.6872300	2.6451890
B	-0.8807390	-0.7233310	1.6986740
B	1.6330420	0.7274490	1.4931690
N	-2.1101400	-1.4394110	1.9303530
N	2.8879840	1.4381620	1.5332870

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C	1.3960320	0.6338880	1.6306050
C	1.3089440	-0.7868780	1.7608640
C	-1.3960320	-0.6338880	1.6306050
C	-1.3089440	0.7868780	1.7608640
C	2.6385680	1.2948840	1.6238960
C	3.8438950	0.5029110	1.7820380
C	3.7568640	-0.9358670	1.8513570
C	2.4604700	-1.5807790	1.9145040
C	1.3850440	3.4755890	1.3995070
C	2.5809330	2.7260190	1.3945210
C	-2.4604700	1.5807790	1.9145040
C	-2.2236530	2.9782270	2.2190750
C	-0.9557480	3.5924450	2.1537890
C	-2.6385680	-1.2948840	1.6238960
C	-3.8438950	-0.5029110	1.7820380
C	-3.7568640	0.9358670	1.8513570
C	-1.3850440	-3.4755890	1.3995070
C	-2.5809330	-2.7260190	1.3945210
C	2.2236530	-2.9782270	2.2190750
C	0.9557480	-3.5924450	2.1537890
C	5.1299850	1.0869740	1.8944270
C	6.2874060	0.3340450	1.9507300
C	6.2069170	-1.0651460	1.8788380
C	4.9664490	-1.6724630	1.8429000
C	-5.1299850	-1.0869740	1.8944270
C	-6.2874060	-0.3340450	1.9507300
C	-6.2069170	1.0651460	1.8788380
C	-4.9664490	1.6724630	1.8429000
C	1.5517210	4.8183540	0.9542090
C	2.8481370	5.1127740	0.6438930
S	3.8856210	3.7686400	0.8765380
S	-3.3496080	4.0925870	2.9644170
C	-2.1506740	5.3011850	3.1794380
C	-0.9295190	4.9049620	2.7119150
S	3.3496080	-4.0925870	2.9644170
C	2.1506740	-5.3011850	3.1794380

C	0.9295190	-4.9049620	2.7119150	C	-3.8438950	0.5029110	-1.7820380
C	-1.5517210	-4.8183540	0.9542090	C	-0.9557480	-3.5924450	-2.1537890
C	-2.8481370	-5.1127740	0.6438930	C	-2.2236530	-2.9782270	-2.2190750
S	-3.8856210	-3.7686400	0.8765380	C	2.5809330	-2.7260190	-1.3945210
H	5.2231490	2.1632230	1.9614420	C	1.3850440	-3.4755890	-1.3995070
H	7.2514260	0.8298120	2.0340730	C	4.9664490	1.6724630	-1.8429000
H	7.1089740	-1.6716780	1.8569090	C	6.2069170	1.0651460	-1.8788380
H	4.9274730	-2.7509500	1.7660640	C	6.2874060	-0.3340450	-1.9507300
H	-5.2231490	-2.1632230	1.9614420	C	5.1299850	-1.0869740	-1.8944270
H	-7.2514260	-0.8298120	2.0340730	C	-4.9664490	-1.6724630	-1.8429000
H	-7.1089740	1.6716780	1.8569090	C	-6.2069170	-1.0651460	-1.8788380
H	-4.9274730	2.7509500	1.7660640	C	-6.2874060	0.3340450	-1.9507300
H	0.7357300	5.5154590	0.8287060	C	-5.1299850	1.0869740	-1.8944270
H	3.2443000	6.0446940	0.2622380	C	0.9295190	4.9049620	-2.7119150
H	-2.4043190	6.2391250	3.6573140	C	2.1506740	5.3011850	-3.1794380
H	-0.0341130	5.5027540	2.8137640	S	3.3496080	4.0925870	-2.9644170
H	2.4043190	-6.2391250	3.6573140	S	-3.8856210	3.7686400	-0.8765380
H	0.0341130	-5.5027540	2.8137640	C	-2.8481370	5.1127740	-0.6438930
H	-0.7357300	-5.5154590	0.8287060	C	-1.5517210	4.8183540	-0.9542090
H	-3.2443000	-6.0446940	0.2622380	S	3.8856210	-3.7686400	-0.8765380
N	0.1642420	2.8749280	1.7192970	C	2.8481370	-5.1127740	-0.6438930
N	-0.1642420	-2.8749280	1.7192970	C	1.5517210	-4.8183540	-0.9542090
B	0.0819440	1.4293890	1.6731480	C	-0.9295190	-4.9049620	-2.7119150
B	-0.0819440	-1.4293890	1.6731480	C	-2.1506740	-5.3011850	-3.1794380
C	1.3089440	0.7868780	-1.7608640	S	-3.3496080	-4.0925870	-2.9644170
C	1.3960320	-0.6338880	-1.6306050	H	4.9274730	2.7509500	-1.7660640
C	-1.3089440	-0.7868780	-1.7608640	H	7.1089740	1.6716780	-1.8569090
C	-1.3960320	0.6338880	-1.6306050	H	7.2514260	-0.8298120	-2.0340730
C	2.4604700	1.5807790	-1.9145040	H	5.2231490	-2.1632230	-1.9614420
C	3.7568640	0.9358670	-1.8513570	H	-4.9274730	-2.7509500	-1.7660640
C	3.8438950	-0.5029110	-1.7820380	H	-7.1089740	-1.6716780	-1.8569090
C	2.6385680	-1.2948840	-1.6238960	H	-7.2514260	0.8298120	-2.0340730
C	0.9557480	3.5924450	-2.1537890	H	-5.2231490	2.1632230	-1.9614420
C	2.2236530	2.9782270	-2.2190750	H	0.0341130	5.5027540	-2.8137640
C	-2.6385680	1.2948840	-1.6238960	H	2.4043190	6.2391250	-3.6573140
C	-2.5809330	2.7260190	-1.3945210	H	-3.2443000	6.0446940	-0.2622380
C	-1.3850440	3.4755890	-1.3995070	H	-0.7357300	5.5154590	-0.8287060
C	-2.4604700	-1.5807790	-1.9145040	H	3.2443000	-6.0446940	-0.2622380
C	-3.7568640	-0.9358670	-1.8513570	H	0.7357300	-5.5154590	-0.8287060

H	-0.0341130	-5.5027540	-2.8137640
H	-2.4043190	-6.2391250	-3.6573140
N	-0.1642420	2.8749280	-1.7192970
N	0.1642420	-2.8749280	-1.7192970
B	-0.0819440	1.4293890	-1.6731480
B	0.0819440	-1.4293890	-1.6731480

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C	-1.4976410	0.3328830	1.5529420
C	-0.5757360	1.4102610	1.7244560
C	1.4976410	-0.3328830	1.5529420
C	0.5757360	-1.4102610	1.7244560
C	-2.8875950	0.5490640	1.5217840
C	-3.3761240	1.9039600	1.7031270
C	-2.4423930	2.9903670	1.8957470
C	-1.0181660	2.7247630	1.9580050
C	-3.1811170	-1.9507580	1.3255240
C	-3.6914860	-0.6347560	1.2776580
C	1.0181660	-2.7247630	1.9580050
C	-0.0170180	-3.6776430	2.3095720
C	-1.3975970	-3.4139140	2.1920570
C	2.8875950	-0.5490640	1.5217840
C	3.3761240	-1.9039600	1.7031270
C	2.4423930	-2.9903670	1.8957470
C	3.1811170	1.9507580	1.3255240
C	3.6914860	0.6347560	1.2776580
C	0.0170180	3.6776430	2.3095720
C	1.3975970	3.4139140	2.1920570
C	-4.7582780	2.2152100	1.7336010
C	-5.2321080	3.5066590	1.8659800
C	-4.3227410	4.5702400	1.9685330
C	-2.9671230	4.3028980	1.9917440
C	4.7582780	-2.2152100	1.7336010
C	5.2321080	-3.5066590	1.8659800
C	4.3227410	-4.5702400	1.9685330
C	2.9671230	-4.3028980	1.9917440
C	-4.1033840	-2.9401010	0.8811290

C	-5.3105060	-2.4087670	0.5280160
S	-5.3454040	-0.7055990	0.7187560
S	0.1933750	-5.1975370	3.1514400
C	-1.4976410	-5.4424540	3.3207630
C	-2.2223680	-4.4226320	2.7731350
S	-0.1933750	5.1975370	3.1514400
C	1.4976410	5.4424540	3.3207630
C	2.2223680	4.4226320	2.7731350
C	4.1033840	2.9401010	0.8811290
C	5.3105060	2.4087670	0.5280160
S	5.3454040	0.7055990	0.7187560
H	-5.4864600	1.4176880	1.6727000
H	-6.3036020	3.6900270	1.8826980
H	-4.6748770	5.5969150	2.0349100
H	-2.2855670	5.1412240	2.0526410
H	5.4864600	-1.4176880	1.6727000
H	6.3036020	-3.6900270	1.8826980
H	4.6748770	-5.5969150	2.0349100
H	2.2855670	-5.1412240	2.0526410
H	-3.8536400	-3.9862080	0.7697030
H	-6.1699290	-2.9256850	0.1220550
H	-1.8705430	-6.3202800	3.8332680
H	-3.3011190	-4.3654170	2.8251860
H	1.8705430	6.3202800	3.8332680
H	3.3011190	4.3654170	2.8251860
H	3.8536400	3.9862080	0.7697030
H	6.1699290	2.9256850	0.1220550
N	-1.8531340	-2.1919220	1.6882610
N	1.8531340	2.1919220	1.6882610
B	-0.9207410	-1.0901530	1.6122790
B	0.9207410	1.0901530	1.6122790
C	-1.5303650	0.0171680	-1.7675190
C	-0.8615190	-1.2432050	-1.6798220
C	1.5303650	-0.0171680	-1.7675190
C	0.8615190	1.2432050	-1.6798220
C	-2.9199000	0.1021200	-1.9827730
C	-3.6295370	-1.1227120	-2.3317800
C	-2.9533630	-2.3930540	-2.2272940
C	-1.5794480	-2.4452500	-1.7759270

C	-2.7221740	2.6192060	-1.7287780	H	3.0967680	4.5021220	-2.6836970
C	-3.4811070	1.4356010	-1.9161770	H	-3.1066460	4.8086840	-1.8632850
C	1.5794480	2.4452500	-1.7759270	H	-5.6369890	4.2713960	-2.1294300
C	0.8526960	3.6364860	-1.4048870	H	-0.0024140	6.7466930	0.0936720
C	-0.5450940	3.6866780	-1.2170840	H	-1.9809650	5.0992810	-0.2790380
C	2.9199000	-0.1021200	-1.9827730	H	0.0024140	-6.7466930	0.0936720
C	3.6295370	1.1227120	-2.3317800	H	1.9809650	-5.0992810	-0.2790380
C	2.9533630	2.3930540	-2.2272940	H	3.1066460	-4.8086840	-1.8632850
C	2.7221740	-2.6192060	-1.7287780	H	5.6369890	-4.2713960	-2.1294300
C	3.4811070	-1.4356010	-1.9161770	N	-1.3387970	2.5665010	-1.5186340
C	-0.8526960	-3.6364860	-1.4048870	N	1.3387970	-2.5665010	-1.5186340
C	0.5450940	-3.6866780	-1.2170840	B	-0.6745610	1.2771010	-1.5995590
C	-4.9459090	-1.1342540	-2.8551150	B	0.6745610	-1.2771010	-1.5995590
C	-5.5875090	-2.2943590	-3.2502810				
C	-4.9180510	-3.5243570	-3.1635240				
C	-3.6266270	-3.5571760	-2.6730440	120			
C	4.9459090	1.1342540	-2.8551150	molecule5_TD1			
C	5.5875090	2.2943590	-3.2502810	C	1.3960320	0.6338880	1.6306050
C	4.9180510	3.5243570	-3.1635240	C	1.3089440	-0.7868780	1.7608640
C	3.6266270	3.5571760	-2.6730440	C	-1.3960320	-0.6338880	1.6306050
C	-3.5056300	3.8064100	-1.8502170	C	-1.3089440	0.7868780	1.7608640
C	-4.8350340	3.5520960	-2.0237430	C	2.6385680	1.2948840	1.6238960
S	-5.1661010	1.8753390	-2.0914700	C	3.8438950	0.5029110	1.7820380
S	1.5635780	5.1396500	-0.8725030	C	3.7568640	-0.9358670	1.8513570
C	0.0514490	5.7754610	-0.3798070	C	2.4604700	-1.5807790	1.9145040
C	-0.9748780	4.9059510	-0.6149480	C	1.3850440	3.4755890	1.3995070
S	-1.5635780	-5.1396500	-0.8725030	C	2.5809330	2.7260190	1.3945210
C	-0.0514490	-5.7754610	-0.3798070	C	-2.4604700	1.5807790	1.9145040
C	0.9748780	-4.9059510	-0.6149480	C	-2.2236530	2.9782270	2.2190750
C	3.5056300	-3.8064100	-1.8502170	C	-0.9557480	3.5924450	2.1537890
C	4.8350340	-3.5520960	-2.0237430	C	-2.6385680	-1.2948840	1.6238960
S	5.1661010	-1.8753390	-2.0914700	C	-3.8438950	-0.5029110	1.7820380
H	-5.4740420	-0.2028670	-3.0019560	C	-3.7568640	0.9358670	1.8513570
H	-6.5944600	-2.2399800	-3.6571900	C	-1.3850440	-3.4755890	1.3995070
H	-5.3924150	-4.4398160	-3.5091160	C	-2.5809330	-2.7260190	1.3945210
H	-3.0967680	-4.5021220	-2.6836970	C	2.2236530	-2.9782270	2.2190750
H	5.4740420	0.2028670	-3.0019560	C	0.9557480	-3.5924450	2.1537890
H	6.5944600	2.2399800	-3.6571900	C	5.1299850	1.0869740	1.8944270
H	5.3924150	4.4398160	-3.5091160	C	6.2874060	0.3340450	1.9507300

C	6.2069170	-1.0651460	1.8788380	C	1.3960320	-0.6338880	-1.6306050
C	4.9664490	-1.6724630	1.8429000	C	-1.3089440	-0.7868780	-1.7608640
C	-5.1299850	-1.0869740	1.8944270	C	-1.3960320	0.6338880	-1.6306050
C	-6.2874060	-0.3340450	1.9507300	C	2.4604700	1.5807790	-1.9145040
C	-6.2069170	1.0651460	1.8788380	C	3.7568640	0.9358670	-1.8513570
C	-4.9664490	1.6724630	1.8429000	C	3.8438950	-0.5029110	-1.7820380
C	1.5517210	4.8183540	0.9542090	C	2.6385680	-1.2948840	-1.6238960
C	2.8481370	5.1127740	0.6438930	C	0.9557480	3.5924450	-2.1537890
S	3.8856210	3.7686400	0.8765380	C	2.2236530	2.9782270	-2.2190750
S	-3.3496080	4.0925870	2.9644170	C	-2.6385680	1.2948840	-1.6238960
C	-2.1506740	5.3011850	3.1794380	C	-2.5809330	2.7260190	-1.3945210
C	-0.9295190	4.9049620	2.7119150	C	-1.3850440	3.4755890	-1.3995070
S	3.3496080	-4.0925870	2.9644170	C	-2.4604700	-1.5807790	-1.9145040
C	2.1506740	-5.3011850	3.1794380	C	-3.7568640	-0.9358670	-1.8513570
C	0.9295190	-4.9049620	2.7119150	C	-3.8438950	0.5029110	-1.7820380
C	-1.5517210	-4.8183540	0.9542090	C	-0.9557480	-3.5924450	-2.1537890
C	-2.8481370	-5.1127740	0.6438930	C	-2.2236530	-2.9782270	-2.2190750
S	-3.8856210	-3.7686400	0.8765380	C	2.5809330	-2.7260190	-1.3945210
H	5.2231490	2.1632230	1.9614420	C	1.3850440	-3.4755890	-1.3995070
H	7.2514260	0.8298120	2.0340730	C	4.9664490	1.6724630	-1.8429000
H	7.1089740	-1.6716780	1.8569090	C	6.2069170	1.0651460	-1.8788380
H	4.9274730	-2.7509500	1.7660640	C	6.2874060	-0.3340450	-1.9507300
H	-5.2231490	-2.1632230	1.9614420	C	5.1299850	-1.0869740	-1.8944270
H	-7.2514260	-0.8298120	2.0340730	C	-4.9664490	-1.6724630	-1.8429000
H	-7.1089740	1.6716780	1.8569090	C	-6.2069170	-1.0651460	-1.8788380
H	-4.9274730	2.7509500	1.7660640	C	-6.2874060	0.3340450	-1.9507300
H	0.7357300	5.5154590	0.8287060	C	-5.1299850	1.0869740	-1.8944270
H	3.2443000	6.0446940	0.2622380	C	0.9295190	4.9049620	-2.7119150
H	-2.4043190	6.2391250	3.6573140	C	2.1506740	5.3011850	-3.1794380
H	-0.0341130	5.5027540	2.8137640	S	3.3496080	4.0925870	-2.9644170
H	2.4043190	-6.2391250	3.6573140	S	-3.8856210	3.7686400	-0.8765380
H	0.0341130	-5.5027540	2.8137640	C	-2.8481370	5.1127740	-0.6438930
H	-0.7357300	-5.5154590	0.8287060	C	-1.5517210	4.8183540	-0.9542090
H	-3.2443000	-6.0446940	0.2622380	S	3.8856210	-3.7686400	-0.8765380
N	0.1642420	2.8749280	1.7192970	C	2.8481370	-5.1127740	-0.6438930
N	-0.1642420	-2.8749280	1.7192970	C	1.5517210	-4.8183540	-0.9542090
B	0.0819440	1.4293890	1.6731480	C	-0.9295190	-4.9049620	-2.7119150
B	-0.0819440	-1.4293890	1.6731480	C	-2.1506740	-5.3011850	-3.1794380
C	1.3089440	0.7868780	-1.7608640	S	-3.3496080	-4.0925870	-2.9644170

H	4.9274730	2.7509500	-1.7660640	C	2.4423930	-2.9903670	1.8957470
H	7.1089740	1.6716780	-1.8569090	C	3.1811170	1.9507580	1.3255240
H	7.2514260	-0.8298120	-2.0340730	C	3.6914860	0.6347560	1.2776580
H	5.2231490	-2.1632230	-1.9614420	C	0.0170180	3.6776430	2.3095720
H	-4.9274730	-2.7509500	-1.7660640	C	1.3975970	3.4139140	2.1920570
H	-7.1089740	-1.6716780	-1.8569090	C	-4.7582780	2.2152100	1.7336010
H	-7.2514260	0.8298120	-2.0340730	C	-5.2321080	3.5066590	1.8659800
H	-5.2231490	2.1632230	-1.9614420	C	-4.3227410	4.5702400	1.9685330
H	0.0341130	5.5027540	-2.8137640	C	-2.9671230	4.3028980	1.9917440
H	2.4043190	6.2391250	-3.6573140	C	4.7582780	-2.2152100	1.7336010
H	-3.2443000	6.0446940	-0.2622380	C	5.2321080	-3.5066590	1.8659800
H	-0.7357300	5.5154590	-0.8287060	C	4.3227410	-4.5702400	1.9685330
H	3.2443000	-6.0446940	-0.2622380	C	2.9671230	-4.3028980	1.9917440
H	0.7357300	-5.5154590	-0.8287060	C	-4.1033840	-2.9401010	0.8811290
H	-0.0341130	-5.5027540	-2.8137640	C	-5.3105060	-2.4087670	0.5280160
H	-2.4043190	-6.2391250	-3.6573140	S	-5.3454040	-0.7055990	0.7187560
N	-0.1642420	2.8749280	-1.7192970	S	0.1933750	-5.1975370	3.1514400
N	0.1642420	-2.8749280	-1.7192970	C	-1.4976410	-5.4424540	3.3207630
B	-0.0819440	1.4293890	-1.6731480	C	-2.2223680	-4.4226320	2.7731350
B	0.0819440	-1.4293890	-1.6731480	S	-0.1933750	5.1975370	3.1514400
				C	1.4976410	5.4424540	3.3207630
				C	2.2223680	4.4226320	2.7731350
				C	4.1033840	2.9401010	0.8811290
				C	5.3105060	2.4087670	0.5280160
				S	5.3454040	0.7055990	0.7187560
				H	-5.4864600	1.4176880	1.6727000
				H	-6.3036020	3.6900270	1.8826980
				H	-4.6748770	5.5969150	2.0349100
				H	-2.2855670	5.1412240	2.0526410
				H	5.4864600	-1.4176880	1.6727000
				H	6.3036020	-3.6900270	1.8826980
				H	4.6748770	-5.5969150	2.0349100
				H	2.2855670	-5.1412240	2.0526410
				H	-3.8536400	-3.9862080	0.7697030
				H	-6.1699290	-2.9256850	0.1220550
				H	-1.8705430	-6.3202800	3.8332680
				H	-3.3011190	-4.3654170	2.8251860
				H	1.8705430	6.3202800	3.8332680
				H	3.3011190	4.3654170	2.8251860

120							
molecule5_TD2							
C	-1.4976410	0.3328830	1.5529420				
C	-0.5757360	1.4102610	1.7244560				
C	1.4976410	-0.3328830	1.5529420				
C	0.5757360	-1.4102610	1.7244560				
C	-2.8875950	0.5490640	1.5217840				
C	-3.3761240	1.9039600	1.7031270				
C	-2.4423930	2.9903670	1.8957470				
C	-1.0181660	2.7247630	1.9580050				
C	-3.1811170	-1.9507580	1.3255240				
C	-3.6914860	-0.6347560	1.2776580				
C	1.0181660	-2.7247630	1.9580050				
C	-0.0170180	-3.6776430	2.3095720				
C	-1.3975970	-3.4139140	2.1920570				
C	2.8875950	-0.5490640	1.5217840				
C	3.3761240	-1.9039600	1.7031270				

H	3.8536400	3.9862080	0.7697030	C	-0.9748780	4.9059510	-0.6149480
H	6.1699290	2.9256850	0.1220550	S	-1.5635780	-5.1396500	-0.8725030
N	-1.8531340	-2.1919220	1.6882610	C	-0.0514490	-5.7754610	-0.3798070
N	1.8531340	2.1919220	1.6882610	C	0.9748780	-4.9059510	-0.6149480
B	-0.9207410	-1.0901530	1.6122790	C	3.5056300	-3.8064100	-1.8502170
B	0.9207410	1.0901530	1.6122790	C	4.8350340	-3.5520960	-2.0237430
C	-1.5303650	0.0171680	-1.7675190	S	5.1661010	-1.8753390	-2.0914700
C	-0.8615190	-1.2432050	-1.6798220	H	-5.4740420	-0.2028670	-3.0019560
C	1.5303650	-0.0171680	-1.7675190	H	-6.5944600	-2.2399800	-3.6571900
C	0.8615190	1.2432050	-1.6798220	H	-5.3924150	-4.4398160	-3.5091160
C	-2.9199000	0.1021200	-1.9827730	H	-3.0967680	-4.5021220	-2.6836970
C	-3.6295370	-1.1227120	-2.3317800	H	5.4740420	0.2028670	-3.0019560
C	-2.9533630	-2.3930540	-2.2272940	H	6.5944600	2.2399800	-3.6571900
C	-1.5794480	-2.4452500	-1.7759270	H	5.3924150	4.4398160	-3.5091160
C	-2.7221740	2.6192060	-1.7287780	H	3.0967680	4.5021220	-2.6836970
C	-3.4811070	1.4356010	-1.9161770	H	-3.1066460	4.8086840	-1.8632850
C	1.5794480	2.4452500	-1.7759270	H	-5.6369890	4.2713960	-2.1294300
C	0.8526960	3.6364860	-1.4048870	H	-0.0024140	6.7466930	0.0936720
C	-0.5450940	3.6866780	-1.2170840	H	-1.9809650	5.0992810	-0.2790380
C	2.9199000	-0.1021200	-1.9827730	H	0.0024140	-6.7466930	0.0936720
C	3.6295370	1.1227120	-2.3317800	H	1.9809650	-5.0992810	-0.2790380
C	2.9533630	2.3930540	-2.2272940	H	3.1066460	-4.8086840	-1.8632850
C	2.7221740	-2.6192060	-1.7287780	H	5.6369890	-4.2713960	-2.1294300
C	3.4811070	-1.4356010	-1.9161770	N	-1.3387970	2.5665010	-1.5186340
C	-0.8526960	-3.6364860	-1.4048870	N	1.3387970	-2.5665010	-1.5186340
C	0.5450940	-3.6866780	-1.2170840	B	-0.6745610	1.2771010	-1.5995590
C	-4.9459090	-1.1342540	-2.8551150	B	0.6745610	-1.2771010	-1.5995590
C	-5.5875090	-2.2943590	-3.2502810				
C	-4.9180510	-3.5243570	-3.1635240				
C	-3.6266270	-3.5571760	-2.6730440				
C	4.9459090	1.1342540	-2.8551150	120			
C	5.5875090	2.2943590	-3.2502810	molecule6_UD1			
C	4.9180510	3.5243570	-3.1635240	C	2.0252590	1.3663890	0.7145470
C	3.6266270	3.5571760	-2.6730440	C	2.0252590	1.3663890	-0.7145470
C	-3.5056300	3.8064100	-1.8502170	C	-0.6354120	1.7755010	-0.7160510
C	-4.8350340	3.5520960	-2.0237430	C	-0.6354120	1.7755010	0.7160510
S	-5.1661010	1.8753390	-2.0914700	C	3.2227450	1.2934370	1.4366500
S	1.5635780	5.1396500	-0.8725030	C	4.4666380	1.4850710	0.7219670
C	0.0514490	5.7754610	-0.3798070	C	4.4666380	1.4850710	-0.7219670
				C	3.2227450	1.2934370	-1.4366500

C	1.8835690	1.2413420	3.5422490	H	-2.5766550	3.8250620	5.7645180
C	3.1066370	1.0617270	2.8677480	H	5.0874530	0.2352030	-3.4456430
C	-1.8071960	2.0374300	1.4381310	H	4.1831680	-0.0799700	-5.8777760
C	-1.6536500	2.3415150	2.8525350	H	-2.5766550	3.8250620	-5.7645180
C	-0.4355360	2.1192350	3.5267440	H	-3.5442090	3.3904460	-3.3791210
C	-1.8071960	2.0374300	-1.4381310	H	7.7497130	2.3283670	1.2516950
C	-3.0667230	2.0116300	-0.7219100	H	7.7497130	2.3283670	-1.2516950
C	-3.0667230	2.0116300	0.7219100	H	-6.4307570	1.6091390	1.2486010
C	-0.4355360	2.1192350	-3.5267440	H	-6.4307570	1.6091390	-1.2486010
C	-1.6536500	2.3415150	-2.8525350	N	0.7050480	1.6200730	2.9046450
C	3.1066370	1.0617270	-2.8677480	N	0.7050480	1.6200730	-2.9046450
C	1.8835690	1.2413420	-3.5422490	B	0.6918790	1.5476300	1.4422940
C	5.6754800	1.8074570	1.3892150	B	0.6918790	1.5476300	-1.4422940
C	6.8465900	2.0709450	0.7031330	C	0.6354120	-1.7755010	0.7160510
C	6.8465900	2.0709450	-0.7031330	C	0.6354120	-1.7755010	-0.7160510
C	5.6754800	1.8074570	-1.3892150	C	-2.0252590	-1.3663890	-0.7145470
C	-4.3078030	1.8682970	-1.3878070	C	-2.0252590	-1.3663890	0.7145470
C	-5.5027600	1.7557510	-0.7020290	C	1.8071960	-2.0374300	1.4381310
C	-5.5027600	1.7557510	0.7020290	C	3.0667230	-2.0116300	0.7219100
C	-4.3078030	1.8682970	1.3878070	C	3.0667230	-2.0116300	-0.7219100
S	1.9923900	0.7796410	5.2168890	C	1.8071960	-2.0374300	-1.4381310
C	3.6436160	0.3232200	5.0306760	C	0.4355360	-2.1192350	3.5267440
C	4.0923820	0.5207930	3.7582780	C	1.6536500	-2.3415150	2.8525350
C	-2.5723930	3.0433950	3.7038450	C	-3.2227450	-1.2934370	1.4366500
C	-2.0850470	3.3114620	4.9482360	C	-3.1066370	-1.0617270	2.8677480
S	-0.4700790	2.7405270	5.1541940	C	-1.8835690	-1.2413420	3.5422490
C	4.0923820	0.5207930	-3.7582780	C	-3.2227450	-1.2934370	-1.4366500
C	3.6436160	0.3232200	-5.0306760	C	-4.4666380	-1.4850710	-0.7219670
S	1.9923900	0.7796410	-5.2168890	C	-4.4666380	-1.4850710	0.7219670
S	-0.4700790	2.7405270	-5.1541940	C	-1.8835690	-1.2413420	-3.5422490
C	-2.0850470	3.3114620	-4.9482360	C	-3.1066370	-1.0617270	-2.8677480
C	-2.5723930	3.0433950	-3.7038450	C	1.6536500	-2.3415150	-2.8525350
H	5.6701130	1.9207230	2.4656900	C	0.4355360	-2.1192350	-3.5267440
H	5.6701130	1.9207230	-2.4656900	C	4.3078030	-1.8682970	1.3878070
H	-4.3126910	1.7558200	-2.4629830	C	5.5027600	-1.7557510	0.7020290
H	-4.3126910	1.7558200	2.4629830	C	5.5027600	-1.7557510	-0.7020290
H	4.1831680	-0.0799700	5.8777760	C	4.3078030	-1.8682970	-1.3878070
H	5.0874530	0.2352030	3.4456430	C	-5.6754800	-1.8074570	-1.3892150
H	-3.5442090	3.3904460	3.3791210	C	-6.8465900	-2.0709450	-0.7031330

C	-6.8465900	-2.0709450	0.7031330
C	-5.6754800	-1.8074570	1.3892150
S	0.4700790	-2.7405270	5.1541940
C	2.0850470	-3.3114620	4.9482360
C	2.5723930	-3.0433950	3.7038450
C	-4.0923820	-0.5207930	3.7582780
C	-3.6436160	-0.3232200	5.0306760
S	-1.9923900	-0.7796410	5.2168890
C	2.5723930	-3.0433950	-3.7038450
C	2.0850470	-3.3114620	-4.9482360
S	0.4700790	-2.7405270	-5.1541940
S	-1.9923900	-0.7796410	-5.2168890
C	-3.6436160	-0.3232200	-5.0306760
C	-4.0923820	-0.5207930	-3.7582780
H	4.3126910	-1.7558200	2.4629830
H	4.3126910	-1.7558200	-2.4629830
H	-5.6701130	-1.9207230	-2.4656900
H	-5.6701130	-1.9207230	2.4656900
H	2.5766550	-3.8250620	5.7645180
H	3.5442090	-3.3904460	3.3791210
H	-5.0874530	-0.2352030	3.4456430
H	-4.1831680	0.0799700	5.8777760
H	3.5442090	-3.3904460	-3.3791210
H	2.5766550	-3.8250620	-5.7645180
H	-4.1831680	0.0799700	-5.8777760
H	-5.0874530	-0.2352030	-3.4456430
H	6.4307570	-1.6091390	1.2486010
H	6.4307570	-1.6091390	-1.2486010
H	-7.7497130	-2.3283670	1.2516950
H	-7.7497130	-2.3283670	-1.2516950
N	-0.7050480	-1.6200730	2.9046450
N	-0.7050480	-1.6200730	-2.9046450
B	-0.6918790	-1.5476300	1.4422940
B	-0.6918790	-1.5476300	-1.4422940

120

molecule6_UD2

C	-0.4849060	-1.5246480	-1.5847540
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C	-1.7120850	-0.7981170	-1.4721710
C	-0.3649290	1.5222780	-1.6518750
C	0.8658710	0.7957370	-1.7342910
C	-0.4783770	-2.9211970	-1.6960250
C	-1.7348620	-3.5936460	-1.9580270
C	-2.9738580	-2.8625150	-1.8283070
C	-2.9428500	-1.4637460	-1.4524970
C	2.0184640	-2.8485690	-1.7019790
C	0.8156100	-3.5751120	-1.5886290
C	2.0868420	1.4629160	-1.8949980
C	3.2277910	0.6629960	-2.3099310
C	3.1841670	-0.7455210	-2.2957800
C	-0.3873390	2.9194370	-1.7492550
C	0.8706680	3.6284360	-1.6150990
C	2.1118510	2.8940010	-1.6710580
C	-2.8829390	2.8160290	-1.8364260
C	-1.6818250	3.5398500	-1.9823910
C	-4.1092880	-0.6630440	-1.1163810
C	-4.0770730	0.7431960	-1.1775630
C	-1.7903400	-4.9103330	-2.4810000
C	-2.9854090	-5.5165310	-2.8222410
C	-4.1921920	-4.8072140	-2.6879850
C	-4.1750250	-3.5060480	-2.2209950
C	0.9314790	5.0093260	-1.3075240
C	2.1282850	5.6585920	-1.0654650
C	3.3334740	4.9393850	-1.1034560
C	3.3142260	3.5871240	-1.3906060
S	3.4103770	-3.8585390	-1.4374300
C	2.4164890	-5.2343710	-1.1453920
C	1.0898370	-4.9424860	-1.2577400
C	4.4314640	1.1199340	-2.9451690
C	5.2529560	0.1172210	-3.3657980
S	4.6026460	-1.4447700	-3.0273800
C	-5.3611870	-1.1169910	-0.5860550
C	-6.2404010	-0.1141880	-0.3048810
S	-5.5860600	1.4416370	-0.6575940
S	-4.2695660	3.7573160	-2.3124380
C	-3.2708770	5.1011280	-2.7290390
C	-1.9489460	4.8446560	-2.5175220

H	-0.8667200	-5.4351360	-2.6893480	C	2.8839690	2.8157690	1.8360800
H	-5.0997760	-2.9430260	-2.2204610	C	-3.3128960	3.5890330	1.3897210
H	0.0095600	5.5559950	-1.1708580	C	-3.3316390	4.9412420	1.1022910
H	4.2385650	3.0288840	-1.3239200	C	-2.1261970	5.6600230	1.0643020
H	2.8778520	-6.1780100	-0.8857050	C	-0.9296350	5.0103870	1.3065760
H	0.3182730	-5.6719040	-1.0580700	C	4.1736330	-3.5067490	2.2215780
H	4.6515550	2.1629950	-3.1302930	C	4.1902700	-4.8078950	2.6886410
H	6.2085640	0.1991260	-3.8676530	C	2.9832220	-5.5167890	2.8227310
H	-5.5732760	-2.1552200	-0.3677960	C	1.7884150	-4.9101810	2.4813090
H	-7.2374460	-0.1908540	0.1087200	S	-4.6030060	-1.4420490	3.0280210
H	-3.7250410	6.0005120	-3.1246630	C	-5.2526370	0.1202410	3.3663750
H	-1.1763600	5.5496450	-2.7939910	C	-4.4308520	1.1225760	2.9454200
H	-2.9830250	-6.5214660	-3.2381540	C	-1.0917290	-4.9413000	1.2582140
H	-5.1317650	-5.2593340	-2.9971460	C	-2.4184990	-5.2327300	1.1461050
H	4.2736620	5.4279030	-0.8617290	S	-3.4118540	-3.8565210	1.4381790
H	2.1275500	6.7129380	-0.7992200	C	1.9506910	4.8448420	2.5168390
N	2.0676870	-1.4724970	-1.8967210	C	3.2727080	5.1008660	2.7283600
N	-2.9315510	1.4690530	-1.4927400	S	4.2709210	3.7566270	2.3119910
B	0.8195280	-0.7325530	-1.6986280	S	5.5866880	1.4401920	0.6576310
B	-1.6647540	0.7327240	-1.4981260	C	6.2403980	-0.1159180	0.3050110
C	-0.8655810	0.7968590	1.7341040	C	5.3607600	-1.1183420	0.5862060
C	0.3654900	1.5229330	1.6515700	H	-4.2374140	3.0310920	1.3230030
C	1.7117770	-0.7979840	1.4721910	H	-0.0075120	5.5566990	1.1698440
C	0.4843220	-1.5240400	1.5848090	H	5.0985850	-2.9440600	2.2211580
C	-2.0862990	1.4645090	1.8947440	H	0.8645800	-5.4346580	2.6895290
C	-2.1107930	2.8955590	1.6704840	H	-6.2080990	0.2025770	3.8684360
C	-0.8693410	3.6295350	1.6144440	H	-4.6504950	2.1657430	3.1304670
C	0.3884060	2.9200950	1.7487780	H	-0.3204160	-5.6709370	1.0583790
C	-3.1843930	-0.7434470	2.2960630	H	-2.8802400	-6.1762120	0.8865170
C	-3.2274890	0.6650880	2.3099840	H	1.1783570	5.5501540	2.7931900
C	0.4772650	-2.9205730	1.6962030	H	3.7271870	6.0001370	3.1238790
C	-0.8169750	-3.5740000	1.5889440	H	7.2374100	-0.1930100	-0.1085910
C	-2.0195470	-2.8470070	1.7023810	H	5.5723960	-2.1566640	0.3679520
C	2.9422910	-1.4640800	1.4526650	H	-4.2716250	5.4300380	0.8603390
C	2.9727530	-2.8628190	1.8286510	H	-2.1250710	6.7143120	0.7978280
C	1.7334770	-3.5934850	1.9583010	H	2.9804240	-6.5217110	3.2386740
C	4.0773740	0.7424020	1.1775510	H	5.1296370	-5.2603290	2.9979720
C	4.1090410	-0.6638550	1.1164940	N	-2.0682340	-1.4708960	1.8969670
C	1.6831100	3.5400550	1.9818920	N	2.9321040	1.4687340	1.4925670

B	-0.8198130	-0.7314490	1.6986570	S	5.2338670	-0.9240470	-2.8505060
B	1.6650250	0.7328790	1.4979560	C	-4.0052710	3.1446660	-2.4629580
				C	-5.1886080	2.6452600	-2.9178930
				S	-5.2338670	0.9240470	-2.8505060
				S	-4.9803890	-2.0537860	-2.5794330
120				C	-4.5917410	-3.7307990	-2.5976060
molecule6_S1				C	-3.2970960	-3.9603750	-2.2395970
C	0.5685990	1.4082970	-1.6268640	H	1.8742720	5.1134250	-0.5560150
C	-0.8550130	1.2434570	-1.6468060	H	-3.0132000	4.4888570	-0.5850690
C	-0.5685990	-1.4082970	-1.6268640	H	-1.8742720	-5.1134250	-0.5560150
C	0.8550130	-1.2434570	-1.6468060	H	3.0132000	-4.4888570	-0.5850690
C	1.1464890	2.6827350	-1.5777550	H	5.3460000	4.4495150	-2.8910620
C	0.2926540	3.7918470	-1.1893770	H	2.8637540	4.9507190	-2.2654950
C	-1.1400430	3.6201760	-1.2017500	H	3.7718920	-4.2010130	-2.4887700
C	-1.7028260	2.3533490	-1.6185170	H	6.0422920	-3.1843160	-3.3084140
C	3.3605300	1.6260990	-2.0969970	H	-3.7718920	4.2010130	-2.4887700
C	2.5558210	2.7761350	-1.9146100	H	-6.0422920	3.1843160	-3.3084140
C	1.7028260	-2.3533490	-1.6185170	H	-5.3460000	-4.4495150	-2.8910620
C	3.0785720	-2.1436730	-2.0233840	H	-2.8637540	-4.9507190	-2.2654950
C	3.6162630	-0.8496910	-2.1982960	H	0.4223830	6.9006190	0.2495920
C	-1.1464890	-2.6827350	-1.5777550	H	-2.0561200	6.5841220	0.2553910
C	-0.2926540	-3.7918470	-1.1893770	H	2.0561200	-6.5841220	0.2553910
C	1.1400430	-3.6201760	-1.2017500	H	-0.4223830	-6.9006190	0.2495920
C	-3.3605300	-1.6260990	-2.0969970	N	2.8854450	0.3200050	-1.9818510
C	-2.5558210	-2.7761350	-1.9146100	N	-2.8854450	-0.3200050	-1.9818510
C	-3.0785720	2.1436730	-2.0233840	B	1.4399830	0.1622280	-1.7538990
C	-3.6162630	0.8496910	-2.1982960	B	-1.4399830	-0.1622280	-1.7538990
C	0.8059350	5.0024970	-0.6675340	C	0.4217670	1.4555500	1.7744070
C	-0.0155950	6.0037190	-0.1814260	C	-0.9747180	1.1537190	1.7307460
C	-1.4082140	5.8290970	-0.1815980	C	-0.4217670	-1.4555500	1.7744070
C	-1.9478340	4.6563760	-0.6763040	C	0.9747180	-1.1537190	1.7307460
C	-0.8059350	-5.0024970	-0.6675340	C	0.8757380	2.7597810	2.0050620
C	0.0155950	-6.0037190	-0.1814260	C	-0.0847060	3.7322260	2.4931420
C	1.4082140	-5.8290970	-0.1815980	C	-1.4963210	3.4402170	2.4060810
C	1.9478340	-4.6563760	-0.6763040	C	-1.9302940	2.1638470	1.8745760
S	4.9803890	2.0537860	-2.5794330	C	3.2040840	1.9586480	1.5464210
C	4.5917410	3.7307990	-2.5976060	C	2.2881440	3.0101340	1.7788350
C	3.2970960	3.9603750	-2.2395970	C	1.9302940	-2.1638470	1.8745760
C	4.0052710	-3.1446660	-2.4629580	C	3.2970960	-1.8169890	1.5320040
C	5.1886080	-2.6452600	-2.9178930				

C	3.7080330	-0.4746080	1.3823560
C	-0.8757380	-2.7597810	2.0050620
C	0.0847060	-3.7322260	2.4931420
C	1.4963210	-3.4402170	2.4060810
C	-3.2040840	-1.9586480	1.5464210
C	-2.2881440	-3.0101340	1.7788350
C	-3.2970960	1.8169890	1.5320040
C	-3.7080330	0.4746080	1.3823560
C	0.3077290	4.9037500	3.1873690
C	-0.6118680	5.7893640	3.7194910
C	-1.9860280	5.5141370	3.6168370
C	-2.4069520	4.3530100	2.9951730
C	-0.3077290	-4.9037500	3.1873690
C	0.6118680	-5.7893640	3.7194910
C	1.9860280	-5.5141370	3.6168370
C	2.4069520	-4.3530100	2.9951730
S	4.8090530	2.5650050	1.2438730
C	4.2766360	4.1962430	1.3776290
C	2.9452930	4.2785480	1.6548530
C	4.3646560	-2.7109140	1.1969800
C	5.5262600	-2.0876570	0.8516390
S	5.3803470	-0.3730370	0.9061220
C	-4.3646560	2.7109140	1.1969800
C	-5.5262600	2.0876570	0.8516390
S	-5.3803470	0.3730370	0.9061220
S	-4.8090530	-2.5650050	1.2438730
C	-4.2766360	-4.1962430	1.3776290
C	-2.9452930	-4.2785480	1.6548530
H	1.3586060	5.0778170	3.3781210
H	-3.4595620	4.1014750	3.0267820
H	-1.3586060	-5.0778170	3.3781210
H	3.4595620	-4.1014750	3.0267820
H	4.9826310	5.0011940	1.2201540
H	2.4288960	5.2260140	1.7071200
H	4.2522590	-3.7860050	1.1635020
H	6.4622320	-2.5321360	0.5401850
H	-4.2522590	3.7860050	1.1635020
H	-6.4622320	2.5321360	0.5401850
H	-4.9826310	-5.0011940	1.2201540

H	-2.4288960	-5.2260140	1.7071200
H	-0.2665180	6.6679220	4.2595400
H	-2.7154600	6.1799270	4.0723410
H	2.7154600	-6.1799270	4.0723410
H	0.2665180	-6.6679220	4.2595400
N	2.8466900	0.6127550	1.5246140
N	-2.8466900	-0.6127550	1.5246140
B	1.4132800	0.3064010	1.6090790
B	-1.4132800	-0.3064010	1.6090790

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C	-1.3191860	-0.7571370	-1.6098420
C	-0.1020800	-1.5067550	-1.7009490
C	1.3220000	0.7556620	-1.6091720
C	0.1049430	1.5052640	-1.7011010
C	-2.5614780	-1.3957240	-1.5040320
C	-2.5590210	-2.8144600	-1.1861640
C	-1.3434450	-3.5755560	-1.3589070
C	-0.1272570	-2.9025750	-1.7628840
C	-3.6549260	0.8163130	-1.9455580
C	-3.7437690	-0.5792100	-1.7261390
C	0.1301240	2.9010910	-1.7632300
C	-1.0758550	3.5542040	-2.2409520
C	-2.3017100	2.8647420	-2.3430830
C	2.5642160	1.3943020	-1.5028870
C	2.5615870	2.8131480	-1.1854360
C	1.3460340	3.5742100	-1.3587200
C	3.6579180	-0.8178380	-1.9435390
C	3.7466260	0.5777260	-1.7242580
C	1.0789880	-3.5558060	-2.2398000
C	2.3049050	-2.8663700	-2.3413190
C	-3.6688780	-3.4715240	-0.6038930
C	-3.6411900	-4.8134660	-0.2681860
C	-2.4718720	-5.5609250	-0.4730130
C	-1.3486920	-4.9420250	-0.9899190
C	3.6712620	3.4704100	-0.6030490
C	3.6434770	4.8124360	-0.2677060
C	2.4741910	5.5598100	-0.4730220

C	1.3510790	4.9407430	-0.9898970
S	-5.2280930	1.5253140	-2.1995080
C	-5.9971250	-0.0119520	-2.0935540
C	-5.1058380	-1.0148400	-1.8603170
C	-1.1738700	4.8544630	-2.8369810
C	-2.4049760	5.1413100	-3.3462310
S	-3.5111550	3.8353190	-3.1439460
C	1.1773660	-4.8561430	-2.8356360
C	2.4088080	-5.1431340	-3.3439520
S	3.5148640	-3.8371120	-3.1412110
S	5.2312040	-1.5268150	-2.1968500
C	6.0001560	0.0104690	-2.0906790
C	5.1087510	1.0133540	-1.8578820
H	-4.5395630	-2.8945630	-0.3259840
H	-0.4234720	-5.4993640	-1.0384820
H	4.5419290	2.8935450	-0.3249320
H	0.4258500	5.4980870	-1.0387080
H	-7.0678170	-0.0843710	-2.2340780
H	-5.4147640	-2.0499820	-1.8376220
H	-0.3346600	5.5305970	-2.9362240
H	-2.7323960	6.0432960	-3.8472580
H	0.3382140	-5.5322800	-2.9353140
H	2.7365680	-6.0452200	-3.8445740
H	7.0708840	0.0829430	-2.2309030
H	5.4176520	2.0485110	-1.8353500
H	-4.5075720	-5.2676710	0.2048770
H	-2.4279320	-6.6052740	-0.1740540
H	2.4301420	6.6042060	-0.1742360
H	4.5097310	5.2667720	0.2054850
N	-2.4581500	1.5243130	-1.9870730
N	2.4611680	-1.5258960	-1.9854130
B	-1.2265960	0.7589400	-1.7603990
B	1.2294970	-0.7604650	-1.7595390
C	1.3201490	-0.7539180	1.6091380
C	0.1041870	-1.5052580	1.7013780
C	-1.3229560	0.7552670	1.6081430
C	-0.1070730	1.5066600	1.7008060
C	2.5632730	-1.3907990	1.5030280
C	2.5626020	-2.8098940	1.1866260

C	1.3484650	-3.5728090	1.3617530
C	0.1314270	-2.9009870	1.7651400
C	3.6538150	0.8228620	1.9435420
C	3.7446000	-0.5725240	1.7239950
C	-0.1343800	2.9024320	1.7640940
C	1.0708350	3.5568060	2.2421500
C	2.2978270	2.8690810	2.3428040
C	-2.5659880	1.3920990	1.5009090
C	-2.5651450	2.8110760	1.1839870
C	-1.3511600	3.5741330	1.3596770
C	-3.6568650	-0.8214040	1.9415530
C	-3.7474470	0.5739050	1.7213330
C	-1.0739950	-3.5551840	2.2428920
C	-2.3010210	-2.8674520	2.3426350
C	3.6729140	-3.4658190	0.6039390
C	3.6474230	-4.8084060	0.2707180
C	2.4799490	-5.5578240	0.4788520
C	1.3561060	-4.9401330	0.9957770
C	-3.6751320	3.4666740	0.6002790
C	-3.6495970	4.8092170	0.2668630
C	-2.4823780	5.5588270	0.4756970
C	-1.3586930	4.9413460	0.9932520
S	5.2260830	1.5342770	2.1962680
C	5.9973800	-0.0017920	2.0895550
C	5.1074690	-1.0060450	1.8569860
C	1.1672870	4.8565030	2.8396900
C	2.3984080	5.1448060	3.3481060
S	3.5064450	3.8407680	3.1435750
C	-1.1706940	-4.8546440	2.8409200
C	-2.4020490	-5.1427970	3.3488030
S	-3.5099960	-3.8388310	3.1432610
S	-5.2293500	-1.5325870	2.1936240
C	-6.0004990	0.0034760	2.0856420
C	-5.1103540	1.0075740	1.8532460
H	4.5420700	-2.8875860	0.3238620
H	0.4324820	-5.4998470	1.0476640
H	-4.5440140	2.8882250	0.3197340
H	-0.4352240	5.5012630	1.0456540
H	7.0682970	-0.0725820	2.2291920

H	5.4180620	-2.0406760	1.8340480	C	-3.1809400	4.5235240	1.3892090
H	0.3271300	5.5312150	2.9406160	C	-3.7978520	5.5520560	0.7032970
H	2.7248080	6.0468000	3.8497850	C	-3.7978520	5.5520560	-0.7032970
H	-0.3305350	-5.5292440	2.9425770	C	-3.1809400	4.5235240	-1.3892090
H	-2.7286930	-6.0445960	3.8506730	C	-1.0367430	1.3237560	4.9266600
H	-7.0714890	0.0744450	2.2246300	C	-0.6520120	2.5292730	5.4946070
H	-5.4207960	2.0422550	1.8296670	C	-0.7022840	3.6961860	4.7188960
H	4.5140260	-5.2617990	-0.2027200	C	-1.1548160	3.6452150	3.4097840
H	2.4378580	-6.6030010	0.1825170	C	-2.9400770	-3.7212360	3.3291510
H	-2.4402510	6.6039800	0.1792650	C	-3.4485740	-3.7177370	4.6194930
H	-4.5159450	5.2624540	-0.2071930	C	-3.3624210	-2.5624230	5.4119310
N	2.4560330	1.5291030	1.9859080	C	-2.7910190	-1.4155110	4.8785430
N	-2.4590880	-1.5276460	1.9849520	C	-1.0045770	-4.9128380	-1.3861600
B	1.2254800	0.7620790	1.7595110	C	-0.5617050	-6.0282440	-0.7028090
B	-1.2284000	-0.7606870	1.7590790	C	-0.5617050	-6.0282440	0.7028090
				C	-1.0045770	-4.9128380	1.3861600
				C	-2.7910190	-1.4155110	-4.8785430
				C	-3.3624210	-2.5624230	-5.4119310
				C	-3.4485740	-3.7177370	-4.6194930
144				C	-2.9400770	-3.7212360	-3.3291510
molecule7_UD1				C	-1.1548160	3.6452150	-3.4097840
C	-1.5527840	2.4238260	2.8169010	C	-0.7022840	3.6961860	-4.7188960
C	-1.4717570	1.2352360	3.5877810	C	-0.6520120	2.5292730	-5.4946070
C	-2.2456740	-1.3947860	3.5755810	C	-1.0367430	1.3237560	-4.9266600
C	-2.2959710	-2.5781990	2.7939570	H	-3.2725890	4.4826190	2.4679260
C	-1.8134010	-2.5428610	1.4189300	H	-4.3276530	6.3262630	1.2530640
C	-1.4457150	-3.7456400	0.7123820	H	-4.3276530	6.3262630	-1.2530640
C	-1.4457150	-3.7456400	-0.7123820	H	-3.2725890	4.4826190	-2.4679260
C	-1.8134010	-2.5428610	-1.4189300	H	-0.9594810	0.4163010	5.5119390
C	-2.2959710	-2.5781990	-2.7939570	H	-0.2872650	2.5649660	6.5180170
C	-2.2456740	-1.3947860	-3.5755810	H	-0.3663140	4.6434970	5.1344280
C	-1.4717570	1.2352360	-3.5877810	H	-1.1556770	4.5496150	2.8177150
C	-1.5527840	2.4238260	-2.8169010	H	-3.0848100	-4.5985710	2.7092120
C	-1.9592600	2.3393240	-1.4195960	H	-3.9488900	-4.6055570	5.0002950
C	-2.5052160	3.4732030	-0.7134520	H	-3.7820590	-2.5524290	6.4152470
C	-2.5052160	3.4732030	0.7134520	H	-2.8115940	-0.4991010	5.4586300
C	-1.9592600	2.3393240	1.4195960	H	-0.9631380	-4.9046800	-2.4660200
C	-1.8642800	1.1199830	0.7171620	H	-0.1871180	-6.8877680	-1.2532420
C	-1.7376400	-1.3211660	0.7184130	H	-0.1871180	-6.8877680	1.2532420
C	-1.7376400	-1.3211660	-0.7184130				
C	-1.8642800	1.1199830	-0.7171620				

H	-0.9631380	-4.9046800	2.4660200	C	3.4485740	3.7177370	4.6194930
H	-2.8115940	-0.4991010	-5.4586300	C	2.9400770	3.7212360	3.3291510
H	-3.7820590	-2.5524290	-6.4152470	C	1.1548160	-3.6452150	3.4097840
H	-3.9488900	-4.6055570	-5.0002950	C	0.7022840	-3.6961860	4.7188960
H	-3.0848100	-4.5985710	-2.7092120	C	0.6520120	-2.5292730	5.4946070
H	-1.1556770	4.5496150	-2.8177150	C	1.0367430	-1.3237560	4.9266600
H	-0.3663140	4.6434970	-5.1344280	C	3.1809400	-4.5235240	-1.3892090
H	-0.2872650	2.5649660	-6.5180170	C	3.7978520	-5.5520560	-0.7032970
H	-0.9594810	0.4163010	-5.5119390	C	3.7978520	-5.5520560	0.7032970
N	-1.7640740	-0.0991060	1.4222300	C	3.1809400	-4.5235240	1.3892090
N	-1.7640740	-0.0991060	-1.4222300	C	1.0367430	-1.3237560	-4.9266600
B	-1.7908220	-0.0973140	2.8933030	C	0.6520120	-2.5292730	-5.4946070
B	-1.7908220	-0.0973140	-2.8933030	C	0.7022840	-3.6961860	-4.7188960
C	2.2959710	2.5781990	2.7939570	C	1.1548160	-3.6452150	-3.4097840
C	2.2456740	1.3947860	3.5755810	C	2.9400770	3.7212360	-3.3291510
C	1.4717570	-1.2352360	3.5877810	C	3.4485740	3.7177370	-4.6194930
C	1.5527840	-2.4238260	2.8169010	C	3.3624210	2.5624230	-5.4119310
C	1.9592600	-2.3393240	1.4195960	C	2.7910190	1.4155110	-4.8785430
C	2.5052160	-3.4732030	0.7134520	H	0.9631380	4.9046800	2.4660200
C	2.5052160	-3.4732030	-0.7134520	H	0.1871180	6.8877680	1.2532420
C	1.9592600	-2.3393240	-1.4195960	H	0.1871180	6.8877680	-1.2532420
C	1.5527840	-2.4238260	-2.8169010	H	0.9631380	4.9046800	-2.4660200
C	1.4717570	-1.2352360	-3.5877810	H	2.8115940	0.4991010	5.4586300
C	2.2456740	1.3947860	-3.5755810	H	3.7820590	2.5524290	6.4152470
C	2.2959710	2.5781990	-2.7939570	H	3.9488900	4.6055570	5.0002950
C	1.8134010	2.5428610	-1.4189300	H	3.0848100	4.5985710	2.7092120
C	1.4457150	3.7456400	-0.7123820	H	1.1556770	-4.5496150	2.8177150
C	1.4457150	3.7456400	0.7123820	H	0.3663140	-4.6434970	5.1344280
C	1.8134010	2.5428610	1.4189300	H	0.2872650	-2.5649660	6.5180170
C	1.7376400	1.3211660	0.7184130	H	0.9594810	-0.4163010	5.5119390
C	1.8642800	-1.1199830	0.7171620	H	3.2725890	-4.4826190	-2.4679260
C	1.8642800	-1.1199830	-0.7171620	H	4.3276530	-6.3262630	-1.2530640
C	1.7376400	1.3211660	-0.7184130	H	4.3276530	-6.3262630	1.2530640
C	1.0045770	4.9128380	1.3861600	H	3.2725890	-4.4826190	2.4679260
C	0.5617050	6.0282440	0.7028090	H	0.9594810	-0.4163010	-5.5119390
C	0.5617050	6.0282440	-0.7028090	H	0.2872650	-2.5649660	-6.5180170
C	1.0045770	4.9128380	-1.3861600	H	0.3663140	-4.6434970	-5.1344280
C	2.7910190	1.4155110	4.8785430	H	1.1556770	-4.5496150	-2.8177150
C	3.3624210	2.5624230	5.4119310	H	3.0848100	4.5985710	-2.7092120

H	3.9488900	4.6055570	-5.0002950
H	3.7820590	2.5524290	-6.4152470
H	2.8115940	0.4991010	-5.4586300
N	1.7640740	0.0991060	1.4222300
N	1.7640740	0.0991060	-1.4222300
B	1.7908220	0.0973140	2.8933030
B	1.7908220	0.0973140	-2.8933030

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C	-1.5527840	2.4238260	2.8169010
C	-1.4717570	1.2352360	3.5877810
C	-2.2456740	-1.3947860	3.5755810
C	-2.2959710	-2.5781990	2.7939570
C	-1.8134010	-2.5428610	1.4189300
C	-1.4457150	-3.7456400	0.7123820
C	-1.4457150	-3.7456400	-0.7123820
C	-1.8134010	-2.5428610	-1.4189300
C	-2.2959710	-2.5781990	-2.7939570
C	-2.2456740	-1.3947860	-3.5755810
C	-1.4717570	1.2352360	-3.5877810
C	-1.5527840	2.4238260	-2.8169010
C	-1.9592600	2.3393240	-1.4195960
C	-2.5052160	3.4732030	-0.7134520
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C	-1.9592600	2.3393240	1.4195960
C	-1.8642800	1.1199830	0.7171620
C	-1.7376400	-1.3211660	0.7184130
C	-1.7376400	-1.3211660	-0.7184130
C	-1.8642800	1.1199830	-0.7171620
C	-3.1809400	4.5235240	1.3892090
C	-3.7978520	5.5520560	0.7032970
C	-3.7978520	5.5520560	-0.7032970
C	-3.1809400	4.5235240	-1.3892090
C	-1.0367430	1.3237560	4.9266600
C	-0.6520120	2.5292730	5.4946070
C	-0.7022840	3.6961860	4.7188960
C	-1.1548160	3.6452150	3.4097840

C	-2.9400770	-3.7212360	3.3291510
C	-3.4485740	-3.7177370	4.6194930
C	-3.3624210	-2.5624230	5.4119310
C	-2.7910190	-1.4155110	4.8785430
C	-1.0045770	-4.9128380	-1.3861600
C	-0.5617050	-6.0282440	-0.7028090
C	-0.5617050	-6.0282440	0.7028090
C	-1.0045770	-4.9128380	1.3861600
C	-2.7910190	-1.4155110	-4.8785430
C	-3.3624210	-2.5624230	-5.4119310
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C	-2.9400770	-3.7212360	-3.3291510
C	-1.1548160	3.6452150	-3.4097840
C	-0.7022840	3.6961860	-4.7188960
C	-0.6520120	2.5292730	-5.4946070
C	-1.0367430	1.3237560	-4.9266600
H	-3.2725890	4.4826190	2.4679260
H	-4.3276530	6.3262630	1.2530640
H	-4.3276530	6.3262630	-1.2530640
H	-3.2725890	4.4826190	-2.4679260
H	-0.9594810	0.4163010	5.5119390
H	-0.2872650	2.5649660	6.5180170
H	-0.3663140	4.6434970	5.1344280
H	-1.1556770	4.5496150	2.8177150
H	-3.0848100	-4.5985710	2.7092120
H	-3.9488900	-4.6055570	5.0002950
H	-3.7820590	-2.5524290	6.4152470
H	-2.8115940	-0.4991010	5.4586300
H	-0.9631380	-4.9046800	-2.4660200
H	-0.1871180	-6.8877680	-1.2532420
H	-0.1871180	-6.8877680	1.2532420
H	-0.9631380	-4.9046800	2.4660200
H	-2.8115940	-0.4991010	-5.4586300
H	-3.7820590	-2.5524290	-6.4152470
H	-3.9488900	-4.6055570	-5.0002950
H	-3.0848100	-4.5985710	-2.7092120
H	-1.1556770	4.5496150	-2.8177150
H	-0.3663140	4.6434970	-5.1344280
H	-0.2872650	2.5649660	-6.5180170

H	-0.9594810	0.4163010	-5.5119390	C	3.7978520	-5.5520560	0.7032970
N	-1.7640740	-0.0991060	1.4222300	C	3.1809400	-4.5235240	1.3892090
N	-1.7640740	-0.0991060	-1.4222300	C	1.0367430	-1.3237560	-4.9266600
B	-1.7908220	-0.0973140	2.8933030	C	0.6520120	-2.5292730	-5.4946070
B	-1.7908220	-0.0973140	-2.8933030	C	0.7022840	-3.6961860	-4.7188960
C	2.2959710	2.5781990	2.7939570	C	1.1548160	-3.6452150	-3.4097840
C	2.2456740	1.3947860	3.5755810	C	2.9400770	3.7212360	-3.3291510
C	1.4717570	-1.2352360	3.5877810	C	3.4485740	3.7177370	-4.6194930
C	1.5527840	-2.4238260	2.8169010	C	3.3624210	2.5624230	-5.4119310
C	1.9592600	-2.3393240	1.4195960	C	2.7910190	1.4155110	-4.8785430
C	2.5052160	-3.4732030	0.7134520	H	0.9631380	4.9046800	2.4660200
C	2.5052160	-3.4732030	-0.7134520	H	0.1871180	6.8877680	1.2532420
C	1.9592600	-2.3393240	-1.4195960	H	0.1871180	6.8877680	-1.2532420
C	1.5527840	-2.4238260	-2.8169010	H	0.9631380	4.9046800	-2.4660200
C	1.4717570	-1.2352360	-3.5877810	H	2.8115940	0.4991010	5.4586300
C	2.2456740	1.3947860	-3.5755810	H	3.7820590	2.5524290	6.4152470
C	2.2959710	2.5781990	-2.7939570	H	3.9488900	4.6055570	5.0002950
C	1.8134010	2.5428610	-1.4189300	H	3.0848100	4.5985710	2.7092120
C	1.4457150	3.7456400	-0.7123820	H	1.1556770	-4.5496150	2.8177150
C	1.4457150	3.7456400	0.7123820	H	0.3663140	-4.6434970	5.1344280
C	1.8134010	2.5428610	1.4189300	H	0.2872650	-2.5649660	6.5180170
C	1.7376400	1.3211660	0.7184130	H	0.9594810	-0.4163010	5.5119390
C	1.8642800	-1.1199830	0.7171620	H	3.2725890	-4.4826190	-2.4679260
C	1.8642800	-1.1199830	-0.7171620	H	4.3276530	-6.3262630	-1.2530640
C	1.7376400	1.3211660	-0.7184130	H	4.3276530	-6.3262630	1.2530640
C	1.0045770	4.9128380	1.3861600	H	3.2725890	-4.4826190	2.4679260
C	0.5617050	6.0282440	0.7028090	H	0.9594810	-0.4163010	-5.5119390
C	0.5617050	6.0282440	-0.7028090	H	0.2872650	-2.5649660	-6.5180170
C	1.0045770	4.9128380	-1.3861600	H	0.3663140	-4.6434970	-5.1344280
C	2.7910190	1.4155110	4.8785430	H	1.1556770	-4.5496150	-2.8177150
C	3.3624210	2.5624230	5.4119310	H	3.0848100	4.5985710	-2.7092120
C	3.4485740	3.7177370	4.6194930	H	3.9488900	4.6055570	-5.0002950
C	2.9400770	3.7212360	3.3291510	H	3.7820590	2.5524290	-6.4152470
C	1.1548160	-3.6452150	3.4097840	H	2.8115940	0.4991010	-5.4586300
C	0.7022840	-3.6961860	4.7188960	N	1.7640740	0.0991060	1.4222300
C	0.6520120	-2.5292730	5.4946070	N	1.7640740	0.0991060	-1.4222300
C	1.0367430	-1.3237560	4.9266600	B	1.7908220	0.0973140	2.8933030
C	3.1809400	-4.5235240	-1.3892090	B	1.7908220	0.0973140	-2.8933030
C	3.7978520	-5.5520560	-0.7032970				

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C	-1.8070960	0.8052430	0.7179920
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C	-1.5265350	0.9050030	3.6008570
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C	-1.9339960	-2.8989920	2.8081430
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C	-1.1551540	-4.0647590	0.7113480
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C	-1.2045390	1.1670920	4.9651940
C	-1.0375140	2.4969480	5.2282640
S	-1.3109940	3.4675080	3.8329470
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C	-2.4646410	-1.9905400	4.9066070
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C	-1.2045390	1.1670920	-4.9651940
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H	-3.1039300	4.2721190	2.4594620
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H	-0.5811850	-5.1989440	-2.4633200
H	0.1899420	-7.1676280	-1.2537670
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H	-1.0631980	0.3905990	5.7063440
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H	-1.0631980	0.3905990	-5.7063440
H	-2.5937270	-1.2167240	-5.6550270
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B	-1.6963900	-0.4249580	2.8947910
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N	-1.6728300	-0.4173700	-1.4178350
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C	1.5610130	2.8742540	1.4192990
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C	1.5610130	2.8742540	-1.4192990
C	1.9851380	1.7444410	3.5836180
C	1.9339960	2.8989920	2.8081430
C	1.9325200	-2.0319900	1.4265670
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C	2.4150900	-3.1920020	0.7121240	H	1.0631980	-0.3905990	-5.7063440
C	1.5265350	-0.9050030	-3.6008570	H	0.7554470	-2.9707210	-6.1604510
C	1.6423070	-2.0651710	-2.8380940	B	1.6963900	0.4249580	2.8947910
C	1.9339960	2.8989920	-2.8081430	B	1.6963900	0.4249580	-2.8947910
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C	0.2105400	6.3215100	-0.7014480				
C	0.6675960	5.2113670	-1.3855190				
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C	3.5423380	-5.3686300	-0.7015550	molecule8_UD2			
C	3.5423380	-5.3686300	0.7015550	C	-0.7144850	1.2495860	1.7524970
C	3.0058740	-4.2933330	1.3824000	C	-1.4188060	-0.0010730	1.7533200
C	2.4646410	1.9905400	4.9066070	C	0.7227890	-1.2034110	1.7149580
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S	2.5146100	4.2758060	3.7224540	C	-1.4403330	2.4727530	1.7813980
S	1.3109940	-3.4675080	3.8329470	C	-2.8287810	2.4347610	2.1777810
C	1.0375140	-2.4969480	5.2282640	C	-3.5284830	1.1938030	2.1756330
C	1.2045390	-1.1670920	4.9651940	C	-2.8409860	-0.0146690	1.7817210
S	2.5146100	4.2758060	-3.7224540	C	0.6276630	3.7913370	1.3960710
C	2.7973420	3.2994500	-5.1187860	C	-0.7610930	3.7035250	1.4633940
C	2.4646410	1.9905400	-4.9066070	C	2.8451390	0.0564780	1.8079410
C	1.2045390	-1.1670920	-4.9651940	C	3.5191140	1.2783960	2.1614090
C	1.0375140	-2.4969480	-5.2282640	C	2.8924400	2.5177620	2.0831740
S	1.3109940	-3.4675080	-3.8329470	C	1.4501540	-2.4207350	1.7808930
H	0.5811850	5.1989440	2.4633200	C	2.8610490	-2.3974350	1.4852970
H	-0.1899420	7.1676280	1.2537670	C	3.5629320	-1.1607500	1.5164590
H	-0.1899420	7.1676280	-1.2537670	C	-0.6197940	-3.7419250	2.0999910
H	0.5811850	5.1989440	-2.4633200	C	0.7664710	-3.6341560	2.1385140
H	3.1039300	-4.2721190	-2.4594620	C	-3.5412310	-1.2379090	1.4774100
H	4.0019880	-6.1830910	-1.2559140	C	-2.8965800	-2.4733580	1.4403870
H	4.0019880	-6.1830910	1.2559140	C	-3.4968290	3.5814650	2.6776140
H	3.1039300	-4.2721190	2.4594620	C	-4.8049830	3.5369900	3.1195220
H	2.5937270	1.2167240	5.6550270	C	-5.4963130	2.3151980	3.1134310
H	3.2024790	3.7534030	6.0154870	C	-4.8581630	1.1734130	2.6690270
H	0.7554470	-2.9707210	6.1604510	C	3.5576280	-3.5602930	1.0762270
H	1.0631980	-0.3905990	5.7063440	C	4.8976990	-3.5304380	0.7436600
H	3.2024790	3.7534030	-6.0154870	C	5.5968600	-2.3149510	0.7944990
H	2.5937270	1.2167240	-5.6550270	C	4.9351950	-1.1599120	1.1656070
				C	1.0867440	5.0849500	1.0084460

C	0.0679010	5.9604510	0.7596110	C	2.8928040	-2.5179420	-2.0829560
S	-1.4746520	5.2437080	1.0289870	C	3.5195820	-1.2786140	-2.1610190
S	5.1122480	1.4471360	2.8712340	C	-1.4400120	-2.4726600	-1.7816550
C	4.9214590	3.1549530	3.0353810	C	-0.7608850	-3.7034800	-1.4636200
C	3.7100650	3.5830890	2.5695240	C	0.6278520	-3.7913690	-1.3962160
S	-5.2227020	-1.4317250	1.0269670	C	-2.8405290	0.0148250	-1.7819220
C	-5.0384070	-3.1285800	0.8063620	C	-3.5281160	-1.1936150	-2.1757790
C	-3.7651740	-3.5441370	1.0758470	C	-2.8284480	-2.4345890	-2.1780470
C	-1.0887840	-4.9990060	2.5906610	C	-2.8959890	2.4735520	-1.4408790
C	-0.0785710	-5.8138920	3.0201900	C	-3.5406990	1.2381260	-1.4776750
S	1.4740600	-5.0855230	2.8182110	C	0.7672170	3.6340960	-2.1386690
H	-2.9546800	4.5120380	2.7816090	C	-0.6190530	3.7419390	-2.1003900
H	-5.2724400	4.4361850	3.5133340	C	4.9356150	1.1596110	-1.1648920
H	-6.5100720	2.2502090	3.5008770	C	5.5972920	2.3146220	-0.7937200
H	-5.3777560	0.2291900	2.7619700	C	4.8982140	3.5301660	-0.7431370
H	3.0120690	-4.4858040	0.9542890	C	3.5582120	3.5600930	-1.0759730
H	5.3902090	-4.4357550	0.3992960	C	-4.8578570	-1.1732060	-2.6690090
H	6.6416560	-2.2669980	0.4987260	C	-5.4960250	-2.3149630	-3.1134670
H	5.4681170	-0.2210230	1.1148660	C	-4.8046810	-3.5367460	-3.1197710
H	2.1330090	5.3404010	0.8912200	C	-3.4965000	-3.5812580	-2.6779510
H	0.1292040	6.9875240	0.4215110	C	3.7104650	-3.5833220	-2.5691220
H	5.7209250	3.7427150	3.4707410	C	4.9219720	-3.1552560	-3.0347530
H	3.3913360	4.6190080	2.6045930	S	5.1128690	-1.4474610	-2.8704780
H	-5.8824170	-3.7183420	0.4702310	S	-1.4745610	-5.2435800	-1.0291100
H	-3.4413980	-4.5722550	0.9747590	C	0.0679480	-5.9604270	-0.7597110
H	-2.1375420	-5.2674980	2.6533070	C	1.0868480	-5.0849800	-1.0085220
H	-0.1523770	-6.8044250	3.4534150	S	1.4750030	5.0854430	-2.8182090
B	1.4273750	2.5403450	1.6914900	C	-0.0775450	5.8139140	-3.0204130
B	-1.4089310	-2.5028000	1.7212240	C	-1.0878830	4.9990420	-2.5911510
N	-0.6895800	-1.2128860	1.7110910	C	-3.7645110	3.5443980	-1.0763510
N	0.6992140	1.2564130	1.7059660	C	-5.0377460	3.1289220	-0.8067410
C	1.4272350	-0.0457980	-1.7208120	S	-5.2221190	1.4320500	-1.0271290
C	0.7233230	1.2033690	-1.7150490	H	5.4684430	0.2206780	-1.1139680
C	-1.4183480	0.0011540	-1.7535520	H	6.6420130	2.2666090	-0.4976950
C	-0.7140910	-1.2495400	-1.7527030	H	5.3907150	4.4354840	-0.3987640
C	2.8456170	-0.0566580	-1.8076630	H	3.0127320	4.4856750	-0.9542530
C	3.5634290	1.1605360	-1.5160560	H	-5.3775060	-0.2289970	-2.7617790
C	2.8616200	2.3972660	-1.4850930	H	-6.5098310	-2.2499480	-3.5007840
C	1.4507710	2.4206480	-1.7809140	H	-5.2721630	-4.4358960	-3.5136590

H	-2.9543240	-4.5118060	-2.7820510
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H	5.7214790	-3.7430610	-3.4699780
H	0.1291710	-6.9874920	-0.4215700
H	2.1330960	-5.3404660	-0.8912600
H	-0.1512180	6.8044690	-3.4536090
H	-2.1366110	5.2675870	-2.6540300
H	-3.4407040	4.5725150	-0.9753660
H	-5.8817040	3.7187490	-0.4705980
B	1.4276780	-2.5404230	-1.6915160
B	-1.4083240	2.5028850	-1.7216710
N	-0.6890460	1.2129300	-1.7113530
N	0.6996030	-1.2564490	-1.7060480

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C	0.5967220	1.2794000	-1.6310790
C	-0.8288380	1.1340680	-1.6860660
C	-0.5967220	-1.2794000	-1.6310790
C	0.8288380	-1.1340680	-1.6860660
C	1.1757090	2.5652100	-1.4994610
C	0.3204360	3.6425590	-1.0474480
C	-1.0928930	3.5082640	-1.1653650
C	-1.6450880	2.2878360	-1.7008590
C	3.3891400	1.6949020	-2.2408740
C	2.5569470	2.7521310	-1.8543070
C	1.6450880	-2.2878360	-1.7008590
C	2.9482870	-2.2066270	-2.2955080
C	3.5476420	-0.9924280	-2.6380550
C	-1.1757090	-2.5652100	-1.4994610
C	-0.3204360	-3.6425590	-1.0474480
C	1.0928930	-3.5082640	-1.1653650
C	-3.3891400	-1.6949020	-2.2408740
C	-2.5569470	-2.7521310	-1.8543070
C	-2.9482870	2.2066270	-2.2955080
C	-3.5476420	0.9924280	-2.6380550
C	0.8288380	4.8108610	-0.4381890
C	0.0004050	5.8167320	0.0256570

C	-1.3898900	5.6850170	-0.0949960
C	-1.9189780	4.5461920	-0.6738230
C	-0.8288380	-4.8108610	-0.4381890
C	-0.0004050	-5.8167320	0.0256570
C	1.3898900	-5.6850170	-0.0949960
C	1.9189780	-4.5461920	-0.6738230
C	4.6980820	2.1397050	-2.6017150
C	4.8450170	3.4973050	-2.5384850
S	3.4018890	4.2786650	-2.0155730
S	3.8954760	-3.5563000	-2.8866950
C	5.0677990	-2.4977720	-3.5773350
C	4.7634010	-1.1811460	-3.3639390
S	-3.8954760	3.5563000	-2.8866950
C	-5.0677990	2.4977720	-3.5773350
C	-4.7634010	1.1811460	-3.3639390
C	-4.6980820	-2.1397050	-2.6017150
C	-4.8450170	-3.4973050	-2.5384850
S	-3.4018890	-4.2786650	-2.0155730
H	1.8892910	4.8947330	-0.2476590
H	0.4322010	6.6769550	0.5295420
H	-2.0540440	6.4417400	0.3129610
H	-2.9931530	4.4154260	-0.6767740
H	-1.8892910	-4.8947330	-0.2476590
H	-0.4322010	-6.6769550	0.5295420
H	2.0540440	-6.4417400	0.3129610
H	2.9931530	-4.4154260	-0.6767740
H	5.5053090	1.4795890	-2.8937340
H	5.7237990	4.0891620	-2.7655580
H	5.9156480	-2.9106340	-4.1110980
H	5.3749310	-0.3765610	-3.7538110
H	-5.9156480	2.9106340	-4.1110980
H	-5.3749310	0.3765610	-3.7538110
H	-5.5053090	-1.4795890	-2.8937340
H	-5.7237990	-4.0891620	-2.7655580
B	2.8177570	0.2855960	-2.2381310
B	-2.8177570	-0.2855960	-2.2381310
N	-1.3981240	-0.1424570	-1.8589920
N	1.3981240	0.1424570	-1.8589920
C	0.3207710	1.3641550	1.9135980

C	-1.0403800	0.9473810	1.7893450	H	0.7901780	4.9860120	3.7619780
C	-0.3207710	-1.3641550	1.9135980	H	-1.0189010	6.4590640	4.4218610
C	1.0403800	-0.9473810	1.7893450	H	-3.3922790	5.8360530	3.8871730
C	0.6475240	2.6987070	2.2538980	H	-3.8570990	3.7424540	2.7419460
C	-0.4358470	3.5517550	2.6982080	H	-0.7901780	-4.9860120	3.7619780
C	-1.7898800	3.1824120	2.4201530	H	1.0189010	-6.4590640	4.4218610
C	-2.0803690	1.9061460	1.8068270	H	3.3922790	-5.8360530	3.8871730
C	2.9960670	2.3333220	1.5091500	H	3.8570990	-3.7424540	2.7419460
C	2.0146190	3.1389270	2.1034390	H	5.1317240	2.5503770	0.9363490
C	2.0803690	-1.9061460	1.8068270	H	5.0388970	5.0071390	1.8545390
C	3.3546410	-1.5394000	1.2420580	H	6.5328790	-1.5319950	-0.3536600
C	3.6704480	-0.2233810	0.8811530	H	5.3457700	0.7994750	-0.1563650
C	-0.6475240	-2.6987070	2.2538980	H	-6.5328790	1.5319950	-0.3536600
C	0.4358470	-3.5517550	2.6982080	H	-5.3457700	-0.7994750	-0.1563650
C	1.7898800	-3.1824120	2.4201530	H	-5.1317240	-2.5503770	0.9363490
C	-2.9960670	-2.3333220	1.5091500	H	-5.0388970	-5.0071390	1.8545390
C	-2.0146190	-3.1389270	2.1034390	B	2.6777230	0.8658280	1.2659130
C	-3.3546410	1.5394000	1.2420580	B	-2.6777230	-0.8658280	1.2659130
C	-3.6704480	0.2233810	0.8811530	N	-1.3256520	-0.4196430	1.6138900
C	-0.2110200	4.7365770	3.4379800	N	1.3256520	0.4196430	1.6138900
C	-1.2408650	5.5661890	3.8428480				
C	-2.5661960	5.2172780	3.5455800				
C	-2.8243390	4.0403300	2.8679540	120			
C	0.2110200	-4.7365770	3.4379800	molecule8_S2			
C	1.2408650	-5.5661890	3.8428480	C	1.3985160	-0.1478730	1.6716560
C	2.5661960	-5.2172780	3.5455800	C	0.5446730	-1.2954530	1.5949460
C	2.8243390	-4.0403300	2.8679540	C	-1.3968130	0.1520420	1.6715420
C	4.2479630	3.0036570	1.3661800	C	-0.5430180	1.2996030	1.5939410
C	4.2320250	4.2843270	1.8384840	C	2.8015610	-0.3231410	1.6964180
S	2.6920860	4.7124670	2.4807550	C	3.3327890	-1.5488710	1.1489570
S	4.6621690	-2.6125130	0.7903610	C	2.4699670	-2.6697650	0.9691740
C	5.5827410	-1.3216370	0.1211950	C	1.0968590	-2.5852450	1.4175980
C	4.9450100	-0.1209040	0.2483830	C	3.1087270	1.9566090	2.6432670
S	-4.6621690	2.6125130	0.7903610	C	3.6116920	0.6996360	2.2958870
C	-5.5827410	1.3216370	0.1211950	C	-1.0952070	2.5893090	1.4155380
C	-4.9450100	0.1209040	0.2483830	C	-0.3052160	3.7430860	1.7562210
C	-4.2479630	-3.0036570	1.3661800	C	1.0089860	3.6453040	2.2296440
C	-4.2320250	-4.2843270	1.8384840	C	-2.7998590	0.3272420	1.6959460
S	-2.6920860	-4.7124670	2.4807550	C	-3.3310900	1.5525270	1.1475250

C	-2.4684090	2.6735050	0.9673210	H	-3.8765480	-3.7270620	3.7474080
C	-3.1070850	-1.9518200	2.6444800	H	-6.1290380	-2.4429870	4.0886610
C	-3.6100340	-0.6951320	2.2960930	B	1.6709930	2.2750220	2.2462320
C	0.3073410	-3.7387430	1.7600340	B	-1.6691910	-2.2705210	2.2482080
C	-1.0067590	-3.6406730	2.2336740	N	-0.8321160	-1.1249820	1.8467840
C	4.6711840	-1.6505170	0.6998220	N	0.8338060	1.1292670	1.8458400
C	5.1585100	-2.8003070	0.1068180	C	-1.3981020	-0.1546280	-1.6712120
C	4.3038430	-3.8941130	-0.0881700	C	-0.5421940	-1.3006490	-1.5940430
C	2.9866950	-3.8173390	0.3248930	C	1.3966070	0.1503600	-1.6723640
C	-4.6693910	1.6533860	0.6979000	C	0.5407360	1.2964780	-1.5956060
C	-5.1570090	2.8026980	0.1042620	C	-2.8008630	-0.3323960	-1.6949550
C	-4.3026570	3.8967540	-0.0907550	C	-3.3295210	-1.5585770	-1.1460740
C	-2.9855530	3.8206520	0.3226190	C	-2.4647560	-2.6780210	-0.9664350
C	4.0662120	2.7385430	3.3589250	C	-1.0920040	-2.5913200	-1.4155920
C	5.2525220	2.0902750	3.5634480	C	-3.1127460	1.9458870	-2.6437460
S	5.2538220	0.5102470	2.8750470	C	-3.6132370	0.6883430	-2.2947960
S	-0.8517800	5.4073810	1.8229660	C	1.0905590	2.5873410	-1.4185230
C	0.6628550	5.9454920	2.4428480	C	0.2983370	3.7393130	-1.7601600
C	1.5470940	4.9157070	2.5994800	C	-1.0157420	3.6386440	-2.2332680
S	0.8546660	-5.4026690	1.8292450	C	2.7993030	0.3282140	-1.6974270
C	-0.6595690	-5.9403720	2.4505790	C	3.3283660	1.5549780	-1.1501480
C	-1.5441860	-4.9106950	2.6058020	C	2.4636690	2.6745090	-0.9706490
C	-4.0645460	-2.7331630	3.3608180	C	3.1106750	-1.9511850	-2.6438220
C	-5.2508020	-2.0846450	3.5649430	C	3.6112680	-0.6931480	-2.2968210
S	-5.2521350	-0.5052360	2.8752070	C	-0.3003420	-3.7435900	-1.7573240
H	5.3169310	-0.7846670	0.7573340	C	1.0135210	-3.6434810	-2.2312460
H	6.1819150	-2.8278000	-0.2567700	C	-4.6672720	-1.6618710	-0.6954250
H	4.6540150	-4.7813390	-0.6087630	C	-5.1523630	-2.8120910	-0.1014590
H	2.3210440	-4.6294710	0.0677650	C	-4.2959670	-3.9046410	0.0929950
H	-5.3146380	0.7871700	0.7555380	C	-2.9793000	-3.8260900	-0.3212530
H	-6.1802700	2.8296800	-0.2597480	C	4.6665590	1.6587700	-0.7008980
H	-4.6529690	4.7837570	-0.6116550	C	5.1521720	2.8095480	-0.1084350
H	-2.3205870	4.6333160	0.0653640	C	4.2958590	3.9021850	0.0859040
H	3.8780590	3.7326380	3.7449510	C	2.9787720	3.8231520	-0.3269320
H	6.1307500	2.4489790	4.0869270	C	-4.0721540	2.7255110	-3.3593490
H	0.8155070	6.9986150	2.6469550	C	-5.2574870	2.0749730	-3.5623130
H	2.5584920	5.0674400	2.9539570	S	-5.2554940	0.4955750	-2.8724820
H	-0.8117030	-6.9932160	2.6564950	S	0.8416620	5.4046130	-1.8280550
H	-2.5554150	-5.0623150	2.9608260	C	-0.6742690	5.9394240	-2.4477220

C	-1.5563990	4.9077890	-2.6038070
S	-0.8446330	-5.4085580	-1.8251520
C	0.6704600	-5.9440110	-2.4462730
C	1.5531970	-4.9128700	-2.6024200
C	4.0696540	-2.7315140	-3.3592460
C	5.2546140	-2.0809350	-3.5642200
S	5.2529140	-0.5006850	-2.8763940
H	-5.3141390	-0.7968150	-0.7522740
H	-6.1753100	-2.8408260	0.2633230
H	-4.6443210	-4.7921900	0.6142670
H	-2.3122100	-4.6370800	-0.0642690
H	5.3133750	0.7936780	-0.7575800
H	6.1754760	2.8386870	0.2553120
H	4.6446640	4.7902690	0.6059580
H	2.3119800	4.6343970	-0.0698770
H	-3.8859790	3.7196150	-3.7463240
H	-6.1367780	2.4315820	-4.0854430
H	-0.8288910	6.9921450	-2.6524300
H	-2.5684740	5.0572650	-2.9573370
H	0.8244680	-6.9967580	-2.6512930
H	2.5644840	-5.0630050	-2.9579350
H	3.8835430	-3.7262620	-3.7445750
H	6.1335190	-2.4381200	-4.0876060
B	-1.6753540	2.2672550	-2.2480220
B	1.6734640	-2.2721640	-2.2469710
N	0.8342400	-1.1278370	-1.8464230
N	-0.8358560	1.1233520	-1.8468690

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C	0.8385080	1.7899200	0.9642250
C	0.8504500	1.7435250	-0.4721460
C	-1.5936220	1.5790720	-0.4783330
C	-1.6063360	1.6757820	0.9559620
C	2.0625340	1.8560820	1.6715480
C	3.2424070	2.2930370	0.9663950
C	3.2510430	2.2747230	-0.4576990
C	2.0845990	1.8009960	-1.1661610

C	0.9280850	1.7011610	3.8388460
C	2.1039010	1.6083130	3.0964630
C	-2.8450350	1.7645220	1.6383990
C	-2.8939510	2.2416370	3.0022850
C	-1.7300640	2.2341800	3.7698690
C	-2.8195280	1.5203870	-1.1795360
C	-4.0128370	1.1689200	-0.4537630
C	-4.0401690	1.3285830	0.9588970
C	-1.7034960	1.8481220	-3.3373240
C	-2.8794390	1.8320340	-2.5889580
C	2.1527070	1.4857440	-2.5774910
C	0.9789500	1.4681720	-3.3328770
C	4.3382370	2.8908910	1.6430010
C	5.4178230	3.4159020	0.9603620
C	5.4254180	3.4018010	-0.4445050
C	4.3544040	2.8624900	-1.1302260
C	-5.1294190	0.5783340	-1.0955690
C	-6.2536210	0.1942500	-0.3921860
C	-6.2994600	0.3861020	0.9993060
C	-5.2127770	0.9334910	1.6541340
S	1.2311470	1.4386570	5.5185030
C	2.9020760	1.1360200	5.2338890
C	3.2286720	1.2508900	3.9113080
C	-4.0048620	2.8107140	3.7124090
C	-3.6777950	3.1750780	4.9906530
S	-2.0245630	2.8546870	5.3562450
C	3.3026880	1.1619890	-3.3708120
C	2.9943880	0.9589790	-4.6869040
S	1.3126150	1.1410650	-4.9949950
S	-2.0123040	2.3292270	-4.9677650
C	-3.6913130	2.5461350	-4.6532570
C	-4.0172960	2.2510190	-3.3574020
H	4.2986250	3.0085630	2.7179460
H	4.3286790	2.9636930	-2.2068700
H	-5.0726590	0.3658090	-2.1546910
H	-5.2315480	0.9845430	2.7341430
H	3.5553350	0.8553250	6.0505940
H	4.2223620	1.0529640	3.5341970
H	-4.9830660	2.9903620	3.2842170

H	-4.3212850	3.6430640	5.7261460	C	-5.4254180	-3.4018010	0.4445050
H	4.3003560	1.0357200	-2.9780470	C	-4.3544040	-2.8624900	1.1302260
H	3.6693750	0.6731700	-5.4842460	S	2.0123040	-2.3292270	4.9677650
H	-4.3533370	2.9026250	-5.4334210	C	3.6913130	-2.5461350	4.6532570
H	-5.0172680	2.3720340	-2.9601260	C	4.0172960	-2.2510190	3.3574020
H	6.2281060	3.8874580	1.5113180	C	-3.3026880	-1.1619890	3.3708120
H	6.2414560	3.8626510	-0.9958560	C	-2.9943880	-0.9589790	4.6869040
H	-7.1643450	0.0576790	1.5704640	S	-1.3126150	-1.1410650	4.9949950
H	-7.0748800	-0.2957800	-0.9080120	C	4.0048620	-2.8107140	-3.7124090
N	-0.3897040	1.7642810	1.6642680	C	3.6777950	-3.1750780	-4.9906530
N	-0.3689580	1.6293680	-1.1817980	S	2.0245630	-2.8546870	-5.3562450
B	-0.4011550	1.8827730	3.1420500	S	-1.2311470	-1.4386570	-5.5185030
B	-0.3667090	1.6312520	-2.6649650	C	-2.9020760	-1.1360200	-5.2338890
C	1.5936220	-1.5790720	0.4783330	C	-3.2286720	-1.2508900	-3.9113080
C	1.6063360	-1.6757820	-0.9559620	H	5.0726590	-0.3658090	2.1546910
C	-0.8385080	-1.7899200	-0.9642250	H	5.2315480	-0.9845430	-2.7341430
C	-0.8504500	-1.7435250	0.4721460	H	-4.2986250	-3.0085630	-2.7179460
C	2.8195280	-1.5203870	1.1795360	H	-4.3286790	-2.9636930	2.2068700
C	4.0128370	-1.1689200	0.4537630	H	4.3533370	-2.9026250	5.4334210
C	4.0401690	-1.3285830	-0.9588970	H	5.0172680	-2.3720340	2.9601260
C	2.8450350	-1.7645220	-1.6383990	H	-4.3003560	-1.0357200	2.9780470
C	1.7034960	-1.8481220	3.3373240	H	-3.6693750	-0.6731700	5.4842460
C	2.8794390	-1.8320340	2.5889580	H	4.9830660	-2.9903620	-3.2842170
C	-2.0845990	-1.8009960	1.1661610	H	4.3212850	-3.6430640	-5.7261460
C	-2.1527070	-1.4857440	2.5774910	H	-3.5553350	-0.8553250	-6.0505940
C	-0.9789500	-1.4681720	3.3328770	H	-4.2223620	-1.0529640	-3.5341970
C	-2.0625340	-1.8560820	-1.6715480	H	7.0748800	0.2957800	0.9080120
C	-3.2424070	-2.2930370	-0.9663950	H	7.1643450	-0.0576790	-1.5704640
C	-3.2510430	-2.2747230	0.4576990	H	-6.2414560	-3.8626510	0.9958560
C	-0.9280850	-1.7011610	-3.8388460	H	-6.2281060	-3.8874580	-1.5113180
C	-2.1039010	-1.6083130	-3.0964630	N	0.3689580	-1.6293680	1.1817980
C	2.8939510	-2.2416370	-3.0022850	N	0.3897040	-1.7642810	-1.6642680
C	1.7300640	-2.2341800	-3.7698690	B	0.3667090	-1.6312520	2.6649650
C	5.1294190	-0.5783340	1.0955690	B	0.4011550	-1.8827730	-3.1420500
C	6.2536210	-0.1942500	0.3921860				
C	6.2994600	-0.3861020	-0.9993060				
C	5.2127770	-0.9334910	-1.6541340				
C	-4.3382370	-2.8908910	-1.6430010				
C	-5.4178230	-3.4159020	-0.9603620				
				120			
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				C	-0.0281680	1.4181480	-1.7531120

C	1.2230220	0.7111390	-1.7448370	H	0.1953270	5.3361430	-2.8140160
C	0.0167640	-1.4213980	-1.7533510	H	4.4981280	2.9371840	-2.7088800
C	-1.2346610	-0.7145410	-1.7421530	H	-0.2292230	-5.4339640	-1.0973800
C	-0.0319340	2.8339590	-1.7570110	H	-4.5142590	-2.9972130	-0.9631570
C	1.1743930	3.5241860	-2.1418410	H	-3.0708320	6.2500760	-0.5173750
C	2.4161290	2.8263600	-2.1171400	H	-0.5664420	5.6144570	-0.8799070
C	2.4392270	1.4377590	-1.7253340	H	-4.9894680	-2.4271270	-2.9674240
C	-2.4727600	2.9117960	-1.5267910	H	-6.7655930	-0.6052090	-3.5615420
C	-1.2434350	3.5668740	-1.4572670	H	5.0829000	2.3969320	-0.7702810
C	-2.4469330	-1.4414410	-1.8173110	H	6.9108860	0.5731220	-0.4234990
C	-3.6737600	-0.7842550	-2.2104640	H	2.9803140	-6.0594370	-3.6549350
C	-3.7518700	0.6065670	-2.1559250	H	0.4937230	-5.4819260	-3.0938580
C	0.0195000	-2.8329770	-1.8572420	H	2.2293900	6.4627710	-3.5580690
C	-1.1894490	-3.5502190	-1.5417420	H	4.4190950	5.2433860	-3.4954970
C	-2.4274020	-2.8493650	-1.5101710	H	-4.4469350	-5.3662610	-0.3663220
C	2.4501260	-2.8927070	-2.1677550	H	-2.2737480	-6.6073050	-0.4404780
C	1.2175760	-3.5359070	-2.2620180	N	-1.2456010	0.6981160	-1.7426570
C	3.6860960	0.7732080	-1.4076520	N	1.2325130	-0.7026220	-1.7414730
C	3.7560390	-0.6177450	-1.4868580	B	-2.5354350	1.4255310	-1.7909390
C	1.1465620	4.8377510	-2.6799420	B	2.5203600	-1.4340920	-1.7775710
C	2.2923170	5.4657000	-3.1286000	C	1.2346930	-0.7143180	1.7420740
C	3.5197840	4.7809800	-3.0957230	C	-0.0167040	-1.4212270	1.7533190
C	3.5689800	3.4844660	-2.6209290	C	-1.2230430	0.7112630	1.7447160
C	-1.1751890	-4.9148280	-1.1581860	C	0.0281180	1.4183230	1.7529870
C	-2.3259310	-5.5709090	-0.7650170	C	2.4469940	-1.4411660	1.8172550
C	-3.5464880	-4.8759990	-0.7263310	C	2.4275130	-2.8491140	1.5102230
C	-3.5880120	-3.5423240	-1.0841170	C	1.1895980	-3.5500290	1.5419170
S	-3.7722860	3.9882730	-1.1614810	C	-0.0193830	-2.8328010	1.8573330
C	-2.6934110	5.2926340	-0.8542680	C	3.7518520	0.6069090	2.1558200
C	-1.3888030	4.9351110	-1.0496640	C	3.6737970	-0.7839160	2.2103820
C	-4.8580770	-1.3701000	-2.7739970	C	0.0318230	2.8341350	1.7568980
C	-5.7984950	-0.4332340	-3.1042950	C	1.2432890	3.5670960	1.4571430
S	-5.2733230	1.1701270	-2.7522900	C	2.4726440	2.9120740	1.5266760
C	4.9286840	1.3474980	-0.9775700	C	-2.4392720	1.4378370	1.7252050
C	5.9016530	0.4081920	-0.7793970	C	-2.4162370	2.8264310	2.1170340
S	5.3395750	-1.1855780	-1.1016260	C	-1.1745310	3.5243060	2.1417650
S	3.7243330	-3.8939870	-2.7676010	C	-3.7560220	-0.6177160	1.4868290
C	2.6238230	-5.1540040	-3.1784990	C	-3.6861160	0.7732350	1.4075500
C	1.3310270	-4.8354120	-2.8627170	C	-1.2174370	-3.5357440	2.2621420

C	-2.4500150	-2.8926000	2.1678190
C	3.5881470	-3.5420500	1.0841970
C	3.5466920	-4.8757780	0.7266030
C	2.3261880	-5.5707720	0.7654830
C	1.1754170	-4.9147090	1.1585990
C	-3.5691200	3.4844600	2.6208490
C	-3.5199790	4.7809450	3.0957240
C	-2.2925350	5.4657060	3.1286580
C	-1.1467540	4.8378330	2.6799620
S	5.2732850	1.1705330	2.7521810
C	5.7985120	-0.4328000	3.1042230
C	4.8581290	-1.3697060	2.7739390
C	1.3885990	4.9353300	1.0495210
C	2.6931930	5.2929230	0.8541580
S	3.7721260	3.9886130	1.1613880
C	-1.3308440	-4.8352200	2.8629100
C	-2.6236320	-5.1538500	3.1786870
S	-3.7241880	-3.8939010	2.7677060
S	-5.3395620	-1.1855990	1.1016760
C	-5.9016810	0.4081440	0.7793720
C	-4.9287260	1.3474810	0.9774740
H	4.5143500	-2.9968910	0.9631140
H	0.2294930	-5.4339430	1.0979600
H	-4.4982470	2.9371340	2.7087570
H	-0.1955420	5.3362530	2.8140830
H	6.7656150	-0.6047270	3.5614770
H	4.9895540	-2.4267250	2.9673860
H	0.5662110	5.6146230	0.8797020
H	3.0705680	6.2503800	0.5172540
H	-0.4935170	-5.4816860	3.0940980
H	-2.9800940	-6.0592740	3.6551660
H	-6.9109280	0.5730350	0.4234980
H	-5.0829640	2.3969040	0.7701460
H	4.4471530	-5.3660370	0.3666190
H	2.2740670	-6.6072330	0.4411460
H	-2.2296480	6.4627480	3.5581990
H	-4.4193100	5.2432900	3.4955220
N	1.2455790	0.6983390	1.7425320
N	-1.2324810	-0.7024980	1.7413990

B	2.5353840	1.4258130	1.7908240
B	-2.5203080	-1.4340110	1.7775540
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C	-1.3856110	-1.5571890	0.7192550
C	-1.3856110	-1.5571890	-0.7192550
C	1.0433990	-1.6783890	-0.7199500
C	1.0433990	-1.6783890	0.7199500
C	-2.6116050	-1.4630300	1.4154000
C	-3.7450980	-0.9141360	0.7112210
C	-3.7450980	-0.9141360	-0.7112210
C	-2.6116050	-1.4630300	-1.4154000
C	-1.5693490	-2.2692530	3.4876460
C	-2.7255430	-1.9495810	2.7707570
C	2.2721800	-1.7051660	1.4179990
C	2.3320250	-2.1840320	2.7816110
C	1.1468650	-2.3783000	3.4974630
C	2.2721800	-1.7051660	-1.4179990
C	3.4584790	-1.2844170	-0.7115340
C	3.4584790	-1.2844170	0.7115340
C	1.1468650	-2.3783000	-3.4974630
C	2.3320250	-2.1840320	-2.7816110
C	-2.7255430	-1.9495810	-2.7707570
C	-1.5693490	-2.2692530	-3.4876460
C	-4.8248590	-0.2977090	1.3864930
C	-5.8662710	0.3003390	0.7022510
C	-5.8662710	0.3003390	-0.7022510
C	-4.8248590	-0.2977090	-1.3864930
C	4.5997650	-0.7872940	-1.3858520
C	5.7020540	-0.3119440	-0.7019090
C	5.7020540	-0.3119440	0.7019090
C	4.5997650	-0.7872940	1.3858520
S	-1.9632020	-2.9321180	5.0347090
C	-3.6533080	-2.8231370	4.7253230
C	-3.9195820	-2.2935630	3.4930520
C	3.4820870	-2.6313730	3.5187790
C	3.1588810	-3.1078490	4.7594640

S	1.4661570	-3.0396260	5.0613050	C	1.5293580	1.2913850	3.5081910
C	-3.9195820	-2.2935630	-3.4930520	C	2.6129650	2.0185370	-1.4235790
C	-3.6533080	-2.8231370	-4.7253230	C	3.7321010	2.5933060	-0.7136780
S	-1.9632020	-2.9321180	-5.0347090	C	3.7321010	2.5933060	0.7136780
S	1.4661570	-3.0396260	-5.0613050	C	1.5293580	1.2913850	-3.5081910
C	3.1588810	-3.1078490	-4.7594640	C	2.6981110	1.6193080	-2.8119180
C	3.4820870	-2.6313730	-3.5187790	C	-2.3395970	1.7759720	-2.8115060
H	-4.7931110	-0.2270200	2.4637080	C	-1.1917280	1.3732620	-3.5064360
H	-4.7931110	-0.2270200	-2.4637080	C	-4.2939020	3.5836640	1.3878620
H	4.5729150	-0.6974950	-2.4611750	C	-5.2698360	4.2839200	0.7024920
H	4.5729150	-0.6974950	2.4611750	C	-5.2698360	4.2839200	-0.7024920
H	-4.3689040	-3.1790900	5.4568740	C	-4.2939020	3.5836640	-1.3878620
H	-4.9251150	-2.2058980	3.1027980	C	4.7725980	3.2807430	-1.3877330
H	4.4935830	-2.6542410	3.1355930	C	5.8013190	3.9011790	-0.7025720
H	3.8329020	-3.5170830	5.5024150	C	5.8013190	3.9011790	0.7025720
H	-4.9251150	-2.2058980	-3.1027980	C	4.7725980	3.2807430	1.3877330
H	-4.3689040	-3.1790900	-5.4568740	S	-1.5713640	0.9013160	5.1208920
H	3.8329020	-3.5170830	-5.5024150	C	-3.2491310	1.1892380	4.8813170
H	4.4935830	-2.6542410	-3.1355930	C	-3.5178700	1.6538390	3.6231930
H	-6.6556730	0.8074810	1.2510120	C	3.8694830	1.4142570	3.6191540
H	-6.6556730	0.8074810	-1.2510120	C	3.5728020	0.9703440	4.8783410
H	6.5411510	0.1071090	1.2513990	S	1.8800190	0.7914040	5.1210720
H	6.5411510	0.1071090	-1.2513990	C	-3.5178700	1.6538390	-3.6231930
N	-0.1801930	-1.7902250	1.4145480	C	-3.2491310	1.1892380	-4.8813170
N	-0.1801930	-1.7902250	-1.4145480	S	-1.5713640	0.9013160	-5.1208920
B	-0.2002350	-2.1198840	2.8577100	S	1.8800190	0.7914040	-5.1210720
B	-0.2002350	-2.1198840	-2.8577100	C	3.5728020	0.9703440	-4.8783410
C	-1.0250150	1.9598990	0.7169740	C	3.8694830	1.4142570	-3.6191540
C	-1.0250150	1.9598990	-0.7169740	H	-4.2346850	3.6959340	2.4626240
C	1.3974060	1.8849770	-0.7168730	H	-4.2346850	3.6959340	-2.4626240
C	1.3974060	1.8849770	0.7168730	H	4.7211890	3.3972880	-2.4624990
C	-2.2304300	2.1695720	1.4238390	H	4.7211890	3.3972880	2.4624990
C	-3.3077860	2.8199350	0.7137820	H	-3.9601690	0.9813980	5.6713990
C	-3.3077860	2.8199350	-0.7137820	H	-4.5247450	1.8470570	3.2817280
C	-2.2304300	2.1695720	-1.4238390	H	4.8870640	1.5259460	3.2718210
C	-1.1917280	1.3732620	3.5064360	H	4.2707240	0.7127900	5.6657070
C	-2.3395970	1.7759720	2.8115060	H	-4.5247450	1.8470570	-3.2817280
C	2.6129650	2.0185370	1.4235790	H	-3.9601690	0.9813980	-5.6713990
C	2.6981110	1.6193080	2.8119180	H	4.2707240	0.7127900	-5.6657070

H	4.8870640	1.5259460	-3.2718210
H	-5.9935410	4.8802970	1.2528800
H	-5.9935410	4.8802970	-1.2528800
H	6.5699450	4.4387260	1.2527470
H	6.5699450	4.4387260	-1.2527470
N	0.1792870	1.7003890	1.4060070
N	0.1792870	1.7003890	-1.4060070
B	0.1712160	1.4191130	2.8507830
B	0.1712160	1.4191130	-2.8507830

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C	0.1777090	1.3973880	-1.7093120
C	1.3131720	0.5205980	-1.6526930
C	-0.1720460	-1.3964330	-1.7102000
C	-1.3075980	-0.5196790	-1.6545770
C	0.3808710	2.7936460	-1.7262650
C	1.6180390	3.2982880	-1.1841920
C	2.7303470	2.4168020	-1.0481790
C	2.6121880	1.0576700	-1.5238030
C	-1.8913180	3.1617700	-2.5855850
C	-0.6148010	3.6611330	-2.3109130
C	-2.6067700	-1.0568400	-1.5276460
C	-3.7613560	-0.2883600	-1.9426120
C	-3.5998170	1.0511690	-2.3156830
C	-0.3751560	-2.7926750	-1.7280610
C	-1.6129790	-3.2975890	-1.1877780
C	-2.7255310	-2.4162330	-1.0528790
C	1.8980370	-3.1603830	-2.5849280
C	0.6212430	-3.6598890	-2.3118780
C	3.7673180	0.2893080	-1.9374510
C	3.6062280	-1.0500220	-2.3113720
C	1.7358240	4.6194440	-0.6864200
C	2.9028720	5.0720180	-0.1010040
C	3.9907780	4.1968020	0.0515490
C	3.8920270	2.8922660	-0.3937490
C	-1.7312800	-4.6189210	-0.6906580
C	-2.8991020	-5.0719000	-0.1070760

C	-3.9873700	-4.1969250	0.0441460
C	-3.8881280	-2.8921650	-0.4004590
S	-2.8558130	4.3438940	-3.3937000
C	-1.5706430	5.4901710	-3.3975290
C	-0.4431890	5.0021790	-2.7961780
C	-5.1057470	-0.7462260	-2.1730770
C	-5.9204040	0.2344270	-2.6669650
S	-5.0861150	1.7258030	-2.8824710
C	5.1121200	0.7471350	-2.1655690
C	5.9274960	-0.2334160	-2.6584850
S	5.0934090	-1.7246590	-2.8758640
S	2.8635240	-4.3422430	-3.3922880
C	1.5784130	-5.4886060	-3.3978590
C	0.4502110	-5.0007890	-2.7978150
H	0.8684330	5.2661190	-0.6993840
H	4.6896170	2.1990110	-0.1634300
H	-0.8636910	-5.2653610	-0.7025850
H	-4.6861570	-2.1991610	-0.1709570
H	-1.6998030	6.4574420	-3.8682180
H	0.4843850	5.5586970	-2.7540220
H	-5.4497490	-1.7620100	-2.0335200
H	-6.9656750	0.1452200	-2.9374850
H	5.4559520	1.7628550	-2.0251250
H	6.9732280	-0.1442250	-2.9272220
H	1.7081830	-6.4557100	-3.8687230
H	-0.4774240	-5.5572930	-2.7569510
H	2.9491670	6.0795480	0.3031920
H	4.8836020	4.5190600	0.5799010
H	-4.8809830	-4.5195500	0.5709310
H	-2.9458280	-6.0795740	0.2967200
N	-1.1126640	0.8588880	-1.8788370
N	1.1185090	-0.8578480	-1.8779220
B	-2.2485470	1.7286020	-2.2470490
B	2.2548140	-1.7274060	-2.2451120
C	-0.1782760	1.3964180	1.7096320
C	-1.3134140	0.5192070	1.6526530
C	0.1725700	-1.3973080	1.7099730
C	1.3077540	-0.5200920	1.6540920
C	-0.3819700	2.7926130	1.7272940

C	-1.6193070	3.2970630	1.1854240	H	1.6976870	6.4562280	3.8706080
C	-2.7312340	2.4151620	1.0488010	H	-0.4864620	5.5570430	2.7566900
C	-2.6126110	1.0558450	1.5238390	H	5.4509600	-1.7604330	2.0302010
C	1.8901670	3.1611610	2.5865820	H	6.9661240	0.1470360	2.9348080
C	0.6134180	3.6601550	2.3123480	H	-5.4567160	1.7597970	2.0256630
C	2.6070930	-1.0566650	1.5265460	H	-6.9732530	-0.1481910	2.9267990
C	3.7615520	-0.2877790	1.9412250	H	-1.7056330	-6.4567700	3.8696910
C	3.5994490	1.0514070	2.3152750	H	0.4799670	-5.5574610	2.7586350
C	0.3763510	-2.7934770	1.7281630	H	-2.9515280	6.0786180	-0.3004620
C	1.6142610	-3.2980020	1.1876470	H	-4.8852350	4.5173630	-0.5783690
C	2.7262140	-2.4160310	1.0517680	H	4.8818880	-4.5182790	-0.5731100
C	-1.8969010	-3.1621210	2.5843810	H	2.9481260	-6.0796940	-0.2965390
C	-0.6196870	-3.6609610	2.3121390	N	1.1122930	0.8583430	1.8788020
C	-3.7675240	0.2868990	1.9371040	N	-1.1182230	-0.8592490	1.8775530
C	-3.6059780	-1.0525510	2.3104270	B	2.2478900	1.7283260	2.2472670
C	-1.7376500	4.6184570	0.6883990	B	-2.2542770	-1.7293550	2.2443210
C	-2.9048310	5.0708460	0.1030840				
C	-3.9922900	4.1952220	-0.0501490				
C	-3.8929930	2.8904770	0.3944490				
C	1.7332470	-4.6195170	0.6911060	126			
C	2.9009590	-5.0718460	0.1067700	molecule10_UD1			
C	3.9884690	-4.1961610	-0.0456890	C	0.4970480	-3.7375920	-2.1899430
C	3.8886530	-2.8913550	0.3986360	C	-0.9271420	-3.6453720	-2.1975730
S	2.8543590	4.3432830	3.3950840	C	-1.5599620	-2.3923140	-1.8461810
C	1.5687790	5.4891070	3.3995430	C	-2.9468330	-2.2859690	-1.5232580
C	0.4413640	5.0009100	2.7982890	C	-3.5757800	-1.0221750	-1.5603560
C	5.1063590	-0.7449960	2.1706920	C	-2.8607320	0.1712470	-1.8577410
C	5.9206890	0.2358140	2.6647820	C	-3.4853730	1.4383390	-2.1899430
S	5.0856150	1.7265330	2.8818020	C	-2.6934130	2.6256150	-2.1975730
C	-5.1124640	0.7441520	2.1655640	C	-1.2918230	2.5471230	-1.8461810
C	-5.9275100	-0.2369380	2.6579600	C	-0.5062900	3.6950170	-1.5232580
S	-5.0929010	-1.7279560	2.8746520	C	0.9026600	3.6078040	-1.5603560
S	-2.8620830	-4.3442630	3.3916980	C	1.5786710	2.3918430	-1.8577410
C	-1.5762310	-5.4897790	3.3984930	C	2.9883250	2.2992520	-2.1899430
C	-0.4480530	-5.0015340	2.7987300	C	3.6205560	1.0197570	-2.1975730
H	-0.8707100	5.2657380	0.7020540	C	2.8517850	-0.1548100	-1.8461810
H	-4.6902660	2.1970650	0.1635550	C	3.4531240	-1.4090480	-1.5232580
H	0.8665050	-5.2670810	0.7043970	C	2.6731200	-2.5856290	-1.5603560
H	4.6860740	-2.1978890	0.1684290	C	1.2820620	-2.5630910	-1.8577410
				C	0.6511580	-1.2865760	-1.8581340

C	-0.7895360	-1.2036620	-1.8562390	H	0.0000000	6.8395690	-0.3871300
C	-1.4397860	0.0793680	-1.8581340	H	-3.5352480	-4.3408800	-0.9103540
C	-0.6476340	1.2855890	-1.8562390	H	-5.9232400	-3.4197840	-0.3871300
C	0.7886280	1.2072070	-1.8581340	H	5.5269360	-0.8911740	-0.9103540
C	1.4371700	-0.0819270	-1.8562390	H	5.9232400	-3.4197840	-0.3871300
C	-1.6726200	-4.7486850	-2.6812710	C	0.3863810	-3.7580370	1.4878760
C	-1.0630650	-5.9245500	-3.0806070	C	-1.0341000	-3.6340700	1.5218900
C	0.3359450	-6.0272270	-3.0436180	C	-1.6269150	-2.3438890	1.8019420
C	1.0917550	-4.9453680	-2.6268790	C	-2.9867630	-2.1812550	2.2074070
C	-3.2761720	3.8228730	-2.6812710	C	-3.5798640	-0.9012910	2.1477860
C	-4.5992790	3.8829160	-3.0806070	C	-2.8483370	0.2532630	1.7601750
C	-5.3877040	2.7226770	-3.0436180	C	-3.4477460	1.5444030	1.4878760
C	-4.8286920	1.5271960	-2.6268790	C	-2.6301470	2.7125920	1.5218900
C	4.9487910	0.9258110	-2.6812710	C	-1.2164100	2.5808940	1.8019420
C	5.6623430	2.0416340	-3.0806070	C	-0.3956410	3.6772400	2.2074070
C	5.0517590	3.3045500	-3.0436180	C	1.0093920	3.5508990	2.1477860
C	3.7369370	3.4181720	-2.6268790	C	1.6435010	2.3401010	1.7601750
C	-0.9537440	4.9806200	-1.0706290	C	3.0613660	2.2136340	1.4878760
C	0.0667190	5.8342200	-0.7836580	C	3.6642470	0.9214780	1.5218900
S	1.6121830	5.1314440	-1.0754560	C	2.8433240	-0.2370050	1.8019420
C	-3.8364710	-3.3162770	-1.0706290	C	3.3824030	-1.4959850	2.2074070
C	-5.0859420	-2.8593300	-0.7836580	C	2.5704730	-2.6496080	2.1477860
S	-5.2500520	-1.1695300	-1.0754560	C	1.2048360	-2.5933640	1.7601750
C	4.7902160	-1.6643430	-1.0706290	C	0.6133430	-1.3028400	1.6823680
C	5.0192230	-2.9748900	-0.7836580	C	-0.8252600	-1.1801020	1.6897350
S	3.6378690	-3.9619140	-1.0754560	C	-1.4349640	0.1202490	1.6823680
H	-2.7433470	-4.6490880	-2.8059920	C	-0.6093680	1.3047480	1.6897350
H	-1.6663560	-6.7453030	-3.4612060	C	0.8216210	1.1825910	1.6823680
H	0.8322750	-6.9318290	-3.3864800	C	1.4346290	-0.1246450	1.6897350
H	2.1698900	-5.0161370	-2.7002450	C	-1.8146950	-4.7623220	1.1776040
H	-2.6545550	4.7003520	-2.8059920	C	-1.2385830	-5.9676630	0.8163660
H	-5.0084260	4.8157580	-3.4612060	C	0.1582380	-6.0871700	0.7805700
H	-6.4192770	2.7451440	-3.3864800	C	0.9471060	-4.9983600	1.1088410
H	-5.4290470	0.6288880	-2.7002450	C	-3.2169450	3.9527330	1.1776040
H	5.3979020	-0.0512640	-2.8059920	C	-4.5488570	4.0564760	0.8163660
H	6.6747820	1.9295450	-3.4612060	C	-5.3507630	2.9065470	0.7805700
H	5.5870030	4.1866860	-3.3864800	C	-4.8022600	1.6789620	1.1088410
H	3.2591570	4.3872480	-2.7002450	C	5.0316400	0.8095890	1.1776040
H	-1.9916880	5.2320540	-0.9103540	C	5.7874390	1.9111880	0.8163660

C	5.1925250	3.1806230	0.7805700
C	3.8551540	3.3193980	1.1088410
C	-0.7976170	4.9143630	2.8168720
C	0.2561360	5.6944020	3.1878650
S	1.7799360	4.9775150	2.8094170
C	-3.8571540	-3.1479380	2.8168720
C	-5.0595640	-2.6253810	3.1878650
S	-5.2006220	-0.9472880	2.8094170
C	4.6547720	-1.7664240	2.8168720
C	4.8034290	-3.0690210	3.1878650
S	3.4206870	-4.0302270	2.8094170
H	-2.8899790	-4.6615300	1.1299760
H	-1.8694340	-6.8034990	0.5240290
H	0.6240530	-7.0140700	0.4570440
H	2.0206210	-5.0860070	1.0040190
H	-2.5920140	4.8335610	1.1299760
H	-4.9572860	5.0207270	0.5240290
H	-6.3863890	2.9665890	0.4570440
H	-5.4149220	0.7930940	1.0040190
H	5.4819930	-0.1720300	1.1299760
H	6.8267200	1.7827720	0.5240290
H	5.7623360	4.0474810	0.4570440
H	3.3943000	4.2929130	1.0040190
H	-1.8246890	5.1784100	3.0330210
H	0.2242120	6.6524280	3.6926700
H	-3.5722900	-4.1694320	3.0330210
H	-5.8732780	-3.1320410	3.6926700
H	5.3969800	-1.0089780	3.0330210
H	5.6490660	-3.5203870	3.6926700

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C	-1.9757330	1.5282130	3.5500020
C	-1.8159890	2.7455200	2.8209650
C	-1.4522880	2.6930250	1.4218990
C	-0.9848650	3.8307330	0.6964630
C	-1.0367420	3.8256140	-0.7149920
C	-1.4823200	2.6918100	-1.4506830
C	-1.8381130	2.7132250	-2.8571350

C	-1.9982180	1.4786780	-3.5561090
C	-1.7798490	0.2325310	-2.8544900
C	-1.6142990	-1.0181350	-3.5229400
C	-1.8003550	-2.2212670	-2.8065360
C	-2.0985090	-2.2336330	-1.4144670
C	-2.5979710	-3.3882900	-0.6911510
C	-2.6062540	-3.3685420	0.7363060
C	-2.0893200	-2.2112830	1.4338300
C	-1.7733140	-2.2193450	2.8263450
C	-1.6561670	-0.9952100	3.5217080
C	-1.7882840	0.2616250	2.8667210
C	-1.7766890	0.2428530	1.4427590
C	-1.6142990	1.4772570	0.7141460
C	-1.6215640	1.4748430	-0.7243490
C	-1.7773610	0.2313710	-1.4384490
C	-1.9339790	-1.0030590	-0.7167070
C	-1.9324480	-0.9948130	0.7260960
C	-2.1581600	3.9648430	3.4566050
C	-2.5799190	4.0091800	4.7730800
C	-2.7087340	2.8148880	5.5006430
C	-2.4311100	1.6054420	4.8880510
C	-2.5042850	1.5110160	-4.8791420
C	-2.7832980	2.7018800	-5.5252720
C	-2.5960210	3.9185880	-4.8492850
C	-2.1532380	3.9135320	-3.5383290
C	-3.2500970	-4.4273530	1.4235330
C	-3.8069500	-5.5015840	0.7534140
C	-3.7684830	-5.5391060	-0.6497740
C	-3.1942280	-4.4915590	-1.3479490
C	-1.2015850	-1.2564990	-4.8755790
C	-1.0893970	-2.5789900	-5.1774510
S	-1.4988680	-3.5930380	-3.8484450
C	-0.3782750	5.0254900	1.2071890
C	-0.0013030	5.8958860	0.2309890
S	-0.3798930	5.3190530	-1.3457940
C	-1.4773960	-3.3436540	3.6659060
C	-1.1614460	-2.9926140	4.9424490
S	-1.2281300	-1.2907970	5.1913410
H	-2.1537730	4.8810010	2.8796640

H	-2.8517250	4.9609440	5.2235720	C	1.6215640	-1.4748430	-0.7243490
H	-3.0726710	2.8294380	6.5251440	C	1.7773610	-0.2313710	-1.4384490
H	-2.6282620	0.6949030	5.4402790	C	3.2500970	4.4273530	1.4235330
H	-2.7412120	0.5792480	-5.3773720	C	3.8069500	5.5015840	0.7534140
H	-3.1870390	2.6889880	-6.5349640	C	3.7684830	5.5391060	-0.6497740
H	-2.8444660	4.8611310	-5.3311550	C	3.1942280	4.4915590	-1.3479490
H	-2.1070860	4.8574030	-3.0092940	C	2.1581600	-3.9648430	3.4566050
H	-3.3685860	-4.3649240	2.4980000	C	2.5799190	-4.0091800	4.7730800
H	-4.3089000	-6.2879260	1.3122880	C	2.7087340	-2.8148880	5.5006430
H	-4.2311630	-6.3596940	-1.1927640	C	2.4311100	-1.6054420	4.8880510
H	-3.2596570	-4.4993240	-2.4288200	C	2.5042850	-1.5110160	-4.8791420
H	-0.9488810	-0.4728460	-5.5745390	C	2.7832980	-2.7018800	-5.5252720
H	-0.7496760	-3.0215110	-6.1052500	C	2.5960210	-3.9185880	-4.8492850
H	-0.1853650	5.2019960	2.2550790	C	2.1532380	-3.9135320	-3.5383290
H	0.5182510	6.8384750	0.3477600	C	0.3782750	-5.0254900	1.2071890
H	-1.4504900	-4.3652530	3.3167260	C	0.0013030	-5.8958860	0.2309890
H	-0.8537770	-3.6420270	5.7521580	S	0.3798930	-5.3190530	-1.3457940
C	2.5979710	3.3882900	-0.6911510	C	1.4773960	3.3436540	3.6659060
C	2.6062540	3.3685420	0.7363060	C	1.1614460	2.9926140	4.9424490
C	2.0893200	2.2112830	1.4338300	S	1.2281300	1.2907970	5.1913410
C	1.7733140	2.2193450	2.8263450	C	1.2015850	1.2564990	-4.8755790
C	1.6561670	0.9952100	3.5217080	C	1.0893970	2.5789900	-5.1774510
C	1.7882840	-0.2616250	2.8667210	S	1.4988680	3.5930380	-3.8484450
C	1.9757330	-1.5282130	3.5500020	H	3.3685860	4.3649240	2.4980000
C	1.8159890	-2.7455200	2.8209650	H	4.3089000	6.2879260	1.3122880
C	1.4522880	-2.6930250	1.4218990	H	4.2311630	6.3596940	-1.1927640
C	0.9848650	-3.8307330	0.6964630	H	3.2596570	4.4993240	-2.4288200
C	1.0367420	-3.8256140	-0.7149920	H	2.1537730	-4.8810010	2.8796640
C	1.4823200	-2.6918100	-1.4506830	H	2.8517250	-4.9609440	5.2235720
C	1.8381130	-2.7132250	-2.8571350	H	3.0726710	-2.8294380	6.5251440
C	1.9982180	-1.4786780	-3.5561090	H	2.6282620	-0.6949030	5.4402790
C	1.7798490	-0.2325310	-2.8544900	H	2.7412120	-0.5792480	-5.3773720
C	1.6142990	1.0181350	-3.5229400	H	3.1870390	-2.6889880	-6.5349640
C	1.8003550	2.2212670	-2.8065360	H	2.8444660	-4.8611310	-5.3311550
C	2.0985090	2.2336330	-1.4144670	H	2.1070860	-4.8574030	-3.0092940
C	1.9339790	1.0030590	-0.7167070	H	0.1853650	-5.2019960	2.2550790
C	1.9324480	0.9948130	0.7260960	H	-0.5182510	-6.8384750	0.3477600
C	1.7766890	-0.2428530	1.4427590	H	1.4504900	4.3652530	3.3167260
C	1.6142990	-1.4772570	0.7141460	H	0.8537770	3.6420270	5.7521580

H	0.9488810	0.4728460	-5.5745390
H	0.7496760	3.0215110	-6.1052500
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C	0.4966190	-3.7376540	-2.1775810
C	-0.9275130	-3.6453030	-2.1898160
C	-1.5614140	-2.3921860	-1.8400460
C	-2.9486000	-2.2857620	-1.5175210
C	-3.5747270	-1.0203100	-1.5438930
C	-2.8600810	0.1724910	-1.8436270
C	-3.4852130	1.4387420	-2.1775810
C	-2.6931680	2.6259010	-2.1898160
C	-1.2909860	2.5483170	-1.8400460
C	-0.5052280	3.6964440	-1.5175210
C	0.9037500	3.6059600	-1.5438930
C	1.5794220	2.3906570	-1.8436270
C	2.9885940	2.2989120	-2.1775810
C	3.6206810	1.0194020	-2.1898160
C	2.8524010	-0.1561320	-1.8400460
C	3.4538280	-1.4106820	-1.5175210
C	2.6709780	-2.5856500	-1.5438930
C	1.2806590	-2.5631480	-1.8436270
C	0.6505050	-1.2865960	-1.8488910
C	-0.7902170	-1.2035530	-1.8478930
C	-1.4394780	0.0799440	-1.8488910
C	-0.6471990	1.2861240	-1.8478930
C	0.7889720	1.2066520	-1.8488910
C	1.4374160	-0.0825710	-1.8478930
C	-1.6708940	-4.7497360	-2.6739110
C	-1.0596530	-5.9256760	-3.0707130
C	0.3393540	-6.0273710	-3.0312770
C	1.0933820	-4.9448990	-2.6130130
C	-3.2779450	3.8219050	-2.6739110
C	-4.6019590	3.8805250	-3.0707130
C	-5.3895330	2.7197970	-3.0312770
C	-4.8290990	1.5255530	-2.6130130
C	4.9488390	0.9278310	-2.6739110

C	5.6616130	2.0451510	-3.0707130
C	5.0501800	3.3075740	-3.0312770
C	3.7357170	3.4193460	-2.6130130
C	-0.9525380	4.9845150	-1.0713290
C	0.0679080	5.8343910	-0.7740250
S	1.6139180	5.1257170	-1.0472830
C	-3.8404480	-3.3171800	-1.0713290
C	-5.0866850	-2.8583860	-0.7740250
S	-5.2459600	-1.1651650	-1.0472830
C	4.7929860	-1.6673350	-1.0713290
C	5.0187770	-2.9760050	-0.7740250
S	3.6320420	-3.9605520	-1.0472830
H	-2.7412820	-4.6511950	-2.8016380
H	-1.6617680	-6.7472120	-3.4514400
H	0.8369540	-6.9316770	-3.3731460
H	2.1717800	-5.0146280	-2.6832000
H	-2.6574120	4.6996170	-2.8016380
H	-5.0123730	4.8127400	-3.4514400
H	-6.4214850	2.7410150	-3.3731460
H	-5.4286850	0.6264970	-2.6832000
H	5.3986940	-0.0484230	-2.8016380
H	6.6741410	1.9344730	-3.4514400
H	5.5845310	4.1906620	-3.3731460
H	3.2569050	4.3881310	-2.6832000
H	-1.9901830	5.2391720	-0.9145290
H	0.0000000	6.8400150	-0.3787830
H	-3.5421650	-4.3431350	-0.9145290
H	-5.9236270	-3.4200080	-0.3787830
H	5.5323480	-0.8960370	-0.9145290
H	5.9236270	-3.4200080	-0.3787830
C	3.6988960	0.8060570	1.5245780
C	3.1249230	2.1101230	1.4676290
C	1.7173760	2.2770750	1.7535940
C	1.1513440	3.5235630	2.1564590
C	-0.2514840	3.6824730	2.1596840
C	-1.1317830	2.6291000	1.7894080
C	-2.5475140	2.8003100	1.5245780
C	-3.3898820	1.6512010	1.4676290
C	-2.8306930	0.3487540	1.7535940

C	0.4651890	-1.3629550	-1.8510210	H	6.3284570	2.5818690	-0.3692950
C	-0.9470990	-1.0895010	-1.8509420	H	-5.3583980	1.6361970	-0.9107550
C	-1.4141990	0.2757990	-1.8502340	H	-5.4020970	4.1888810	-0.3685500
C	2.2992600	4.4776560	-2.6748990	C	-3.7728790	-0.2986680	1.5230970
C	1.8528630	5.7249140	-3.0739580	C	-3.3801330	-1.6684360	1.4682970
C	0.4803390	6.0150030	-3.0364430	C	-2.0078180	-2.0229250	1.7543280
C	-0.4135200	5.0456140	-2.6164120	C	-1.6147220	-3.3331630	2.1605470
C	2.7278040	-4.2316590	-2.6779140	C	-0.2464700	-3.6809060	2.1607340
C	4.0315360	-4.4683140	-3.0760500	C	0.7672300	-2.7567580	1.7873470
C	4.9691270	-3.4249310	-3.0359150	C	2.1465970	-3.1178910	1.5213450
C	4.5761630	-2.1665470	-2.6151260	C	3.1366420	-2.0932170	1.4637700
C	-5.0307530	-0.2488290	-2.6733190	C	2.7586410	-0.7270140	1.7494330
C	-5.8882640	-1.2596080	-3.0698480	C	3.6981200	0.2680830	2.1535220
C	-5.4538710	-2.5934070	-3.0291890	C	3.3149600	1.6268320	2.1576280
C	-4.1673220	-2.8823950	-2.6094710	C	2.0068140	2.0433680	1.7879440
C	0.2668280	-5.0665670	-1.0677140	C	1.6295330	3.4191560	1.5255000
C	-0.8590010	-5.7691760	-0.7663470	C	0.2471570	3.7640680	1.4680080
S	-2.2949890	-4.8586930	-1.0404480	C	-0.7470980	2.7530810	1.7519660
C	4.2521550	2.7635940	-1.0664060	C	-2.0791910	3.0688400	2.1544300
C	5.4238370	2.1396060	-0.7670370	C	-3.0646020	2.0578120	2.1551550
S	5.3529430	0.4409050	-1.0437510	C	-2.7707160	0.7166690	1.7854900
C	-4.5218660	2.3005040	-1.0682310	C	-1.3931840	0.3689600	1.6817070
C	-4.5672410	3.6270840	-0.7679330	C	-1.0090600	-1.0228040	1.6777330
S	-3.0608310	4.4151090	-1.0447960	C	0.3797190	-1.3901110	1.6820560
H	3.3467880	4.2353750	-2.8010910	C	1.3930620	-0.3617120	1.6758590
H	2.5607800	6.4570820	-3.4550110	C	1.0168690	1.0246110	1.6822490
H	0.1101220	6.9776910	-3.3805880	C	-0.3805790	1.3879850	1.6768420
H	-1.4725800	5.2605270	-2.6881370	C	-4.3272210	-2.6313640	1.0490170
H	1.9946020	-5.0178220	-2.8053830	C	-5.6310490	-2.2852250	0.7421710
H	4.3119530	-5.4470280	-3.4580320	C	-6.0349230	-0.9465180	0.8497080
H	5.9882070	-3.5853610	-3.3794030	C	-5.1179840	0.0196670	1.2265750
H	5.2920290	-1.3568490	-2.6845350	C	4.4426720	-2.4327320	1.0411250
H	-5.3443280	0.7794370	-2.8015080	C	4.7933770	-3.7350810	0.7328230
H	-6.8764170	-1.0129460	-3.4508320	C	3.8359410	-4.7538010	0.8432700
H	-6.1031790	-3.3958750	-3.3708130	C	2.5418240	-4.4420970	1.2237400
H	-3.8240340	-3.9071950	-2.6789570	C	-0.1119130	5.0653330	1.0467270
H	1.2603700	-5.4604440	-0.9137830	C	0.8407440	6.0208180	0.7405900
H	-0.9276660	-6.7734510	-0.3678240	C	2.2017300	5.7010620	0.8510450
H	4.0960130	3.8207450	-0.9106340	C	2.5788920	4.4240330	1.2298760

C	5.0046700	0.0731360	2.7181910
C	5.5861940	1.2330380	3.1309230
S	4.5896590	2.6133510	2.8426810
C	-2.4352020	-4.3667180	2.7282920
C	-1.7203630	-5.4503480	3.1390750
S	-0.0274760	-5.2778270	2.8457740
C	-2.5644530	4.2973330	2.7195190
C	-3.8609710	4.2212810	3.1282800
S	-4.5582350	2.6690460	2.8358830
H	-4.0056530	-3.6541110	0.9023990
H	-6.3238000	-3.0427860	0.3857520
H	-7.0516360	-0.6566260	0.5963860
H	-5.4322070	1.0545960	1.2277780
H	5.1669770	-1.6429150	0.8919460
H	5.7948320	-3.9565240	0.3737460
H	4.0917660	-5.7792880	0.5886630
H	1.8019620	-5.2310500	1.2271500
H	-1.1580040	5.2979660	0.8973480
H	0.5318950	6.9992100	0.3824510
H	2.9618270	6.4360140	0.5980430
H	3.6321260	4.1777920	1.2329650
H	5.4608280	-0.8972730	2.8646300
H	6.5467000	1.3564560	3.6164440
H	-3.5032440	-4.2763800	2.8777550
H	-2.0922620	-6.3436700	3.6260940
H	-1.9522780	5.1770790	2.8694250
H	-4.4490230	4.9909440	3.6134280

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C	-1.1490240	1.4769220	-1.8394160
C	0.2426480	1.8402730	-1.8273860
C	1.2525730	0.8211430	-1.6895600
C	0.8758330	-0.5687550	-1.6047210
C	-0.5170460	-0.9333730	-1.6243970
C	-1.5278690	0.0905740	-1.7109280
C	-0.8980800	-2.3142920	-1.5879190
C	-2.2706570	-2.6307290	-1.7908310

C	-3.2671420	-1.6419860	-1.8643770
C	-2.9054520	-0.2677600	-1.7045990
C	-3.8854500	0.7661840	-1.5850050
C	-3.5070600	2.1038140	-1.7927700
C	-2.1524770	2.4830670	-2.0088430
C	-1.7491730	3.8151690	-2.3429330
C	-0.3857340	4.1539710	-2.3025210
C	0.6278410	3.2122190	-1.9789660
C	1.9969260	3.5445830	-1.7836680
C	2.9820650	2.5649380	-1.5756500
C	2.6291420	1.1831810	-1.6762710
C	3.6141440	0.1608320	-1.8450250
C	3.2324690	-1.1893120	-1.7507000
C	1.8817490	-1.5823780	-1.5288400
C	1.4856890	-2.9408310	-1.3142530
C	0.1232260	-3.2818070	-1.3819750
C	-5.2650640	0.6449350	-1.2143430
C	-5.9180540	1.8397590	-1.1892760
S	-4.8885820	3.1595710	-1.6029660
S	-2.9421240	-4.2097170	-2.1065730
C	-4.5107020	-3.5496120	-2.3758520
C	-4.5427290	-2.1955510	-2.2183650
C	2.3055270	-4.0789190	-1.0225720
C	1.5924830	-5.2347690	-0.9088410
S	-0.0962660	-4.9936120	-1.1411170
C	4.9822330	0.3069660	-2.2531770
C	5.6104660	-0.8870790	-2.4469760
S	4.5790710	-2.2316080	-2.1415770
S	2.6869020	5.1439680	-1.6724320
C	4.2387340	4.5056200	-1.2775080
C	4.2521960	3.1427250	-1.2520960
C	-2.5598200	4.9229840	-2.7583390
C	-1.8377390	6.0543300	-3.0001570
S	-0.1486580	5.8256900	-2.7425350
H	-5.7320610	-0.2779910	-0.9011900
H	-6.9480430	2.0277680	-0.9131850
H	-5.3261100	-4.2036980	-2.6594610
H	-5.4310870	-1.6122070	-2.4172930
H	3.3708970	-4.0437910	-0.8400180

H	1.9639620	-6.2198580	-0.6568790	S	0.1486580	-5.8256900	2.7425350
H	5.4586950	1.2531150	-2.4690420	C	5.2650640	-0.6449350	1.2143430
H	6.6282820	-1.0541110	-2.7778230	C	5.9180540	-1.8397590	1.1892760
H	5.0521910	5.1817540	-1.0457990	S	4.8885820	-3.1595710	1.6029660
H	5.1180680	2.5758310	-0.9401920	S	2.9421240	4.2097170	2.1065730
H	-3.6286360	4.8833620	-2.9218010	C	4.5107020	3.5496120	2.3758520
H	-2.2045020	7.0135090	-3.3443550	C	4.5427290	2.1955510	2.2183650
C	-0.8758330	0.5687550	1.6047210	C	-2.3055270	4.0789190	1.0225720
C	0.5170460	0.9333730	1.6243970	C	-1.5924830	5.2347690	0.9088410
C	1.5278690	-0.0905740	1.7109280	S	0.0962660	4.9936120	1.1411170
C	1.1490240	-1.4769220	1.8394160	H	-5.4586950	-1.2531150	2.4690420
C	-0.2426480	-1.8402730	1.8273860	H	-6.6282820	1.0541110	2.7778230
C	-1.2525730	-0.8211430	1.6895600	H	-5.0521910	-5.1817540	1.0457990
C	-0.6278410	-3.2122190	1.9789660	H	-5.1180680	-2.5758310	0.9401920
C	-1.9969260	-3.5445830	1.7836680	H	3.6286360	-4.8833620	2.9218010
C	-2.9820650	-2.5649380	1.5756500	H	2.2045020	-7.0135090	3.3443550
C	-2.6291420	-1.1831810	1.6762710	H	5.7320610	0.2779910	0.9011900
C	-3.6141440	-0.1608320	1.8450250	H	6.9480430	-2.0277680	0.9131850
C	-3.2324690	1.1893120	1.7507000	H	5.3261100	4.2036980	2.6594610
C	-1.8817490	1.5823780	1.5288400	H	5.4310870	1.6122070	2.4172930
C	-1.4856890	2.9408310	1.3142530	H	-3.3708970	4.0437910	0.8400180
C	-0.1232260	3.2818070	1.3819750	H	-1.9639620	6.2198580	0.6568790
C	0.8980800	2.3142920	1.5879190				
C	2.2706570	2.6307290	1.7908310				
C	3.2671420	1.6419860	1.8643770	108			
C	2.9054520	0.2677600	1.7045990	molecule11_UD2			
C	3.8854500	-0.7661840	1.5850050	C	1.4164220	-1.6147820	1.4630600
C	3.5070600	-2.1038140	1.7927700	C	2.0803170	-0.3387050	1.4649700
C	2.1524770	-2.4830670	2.0088430	C	1.3101830	0.8731560	1.5900450
C	1.7491730	-3.8151690	2.3429330	C	-0.1235390	0.8117490	1.7357940
C	0.3857340	-4.1539710	2.3025210	C	-0.7874040	-0.4654340	1.7455270
C	-4.9822330	-0.3069660	2.2531770	C	-0.0195970	-1.6747820	1.5884020
C	-5.6104660	0.8870790	2.4469760	C	-2.2049520	-0.5378300	1.9463330
S	-4.5790710	2.2316080	2.1415770	C	-2.7822780	-1.8224920	2.1491610
S	-2.6869020	-5.1439680	1.6724320	C	-2.0436790	-3.0095530	2.0011060
C	-4.2387340	-4.5056200	1.2775080	C	-0.6759280	-2.9375860	1.5903770
C	-4.2521960	-3.1427250	1.2520960	C	0.0665300	-4.0997470	1.2149240
C	2.5598200	-4.9229840	2.7583390	C	1.4691410	-4.0348200	1.1571830
C	1.8377390	-6.0543300	3.0001570	C	2.1805450	-2.8211960	1.3725030

C	3.6063440	-2.7468690	1.4720740	H	4.2957010	-4.8597990	1.7271740
C	4.2357420	-1.4903810	1.4524280	H	6.7362550	-3.9744620	1.8388490
C	3.5090710	-0.2717110	1.3712200	C	-2.0825590	0.3333950	-1.4721700
C	4.1044850	1.0087670	1.2026670	C	-1.3105560	-0.8738520	-1.6066180
C	3.3579070	2.1969680	1.2743130	C	0.1207170	-0.8065390	-1.7689280
C	1.9696900	2.1344460	1.6102000	C	0.7883580	0.4740070	-1.7771310
C	1.2391200	3.2891310	2.0321360	C	0.0175220	1.6784790	-1.6036490
C	-0.1612190	3.2183650	2.1420990	C	-1.4163960	1.6104040	-1.4729260
C	-0.8804040	2.0133890	1.9012260	C	0.6692990	2.9529960	-1.5984310
C	-2.3094230	1.9386650	1.9014280	C	-0.1063950	4.0964610	-1.2604140
C	-2.9357740	0.6815450	1.9635670	C	-1.5036450	4.0430830	-1.1282400
C	-0.4358790	-5.3785340	0.8051590	C	-2.1810930	2.8074300	-1.3685490
C	0.5499900	-6.2603820	0.4824500	C	-3.5999380	2.7358080	-1.5185220
S	2.1246660	-5.5796410	0.6616520	C	-4.2354560	1.4824110	-1.4752280
S	-4.3917350	-2.1655630	2.7288240	C	-3.5065780	0.2674260	-1.3529670
C	-4.0597360	-3.8550580	2.8157500	C	-4.1273940	-1.0083830	-1.1634660
C	-2.7956820	-4.1613460	2.4074920	C	-3.3573870	-2.1749910	-1.3041140
C	-3.2619240	3.0074580	1.8461900	C	-1.9707400	-2.1438230	-1.6154090
C	-4.5531380	2.5751700	1.9032460	C	-1.2118610	-3.2861140	-1.9872880
S	-4.6689560	0.8601270	2.0184280	C	0.1787440	-3.2341650	-2.1807430
C	1.7548700	4.5400420	2.5096410	C	0.8746390	-2.0032910	-1.9462960
C	0.7802410	5.3850540	2.9485770	C	2.3020410	-1.9294780	-1.9347630
S	-0.7962520	4.7064600	2.8027750	C	2.9333980	-0.6728360	-2.0125170
S	5.7703630	1.3527260	0.8105320	C	2.2025490	0.5491430	-1.9925810
C	5.4481590	3.0417140	0.6828010	C	2.8102700	1.8374300	-2.1637520
C	4.1458950	3.3469480	0.9444460	C	2.0452460	2.9968120	-1.9472760
C	4.5523440	-3.8135760	1.6253750	C	-4.5223220	3.7992970	-1.7986010
C	5.8428160	-3.3783630	1.6991060	C	-5.8087510	3.3687620	-1.9313480
S	5.9667290	-1.6618700	1.5924600	S	-5.9558490	1.6622010	-1.7317280
H	-1.4843800	-5.6062480	0.6753780	S	0.4900140	5.6912060	-0.8834930
H	0.4409160	-7.2727090	0.1141830	C	-1.0958070	6.2577920	-0.5181370
H	-4.8203280	-4.5323930	3.1842010	C	-2.0457020	5.2939810	-0.6843820
H	-2.3998400	-5.1664560	2.4556230	C	4.1406730	2.1579130	-2.5940580
H	-3.0084570	4.0494490	1.7062750	C	4.3650780	3.4982470	-2.6957240
H	-5.4554630	3.1702660	1.8425490	S	2.9813620	4.4331650	-2.2730330
H	2.8062290	4.7787820	2.5891270	C	3.2472600	-3.0007000	-1.8140240
H	0.9030800	6.3739610	3.3730200	C	4.5407380	-2.5787260	-1.8550140
H	6.2400100	3.7162870	0.3820740	S	4.6687640	-0.8717640	-2.0232570
H	3.7490370	4.3456070	0.8284340	S	-1.8448840	-4.8536960	-2.4243540

C	-0.2818720	-5.4108100	-2.8913980
C	0.6844730	-4.4660590	-2.7169060
C	-5.4826310	-1.3061940	-0.8047120
C	-5.7229470	-2.6431920	-0.6894520
S	-4.3226430	-3.5943470	-1.0079990
H	-4.2369250	4.8281170	-1.9700730
H	-6.6844670	3.9596590	-2.1706980
H	-1.2343660	7.2714360	-0.1632690
H	-3.0835390	5.4553990	-0.4284580
H	4.9010850	1.4357790	-2.8569070
H	5.2752210	3.9938650	-3.0097390
H	2.9845990	-4.0285870	-1.6118440
H	5.4360830	-3.1762180	-1.7404690
H	-0.1657550	-6.4096090	-3.2936990
H	1.7067800	-4.6294510	-3.0260480
H	-6.2403910	-0.5684250	-0.5798550
H	-6.6477370	-3.1275850	-0.4022220

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C	-0.9149850	2.3277580	0.7244400
C	-0.9056450	2.3270990	-0.7134540
C	-1.3154070	1.1492560	-1.4360610
C	-1.7796410	-0.0163770	-0.7240950
C	-1.7985830	-0.0133950	0.7149840
C	-1.3377800	1.1460440	1.4366960
C	-2.3084910	-1.1484820	1.4307340
C	-2.4928850	-1.0151060	2.8354030
C	-2.0374190	0.1033380	3.5517600
C	-1.3382350	1.1424150	2.8603010
C	-0.6875150	2.2115250	3.5514350
C	-0.3553080	3.3841400	2.8525350
C	-0.5364620	3.5064570	1.4460700
C	-0.3337470	4.7255410	0.7203120
C	-0.3172140	4.6977210	-0.6836420
C	-0.5136830	3.5064140	-1.4312620
C	-0.3338520	3.3950870	-2.8371790
C	-0.6614610	2.2293740	-3.5454710

C	-1.3008090	1.1489910	-2.8601380
C	-1.9915190	0.1090090	-3.5580370
C	-2.4328490	-1.0211720	-2.8496180
C	-2.2455100	-1.1614570	-1.4456880
C	-2.5736780	-2.3523850	-0.7212690
C	-2.6319350	-2.3126710	0.6818170
C	-0.2602390	2.2473580	4.9211280
C	0.3338520	3.4207470	5.2689830
S	0.4175990	4.5444190	3.9407600
S	-3.4164690	-2.0939330	3.8837820
C	-3.2153460	-1.0124390	5.2349880
C	-2.4792190	0.0884450	4.9194550
C	-2.8633360	-3.6596180	-1.2374400
C	-3.1666870	-4.5663390	-0.2693770
S	-3.1049690	-3.8826570	1.3299320
C	-2.4503740	0.1141810	-4.9205680
C	-3.2019190	-0.9752280	-5.2390280
S	-3.3911720	-2.0713060	-3.8993180
S	0.3997710	4.5901780	-3.9135440
C	0.3243480	3.4783170	-5.2562050
C	-0.2464130	2.2906580	-4.9182200
C	-0.1614060	6.0568100	1.2336640
C	-0.0002480	6.9964690	0.2618690
S	-0.0611730	6.3153080	-1.3420000
H	-0.3201830	1.4042010	5.5959700
H	0.7721220	3.6895070	6.2227850
H	-3.6833880	-1.2528370	6.1825870
H	-2.3177000	0.8966630	5.6207040
H	-2.7813240	-3.9434120	-2.2784850
H	-3.3801690	-5.6213750	-0.3898920
H	-2.2950040	0.9315700	-5.6124650
H	-3.6866500	-1.1972310	-6.1827760
H	0.7461030	3.7693420	-6.2108840
H	-0.3001450	1.4566850	-5.6050890
H	-0.2015670	6.3248790	2.2817130
H	0.1193510	8.0667530	0.3831060
C	0.9149850	-2.3277580	0.7244400
C	0.9056450	-2.3270990	-0.7134540
C	1.3154070	-1.1492560	-1.4360610
C	1.7796410	0.0163770	0.7240950
C	1.7985830	0.0133950	-0.7149840
C	1.3377800	-1.1460440	-1.4366960
C	2.3084910	1.1484820	-1.4307340
C	2.4928850	1.0151060	-2.8354030
C	2.0374190	-0.1033380	-3.5517600
C	1.3382350	-1.1424150	-2.8603010
C	0.6875150	-2.2115250	-3.5514350
C	0.3553080	-3.3841400	-2.8525350
C	0.5364620	-3.5064570	-1.4460700
C	0.3337470	-4.7255410	-0.7203120
C	0.3172140	-4.6977210	0.6836420
C	0.5136830	-3.5064140	1.4312620
C	0.3338520	-3.3950870	2.8371790
C	0.6614610	-2.2293740	3.5454710

C	1.7796410	0.0163770	-0.7240950	H	0.3201830	-1.4042010	5.5959700
C	1.7985830	0.0133950	0.7149840	H	-0.7721220	-3.6895070	6.2227850
C	1.3377800	-1.1460440	1.4366960	H	3.6833880	1.2528370	6.1825870
C	2.3084910	1.1484820	1.4307340	H	2.3177000	-0.8966630	5.6207040
C	2.4928850	1.0151060	2.8354030	H	2.7813240	3.9434120	-2.2784850
C	2.0374190	-0.1033380	3.5517600	H	3.3801690	5.6213750	-0.3898920
C	1.3382350	-1.1424150	2.8603010	H	2.2950040	-0.9315700	-5.6124650
C	0.6875150	-2.2115250	3.5514350	H	3.6866500	1.1972310	-6.1827760
C	0.3553080	-3.3841400	2.8525350	H	-0.7461030	-3.7693420	-6.2108840
C	0.5364620	-3.5064570	1.4460700	H	0.3001450	-1.4566850	-5.6050890
C	0.3337470	-4.7255410	0.7203120	H	0.2015670	-6.3248790	2.2817130
C	0.3172140	-4.6977210	-0.6836420	H	-0.1193510	-8.0667530	0.3831060
C	0.5136830	-3.5064140	-1.4312620				
C	0.3338520	-3.3950870	-2.8371790				
C	0.6614610	-2.2293740	-3.5454710				
C	1.3008090	-1.1489910	-2.8601380	108			
C	1.9915190	-0.1090090	-3.5580370	molecule11_UD6			
C	2.4328490	1.0211720	-2.8496180	C	-0.1858640	1.6799400	-1.5965130
C	2.2455100	1.1614570	-1.4456880	C	0.7063630	0.5608040	-1.7549450
C	2.5736780	2.3523850	-0.7212690	C	0.1858570	-0.7842810	-1.7288960
C	2.6319350	2.3126710	0.6818170	C	-1.2304880	-1.0056100	-1.5641970
C	0.2602390	-2.2473580	4.9211280	C	-2.1284790	0.1149220	-1.4709920
C	-0.3338520	-3.4207470	5.2689830	C	-1.6057990	1.4556440	-1.4730260
S	-0.4175990	-4.5444190	3.9407600	C	-3.5454240	-0.1016100	-1.3928780
S	3.4164690	2.0939330	3.8837820	C	-4.3934290	1.0314570	-1.5209610
C	3.2153460	1.0124390	5.2349880	C	-3.8977830	2.3447770	-1.5400850
C	2.4792190	-0.0884450	4.9194550	C	-2.4943520	2.5659960	-1.3814880
C	2.8633360	3.6596180	-1.2374400	C	-1.9487020	3.8618260	-1.1188540
C	3.1666870	4.5663390	-0.2693770	C	-0.5646090	4.0632050	-1.2484050
S	3.1049690	3.8826570	1.3299320	C	0.3286890	3.0151470	-1.6067340
C	2.4503740	-0.1141810	-4.9205680	C	1.6913650	3.2297740	-1.9928470
C	3.2019190	0.9752280	-5.2390280	C	2.5415510	2.1249150	-2.1637420
S	3.3911720	2.0713060	-3.8993180	C	2.1073460	0.7830660	-1.9734740
S	-0.3997710	-4.5901780	-3.9135440	C	2.9634390	-0.3518770	-1.9971270
C	-0.3243480	-3.4783170	-5.2562050	C	2.4776300	-1.6673240	-1.9032940
C	0.2464130	-2.2906580	-4.9182200	C	1.0646550	-1.8958270	-1.8965580
C	0.1614060	-6.0568100	1.2336640	C	0.4998070	-3.1938660	-2.1227950
C	0.0002480	-6.9964690	0.2618690	C	-0.8755650	-3.3914910	-1.9144220
S	0.0611730	-6.3153080	-1.3420000	C	-1.7497910	-2.3375080	-1.5367520
				C	-3.1324930	-2.5371350	-1.2208080

C	-4.0013070	-1.4352940	-1.2089330	C	-1.7049780	-3.2061050	1.9718380
C	-2.6273580	5.0324510	-0.6349750	C	-0.3455370	-2.9967030	1.5778620
C	-1.7952100	6.0868160	-0.4154590	C	0.5199470	-4.0772460	1.2159830
S	-0.1352200	5.7127260	-0.7874000	C	1.9070350	-3.8645630	1.1729810
S	-6.1443800	1.0197500	-1.7536520	C	2.4888200	-2.5855040	1.3927410
C	-6.1674200	2.7559260	-1.9287410	C	3.8991900	-2.3618090	1.5048100
C	-4.9300450	3.3100300	-1.8017610	C	4.3935400	-1.0476480	1.4789550
C	-3.8055180	-3.7621940	-0.8975830	C	3.5481280	0.0895500	1.3758930
C	-5.1416480	-3.6036940	-0.6909460	C	4.0054440	1.4247170	1.1984860
S	-5.6538130	-1.9484110	-0.8642150	C	3.1358200	2.5255300	1.2389880
C	1.1327520	-4.3546910	-2.6894950	C	1.7635240	2.3227220	1.5820790
C	0.2788340	-5.3944480	-2.8890750	C	0.9240400	3.3951130	2.0196370
S	-1.3528000	-5.0234990	-2.4028950	C	-0.4574580	3.1781120	2.1474490
S	4.7265700	-0.3413880	-2.0544550	C	-1.0539140	1.9105040	1.8975020
C	4.7791970	-2.0730970	-1.8817800	C	-2.4683260	1.6925210	1.8930080
C	3.5398000	-2.6282090	-1.8065790	C	-2.9651090	0.3799840	1.9488090
C	2.3371620	4.4668250	-2.3348730	C	0.1550840	-5.4035300	0.8017060
C	3.6277730	4.3082000	-2.7381790	C	1.2218380	-6.1841510	0.4844460
S	4.1325020	2.6423380	-2.7237380	S	2.7391080	-5.3457980	0.6748760
H	-3.6793890	5.0669660	-0.3855870	S	-4.1490460	-2.6113420	2.6894510
H	-2.0460960	7.0637240	-0.0195370	C	-3.6291650	-4.2725670	2.7645570
H	-7.1025330	3.2548360	-2.1556650	C	-2.3374250	-4.4349320	2.3664810
H	-4.7514150	4.3652310	-1.9630070	C	-3.5182430	2.6688330	1.8399820
H	-3.3131800	-4.7162910	-0.7619860	C	-4.7638020	2.1231710	1.8884200
H	-5.8663390	-4.3583430	-0.4094440	S	-4.7278110	0.3853620	1.9928300
H	2.1648910	-4.3948520	-3.0085800	C	1.3258360	4.6823530	2.5173880
H	0.5007790	-6.3634530	-3.3207960	C	0.2881560	5.4200560	2.9980860
H	5.7380040	-2.5694780	-1.7932430	S	-1.2388260	4.5906450	2.8673210
H	3.3931370	-3.6795590	-1.6033170	S	5.6482270	1.9483240	0.8177170
H	1.8533720	5.4354360	-2.3359250	C	5.1203610	3.6013300	0.6469990
H	4.3213940	5.0728040	-3.0679310	C	3.7893270	3.7533170	0.8873340
C	1.6018480	-1.4635410	1.4670640	C	4.9471550	-3.3288630	1.6801600
C	2.1309330	-0.1264140	1.4603390	C	6.1885430	-2.7742890	1.7568690
C	1.2388330	0.9990140	1.5741620	S	6.1520120	-1.0358660	1.6321990
C	-0.1802750	0.7908900	1.7232880	H	-0.8640560	-5.7356500	0.6604960
C	-0.7111480	-0.5468550	1.7303420	H	1.2176720	-7.2023230	0.1141120
C	0.1778040	-1.6718910	1.5794840	H	-4.3152470	-5.0285050	3.1285760
C	-2.1171880	-0.7620060	1.9251590	H	-1.8325870	-5.3903850	2.4212490
C	-2.5588440	-2.1004070	2.1191790	H	-3.3576240	3.7299760	1.7008020

H	-5.7185020	2.6313620	1.8253880
H	2.3534300	5.0159280	2.5792290
H	0.3229420	6.4058900	3.4472350
H	5.8335860	4.3557260	0.3366240
H	3.2728270	4.6938170	0.7468360
H	4.7912190	-4.3937950	1.7989540
H	7.1349840	-3.2780850	1.9150920

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C	-1.8066660	-1.0957250	-1.3976630
C	-2.0031670	0.3200110	-1.5693140
C	-0.8610640	1.1973040	-1.6548070
C	0.4726370	0.6504300	-1.7325310
C	0.6486120	-0.7772130	-1.7635940
C	-0.4760510	-1.6418070	-1.5076210
C	1.9356240	-1.3391510	-2.0465890
C	2.0330640	-2.7553320	-2.1585200
C	0.9615080	-3.6085060	-1.8434240
C	-0.2783910	-3.0461140	-1.4044630
C	-1.3507950	-3.8556300	-0.9205730
C	-2.6526620	-3.3256140	-0.8718420
C	-2.9278920	-1.9626970	-1.1871430
C	-4.2500160	-1.4194770	-1.2807280
C	-4.4209240	-0.0414370	-1.5120230
C	-3.3284860	0.8587940	-1.6468490
C	-3.4653410	2.2495840	-1.9182470
C	-2.3622940	3.1206090	-1.9593480
C	-1.0501640	2.6071790	-1.7108370
C	0.0887900	3.4594590	-1.5614240
C	1.3821820	2.9147740	-1.6635080
C	1.6054030	1.5189070	-1.8437070
C	2.8890480	0.9521530	-2.1305660
C	3.0194060	-0.4442080	-2.2540960
C	-1.2860720	-5.1960510	-0.4172630
C	-2.5030660	-5.6884700	-0.0569800
S	-3.7691350	-4.5452620	-0.2990970
S	3.3874850	-3.6687430	-2.7720550

C	2.5204210	-5.1510470	-2.6429520
C	1.2629830	-4.9787240	-2.1443220
C	4.1318020	1.6209330	-2.3852390
C	5.1472430	0.7679870	-2.6966670
S	4.6501880	-0.8786700	-2.6906910
C	0.1158830	4.8614600	-1.2639670
C	1.3778600	5.3667880	-1.1802210
S	2.5803990	4.1691430	-1.4584900
S	-4.9378140	3.0980920	-2.3187180
C	-4.0827520	4.5719490	-2.5819900
C	-2.7435210	4.4434030	-2.3647890
C	-5.5098980	-2.1014330	-1.2077650
C	-6.5812460	-1.2732730	-1.3635180
S	-6.1150490	0.3658740	-1.6076110
H	-0.3664060	-5.7389860	-0.2521140
H	-2.7270660	-6.6534950	0.3798530
H	2.9841770	-6.0739380	-2.9691120
H	0.5578250	-5.7943380	-2.0653290
H	4.2829410	2.6904290	-2.3634450
H	6.1740530	1.0195840	-2.9294760
H	-0.7606770	5.4507370	-1.0410860
H	1.6741860	6.3772350	-0.9286840
H	-4.6199580	5.4517700	-2.9143620
H	-2.0507900	5.2501100	-2.5582430
H	-5.6357730	-3.1669810	-1.0755010
H	-7.6308380	-1.5401110	-1.3595300
C	-0.3584640	-0.7650830	1.8071000
C	-0.7115350	0.6266210	1.7195920
C	0.3288310	1.6215300	1.6587780
C	1.7097800	1.2241810	1.5361090
C	2.0419750	-0.1715610	1.4204490
C	1.0154930	-1.1630820	1.6208810
C	3.3981550	-0.5758860	1.1891630
C	3.6612770	-1.9680820	1.0516240
C	2.6656120	-2.9430390	1.2407580
C	1.3601830	-2.5429910	1.6594350
C	0.4106750	-3.4726320	2.1910720
C	-0.9200160	-3.0645080	2.3923520
C	-1.3625840	-1.7437040	2.0898460

C	-2.7360040	-1.3432680	2.1166780	H	-3.9067210	-3.2323020	2.3581620
C	-3.0667230	0.0142250	1.9475220	H	-6.0774610	-1.8152710	2.3134520
C	-2.0854380	1.0263490	1.7722150				
C	-2.3789680	2.4113840	1.6292760				
C	-1.3731140	3.3933140	1.6030160				
C	-0.0056610	3.0022010	1.7428520	108			
C	1.0375050	3.9437860	2.0070960	molecule11_S2			
C	2.3790490	3.5427430	1.8798970	C	-1.4310180	0.0517850	1.7588080
C	2.7434610	2.2115630	1.5264060	C	-0.7600520	-1.2162170	1.8278680
C	4.0830230	1.8112090	1.2187580	C	0.6674860	-1.2713880	1.6648530
C	4.3832730	0.4438260	1.0725990	C	1.4318240	-0.0525500	1.7586840
C	0.6534150	-4.7920050	2.7011570	C	0.7608770	1.2154620	1.8278970
C	-0.4529150	-5.3596750	3.2602290	C	-0.6666710	1.2706360	1.6650410
S	-1.8286410	-4.3265830	3.1878230	C	1.5097420	2.4205020	2.0262640
S	5.1718420	-2.7176680	0.6008740	C	0.8099820	3.6512350	1.9256590
C	4.4561660	-4.2857600	0.5887850	C	-0.5707530	3.7282000	1.6568400
C	3.1380150	-4.2602510	0.9329990	C	-1.3253420	2.5211240	1.4894360
C	5.2386370	2.6342640	1.0106370	C	-2.7280280	2.5052290	1.1874460
C	6.3696890	1.9162560	0.7578880	C	-3.4671010	1.3309120	1.4282920
S	6.0821130	0.2187080	0.7471840	C	-2.8562020	0.1070950	1.8137070
C	0.9186660	5.2842640	2.5058800	C	-3.5698460	-1.0602220	2.2421330
C	2.1236510	5.8827400	2.7219530	C	-2.8865480	-2.2819560	2.3602370
S	3.4485810	4.8477760	2.3375450	C	-1.5089050	-2.4212730	2.0261510
S	-3.9523980	3.1350140	1.4280220	C	-0.8091520	-3.6519990	1.9253550
C	-3.2703700	4.7066060	1.2548430	C	0.5715340	-3.7289600	1.6563110
C	-1.9116260	4.7009350	1.3694850	C	1.3261450	-2.5218640	1.4890040
C	-3.9057840	-2.1551490	2.2772730	C	2.7287850	-2.5059220	1.1868330
C	-5.0646760	-1.4396510	2.2438360	C	3.4678730	-1.3316100	1.4277180
S	-4.7925020	0.2450260	2.0196180	C	2.8570140	-0.1078520	1.8133410
H	1.6231250	-5.2696950	2.7270140	C	3.5707150	1.0594120	2.2418320
H	-0.5306080	-6.3274550	3.7404480	C	2.8874680	2.2811550	2.3600450
H	5.0471320	-5.1409880	0.2859180	C	-3.5404590	3.5444440	0.6222820
H	2.5109080	-5.1398060	0.8947560	C	-4.8485630	3.1955570	0.4839880
H	5.2359870	3.7157700	1.0064360	S	-5.1668170	1.5712560	1.0191100
H	7.3648660	2.2947650	0.5599090	S	1.5009210	5.2633910	2.1358890
H	-0.0176720	5.7583850	2.7656930	C	-0.0615700	6.0013950	1.9057610
H	2.3117300	6.8719750	3.1210750	C	-1.0418610	5.0873110	1.6760870
H	-3.9166880	5.5501630	1.0477990	C	4.9347230	1.1559320	2.6813280
H	-1.3153180	5.5902070	1.2258160	C	5.2750270	2.4001050	3.1167220
				S	3.9481420	3.5285970	3.0189670

C	3.5411890	-3.5449910	0.6213490
C	4.8492410	-3.1959950	0.4828040
S	5.1675050	-1.5717430	1.0180930
S	-1.5001810	-5.2641750	2.1351350
C	0.0622580	-6.0021900	1.9047400
C	1.0425640	-5.0880930	1.6751540
C	-4.9338140	-1.1568090	2.6817500
C	-5.2740770	-2.4010340	3.1170040
S	-3.9472000	-3.5295040	3.0190040
H	-3.1564100	4.4770890	0.2336750
H	-5.6471330	3.7778590	0.0411980
H	-0.1576680	7.0785890	1.9734180
H	-2.0759610	5.3825630	1.5752810
H	5.6267090	0.3236070	2.7217000
H	6.2236050	2.7271960	3.5262990
H	3.1572130	-4.4776580	0.2327320
H	5.6477520	-3.7782140	0.0398050
H	0.1583470	-7.0793960	1.9722080
H	2.0766380	-5.3833870	1.5742000
H	-5.6257890	-0.3244880	2.7223140
H	-6.2225970	-2.7281760	3.5266760
C	1.4310240	0.0525300	-1.7589330
C	0.7600590	-1.2154810	-1.8280760
C	-0.6674730	-1.2706430	-1.6650580
C	-1.4317960	-0.0517800	-1.7587260
C	-0.7608520	1.2162330	-1.8277640
C	0.6667120	1.2713750	-1.6650030
C	-1.5097330	2.4212880	-2.0259230
C	-0.8099940	3.6520080	-1.9250080
C	0.5707720	3.7289310	-1.6563560
C	1.3254290	2.5218500	-1.4892420
C	2.7281070	2.5058820	-1.1872780
C	3.4671490	1.3315560	-1.4282700
C	2.8562120	0.1078090	-1.8138130
C	3.5698320	-1.0594600	-2.2424510
C	2.8865490	-2.2811930	-2.3605610
C	1.5088990	-2.4205310	-2.0264620
C	0.8091140	-3.6512530	-1.9257590
C	-0.5715760	-3.7281800	-1.6567370

C	-1.3261670	-2.5211210	-1.4892930
C	-2.7287660	-2.5051620	-1.1869750
C	-3.4678540	-1.3308440	-1.4277720
C	-2.8569930	-0.1070640	-1.8133390
C	-3.5706790	1.0602150	-2.2418330
C	-2.8874400	2.2819920	-2.3597840
C	3.5405810	3.5449420	-0.6218780
C	4.8486510	3.1959430	-0.4835060
S	5.1668240	1.5717140	-1.0188690
S	-1.5010220	5.2642110	-2.1346160
C	0.0614840	6.0022020	-1.9044410
C	1.0418390	5.0880630	-1.6752700
C	-4.9345720	1.1567110	-2.6816920
C	-5.2748060	2.4009080	-3.1171120
S	-3.9480130	3.5294500	-3.0188030
C	-3.5410830	-3.5442730	-0.6214130
C	-4.8491180	-3.1953020	-0.4827640
S	-5.1674720	-1.5710640	-1.0180360
S	1.5000230	-5.2634490	-2.1357590
C	-0.0624730	-6.0014110	-1.9054570
C	-1.0427140	-5.0872840	-1.6757680
C	4.9337310	-1.1559750	-2.6822990
C	5.2739310	-2.4001390	-3.1177890
S	3.9470940	-3.5286490	-3.0196580
H	3.1565960	4.4775480	-0.2331280
H	5.6472180	3.7781500	-0.0405880
H	0.1575230	7.0794220	-1.9717620
H	2.0759690	5.3832550	-1.5746090
H	-5.6264750	0.3243350	-2.7224080
H	-6.2233120	2.7280350	-3.5268240
H	-3.1569650	-4.4769250	-0.2328790
H	-5.6475970	-3.7775100	-0.0396900
H	-0.1585930	-7.0786090	-1.9730350
H	-2.0768320	-5.3824290	-1.5748530
H	5.6256890	-0.3236450	-2.7229160
H	6.2223890	-2.7272220	-3.5276510

molecule12_conf1			
C	2.2842720	3.6106460	0.9577310
C	2.8707570	2.3337260	0.7320700
C	2.1026930	1.1671730	1.0122090
C	0.7697600	1.2919400	1.5028610
C	0.2063970	2.5832180	1.7142040
C	0.9983010	3.7302060	1.4307240
C	2.6646410	-0.1253850	0.7985350
C	-0.0004100	0.1252100	1.7797870
C	0.5653530	-1.1670870	1.5759830
C	1.8993340	-1.2926000	1.0884710
C	-0.2029850	-2.3328600	1.8584000
C	-1.5364860	-2.1766280	2.3291710
C	-2.0835090	-0.9306850	2.5227530
C	-1.3357180	0.2505600	2.2605580
C	-1.8747790	1.5522110	2.4547810
C	-1.1300740	2.6773070	2.1914380
H	-1.5624100	3.6655370	2.3320610
H	-2.9008250	1.6428200	2.8025690
H	2.8741720	4.4992560	0.7408120
H	0.5608330	4.7139500	1.5874580
H	-2.1260970	-3.0695700	2.5243500
H	-3.1096750	-0.8299010	2.8675430
C	4.1923900	2.1792120	0.2280230
C	4.7318990	0.9319320	0.0119280
C	3.9915850	-0.2505540	0.2934220
H	4.7737370	3.0732490	0.0101580
H	5.7440780	0.8319090	-0.3757830
C	4.5274790	-1.5538650	0.0918510
C	3.7925780	-2.6797660	0.3833760
C	2.4650490	-2.5844100	0.8870170
H	5.5405650	-1.6448210	-0.2956240
H	4.2193180	-3.6686200	0.2263860
C	0.3896650	-3.6092020	1.6527190
H	-0.2031980	-4.4962230	1.8649460
C	1.6776460	-3.7310280	1.1854230
H	2.1137980	-4.7158340	1.0289130
C	-0.3921840	3.6099380	-1.6522070
C	0.2013480	2.3340320	-1.8580880

C	-0.5661880	1.1676820	-1.5758700
C	-1.9002490	1.2921820	-1.0883460
C	-2.4668000	2.5835610	-0.8865460
C	-1.6802230	3.7307910	-1.1848270
C	0.0004880	-0.1241920	-1.7797940
C	-2.6647240	0.1243820	-0.7985460
C	-2.1019330	-1.1677620	-1.0125450
C	-0.7689010	-1.2915150	-1.5031230
C	-2.8692360	-2.3348970	-0.7327310
C	-4.1909560	-2.1813740	-0.2285770
C	-4.7312340	-0.9345040	-0.0120740
C	-3.9917090	0.2485470	-0.2932990
C	-4.5284020	1.5514540	-0.0912720
C	-3.7942820	2.6779190	-0.3826240
H	-4.2216350	3.6664520	-0.2252670
H	-5.5414870	1.6416560	0.2963820
H	0.2000250	4.4974110	-1.8643860
H	-2.1170650	4.7152630	-1.0281570
H	-4.7717230	-3.0758500	-0.0109620
H	-5.7434500	-0.8352460	0.3757450
C	1.5350430	2.1787880	-2.3286420
C	2.0829660	0.9332520	-2.5223090
C	1.3359320	-0.2485570	-2.2604240
H	2.1240780	3.0721730	-2.5235550
H	3.1092940	0.8332190	-2.8668380
C	1.8759230	-1.5498090	-2.4547740
C	1.1319190	-2.6754590	-2.1917830
C	-0.2046810	-2.5823750	-1.7147350
H	2.9021020	-1.6396760	-2.8023580
H	1.5649580	-3.6633700	-2.3325100
C	-2.2819620	-3.6113830	-0.9588000
H	-2.8712500	-4.5004470	-0.7420880
C	-0.9958660	-3.7299660	-1.4316940
H	-0.5577170	-4.7133760	-1.5886150

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molecule12_conf2			
C	-1.1995690	3.5523360	1.7318870

C	0.0384710	2.8501910	1.7266980
C	0.0191170	1.4267600	1.7161360
C	-1.2255210	0.7304780	1.7167590
C	-2.4487280	1.4587830	1.7282330
C	-2.3994080	2.8811850	1.7331970
C	1.2446700	0.6970510	1.7168240
C	-1.2449470	-0.6955850	1.7176580
C	-0.0193940	-1.4252820	1.7179150
C	1.2252470	-0.7290150	1.7177610
C	-0.0387690	-2.8487120	1.7290220
C	-1.2950850	-3.5172700	1.7346020
C	-2.4763790	-2.8137900	1.7354510
C	-2.4870750	-1.3906490	1.7294320
C	-3.6943840	-0.6370390	1.7349370
C	-3.6757510	0.7377060	1.7343610
H	-4.6078260	1.2992200	1.7338910
H	-4.6411820	-1.1734970	1.7352330
H	-1.1792370	4.6403410	1.7311750
H	-3.3371430	3.4333430	1.7342140
H	-1.3039210	-4.6054410	1.7346680
H	-3.4288260	-3.3401100	1.7365590
C	1.2947800	3.5187490	1.7319630
C	2.4760770	2.8152690	1.7331950
C	2.4867910	1.3921240	1.7282410
H	1.3036320	4.6069210	1.7315450
H	3.4285220	3.3415940	1.7340710
C	3.6940990	0.6385190	1.7346470
C	3.6754720	-0.7362270	1.7352750
C	2.4484500	-1.4573120	1.7297810
H	4.6408980	1.1749780	1.7346180
H	4.6075470	-1.2977400	1.7353200
C	1.1992710	-3.5508590	1.7345900
H	1.1789400	-4.6388640	1.7343960
C	2.3991160	-2.8797110	1.7356560
H	3.3368460	-3.4318770	1.7370290
C	0.7376400	3.6747630	-1.7351110
C	1.4585410	2.4476450	-1.7289170
C	0.7300510	1.2245540	-1.7169590
C	-0.6960100	1.2441700	-1.7170990

C	-1.3908950	2.4863920	-1.7291800
C	-0.6371050	3.6935860	-1.7353180
C	1.4261500	-0.0201850	-1.7169000
C	-1.4258750	0.0187150	-1.7171470
C	-0.7297770	-1.2260230	-1.7174010
C	0.6962860	-1.2456420	-1.7173360
C	-1.4582470	-2.4491260	-1.7289680
C	-2.8806430	-2.3995970	-1.7342440
C	-3.5516230	-1.1996590	-1.7331240
C	-2.8493040	0.0382850	-1.7279240
C	-3.5176850	1.2946960	-1.7336280
C	-2.8140390	2.4758910	-1.7349630
H	-3.3402270	3.4284110	-1.7362820
H	-4.6058560	1.3036850	-1.7335070
H	1.2992670	4.6067700	-1.7352620
H	-1.1734270	4.6404620	-1.7358280
H	-3.4329410	-3.3372510	-1.7352820
H	-4.6396250	-1.1791750	-1.7326150
C	2.8809320	2.3981150	-1.7343720
C	3.5519080	1.1981800	-1.7329490
C	2.8495820	-0.0397560	-1.7275240
H	3.4332270	3.3357690	-1.7357460
H	4.6399100	1.1776910	-1.7324610
C	3.5179690	-1.2961630	-1.7329160
C	2.8143310	-2.4773620	-1.7340950
C	1.3911860	-2.4878640	-1.7287640
H	4.6061400	-1.3051460	-1.7325930
H	3.3405240	-3.4298800	-1.7349980
C	-0.7373350	-3.6762490	-1.7346390
H	-1.2989750	-4.6082470	-1.7342730
C	0.6374100	-3.6950680	-1.7346200
H	1.1737370	-4.6419410	-1.7346030

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molecule13_conf1

C	-0.2301630	3.7400610	1.6585040
C	-1.5650990	3.4253750	1.6678260
C	-2.0579270	2.0649170	1.6578320

C	-3.4303160	1.6782240	1.6973910
C	-3.8022350	0.3394740	1.7010340
C	-2.8267500	-0.7013770	1.6685430
C	-3.1100600	-2.1201310	1.6795920
C	-2.1320280	-3.0811160	1.6657440
N	-0.7732480	-2.7728110	1.6379330
C	0.2301630	-3.7400610	1.6585040
C	1.5650990	-3.4253750	1.6678260
C	2.0579270	-2.0649170	1.6578320
C	3.4303160	-1.6782240	1.6973910
C	3.8022350	-0.3394740	1.7010340
C	2.8267500	0.7013770	1.6685430
C	3.1100600	2.1201310	1.6795920
C	2.1320280	3.0811160	1.6657440
N	0.7732480	2.7728110	1.6379330
B	0.3844080	1.3767520	1.5977660
C	-1.0957350	1.0387360	1.6136410
C	-1.4739060	-0.3209660	1.6216570
B	-0.3844080	-1.3767520	1.5977660
C	1.0957350	-1.0387360	1.6136410
C	1.4739060	0.3209660	1.6216570
H	0.1070740	4.7737290	1.6698290
H	-2.2727260	4.2508720	1.6879480
H	-4.2032090	2.4452940	1.7224130
H	-4.8600480	0.0812330	1.7288870
H	-4.1429050	-2.4594040	1.6960370
H	-2.3798360	-4.1397320	1.6723380
H	-0.1070740	-4.7737290	1.6698290
H	2.2727260	-4.2508720	1.6879480
H	4.2032090	-2.4452940	1.7224130
H	4.8600480	-0.0812330	1.7288870
H	4.1429050	2.4594040	1.6960370
H	2.3798360	4.1397320	1.6723380
C	-2.1320280	3.0811160	-1.6657440
C	-3.1100600	2.1201310	-1.6795920
C	-2.8267500	0.7013770	-1.6685430
C	-3.8022350	-0.3394740	-1.7010340
C	-3.4303160	-1.6782240	-1.6973910
C	-2.0579270	-2.0649170	-1.6578320

C	-1.5650990	-3.4253750	-1.6678260
C	-0.2301630	-3.7400610	-1.6585040
N	0.7732480	-2.7728110	-1.6379330
C	2.1320280	-3.0811160	-1.6657440
C	3.1100600	-2.1201310	-1.6795920
C	2.8267500	-0.7013770	-1.6685430
C	3.8022350	0.3394740	-1.7010340
C	3.4303160	1.6782240	-1.6973910
C	2.0579270	2.0649170	-1.6578320
C	1.5650990	3.4253750	-1.6678260
C	0.2301630	3.7400610	-1.6585040
N	-0.7732480	2.7728110	-1.6379330
B	-0.3844080	1.3767520	-1.5977660
C	-1.4739060	0.3209660	-1.6216570
C	-1.0957350	-1.0387360	-1.6136410
B	0.3844080	-1.3767520	-1.5977660
C	1.4739060	-0.3209660	-1.6216570
C	1.0957350	1.0387360	-1.6136410
H	-2.3798360	4.1397320	-1.6723380
H	-4.1429050	2.4594040	-1.6960370
H	-4.8600480	-0.0812330	-1.7288870
H	-4.2032090	-2.4452940	-1.7224130
H	-2.2727260	-4.2508720	-1.6879480
H	0.1070740	-4.7737290	-1.6698290
H	2.3798360	-4.1397320	-1.6723380
H	4.1429050	-2.4594040	-1.6960370
H	4.8600480	0.0812330	-1.7288870
H	4.2032090	2.4452940	-1.7224130
H	2.2727260	4.2508720	-1.6879480
H	-0.1070740	4.7737290	-1.6698290

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molecule13_conf2

C	-1.2259940	3.5401360	1.6574230
C	-2.4269720	2.8789400	1.6734620
C	-2.5353940	1.4368140	1.6557850
C	-3.7538340	0.6946810	1.7006660
C	-3.7538340	-0.6946810	1.7006660
C	-2.5353940	-1.4368140	1.6557850

C	-2.4269720	-2.8789400	1.6734620
C	-1.2259940	-3.5401360	1.6574230
N	0.0000000	-2.8779370	1.6248680
C	1.2259940	-3.5401360	1.6574230
C	2.4269720	-2.8789400	1.6734620
C	2.5353940	-1.4368140	1.6557850
C	3.7538340	-0.6946810	1.7006660
C	3.7538340	0.6946810	1.7006660
C	2.5353940	1.4368140	1.6557850
C	2.4269720	2.8789400	1.6734620
C	1.2259940	3.5401360	1.6574230
N	0.0000000	2.8779370	1.6248680
B	0.0000000	1.4299260	1.5760830
C	-1.3347390	0.7062350	1.5967660
C	-1.3347390	-0.7062350	1.5967660
B	0.0000000	-1.4299260	1.5760830
C	1.3347390	-0.7062350	1.5967660
C	1.3347390	0.7062350	1.5967660
H	-1.1792020	4.6263100	1.6693000
H	-3.3301510	3.4837770	1.6983260
H	-4.7035210	1.2269100	1.7391960
H	-4.7035210	-1.2269100	1.7391960
H	-3.3301510	-3.4837770	1.6983260
H	-1.1792020	-4.6263100	1.6693000
H	1.1792020	-4.6263100	1.6693000
H	3.3301510	-3.4837770	1.6983260
H	4.7035210	-1.2269100	1.7391960
H	4.7035210	1.2269100	1.7391960
H	3.3301510	3.4837770	1.6983260
H	1.1792020	4.6263100	1.6693000
C	3.5401360	1.2259940	-1.6574230
C	2.8789400	2.4269720	-1.6734620
C	1.4368140	2.5353940	-1.6557850
C	0.6946810	3.7538340	-1.7006660
C	-0.6946810	3.7538340	-1.7006660
C	-1.4368140	2.5353940	-1.6557850
C	-2.8789400	2.4269720	-1.6734620
C	-3.5401360	1.2259940	-1.6574230
N	-2.8779370	0.0000000	-1.6248680

C	-3.5401360	-1.2259940	-1.6574230
C	-2.8789400	-2.4269720	-1.6734620
C	-1.4368140	-2.5353940	-1.6557850
C	-0.6946810	-3.7538340	-1.7006660
C	0.6946810	-3.7538340	-1.7006660
C	1.4368140	-2.5353940	-1.6557850
C	2.8789400	-2.4269720	-1.6734620
C	3.5401360	-1.2259940	-1.6574230
N	2.8779370	0.0000000	-1.6248680
B	1.4299260	0.0000000	-1.5760830
C	0.7062350	1.3347390	-1.5967660
C	-0.7062350	1.3347390	-1.5967660
B	-1.4299260	0.0000000	-1.5760830
C	-0.7062350	-1.3347390	-1.5967660
C	0.7062350	-1.3347390	-1.5967660
H	4.6263100	1.1792020	-1.6693000
H	3.4837770	3.3301510	-1.6983260
H	1.2269100	4.7035210	-1.7391960
H	-1.2269100	4.7035210	-1.7391960
H	-3.4837770	3.3301510	-1.6983260
H	-4.6263100	1.1792020	-1.6693000
H	-4.6263100	-1.1792020	-1.6693000
H	-3.4837770	-3.3301510	-1.6983260
H	-1.2269100	-4.7035210	-1.7391960
H	1.2269100	-4.7035210	-1.7391960
H	3.4837770	-3.3301510	-1.6983260
H	4.6263100	-1.1792020	-1.6693000

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molecule13_conf3

C	1.9826250	0.2219410	3.8514030
C	2.3372630	-0.9384430	3.2110140
C	2.2673470	-1.1043770	1.7758420
C	2.6396340	-2.2778180	1.0561650
C	2.5469310	-2.3355120	-0.3286440
C	2.0751520	-1.2227240	-1.0859010
C	1.9426600	-1.1820100	-2.5259040
C	1.4944920	-0.0792740	-3.2058510

N	1.1275910	1.1045260	-2.5673720	C	-2.2673470	1.1043770	-1.7758420
C	0.6978590	2.2394910	-3.2489730	C	-2.6396340	2.2778180	-1.0561650
C	0.3565620	3.4056620	-2.6115590	C	-2.5469310	2.3355120	0.3286440
C	0.4094300	3.5658530	-1.1750080	C	-2.0751520	1.2227240	1.0859010
C	0.0708340	4.7528000	-0.4593210	C	-1.9426600	1.1820100	2.5259040
C	0.1559840	4.8097720	0.9277250	C	-1.4944920	0.0792740	3.2058510
C	0.5902730	3.6839430	1.6895630	N	-1.1275910	-1.1045260	2.5673720
C	0.7245080	3.6420930	3.1299950	B	-1.1967750	-1.1554280	1.1196680
C	1.1671280	2.5351640	3.8100390	C	-0.8270100	-2.4519300	0.4230550
N	1.5212700	1.3486170	3.1703650	C	-0.9186210	-2.5108990	-0.9828580
B	1.3936810	1.2775020	1.7282530	B	-1.3936810	-1.2775020	-1.7282530
C	1.7897700	-0.0097610	1.0294810	C	-1.7897700	0.0097610	-1.0294810
C	1.6992560	-0.0676220	-0.3773200	C	-1.6992560	0.0676220	0.3773200
B	1.1967750	1.1554280	-1.1196680	H	-0.6411260	-2.1511800	4.3309330
C	0.8270100	2.4519300	-0.4230550	H	-0.0325690	-4.2372880	3.2330740
C	0.9186210	2.5108990	0.9828580	H	0.2616230	-5.6336090	1.0077100
H	2.0517880	0.3145000	4.9329910	H	0.1091430	-5.7347120	-1.4390390
H	2.6836880	-1.7637490	3.8281510	H	-0.4764400	-4.5229820	-3.7178230
H	2.9924960	-3.1516150	1.6015020	H	-1.2645380	-2.5396730	-4.8934090
H	2.8227340	-3.2547600	-0.8417920	H	-2.0517880	-0.3145000	-4.9329910
H	2.1903030	-2.0628360	-3.1116540	H	-2.6836880	1.7637490	-3.8281510
H	1.3973490	-0.0849610	-4.2886870	H	-2.9924960	3.1516150	-1.6015020
H	0.6411260	2.1511800	-4.3309330	H	-2.8227340	3.2547600	0.8417920
H	0.0325690	4.2372880	-3.2330740	H	-2.1903030	2.0628360	3.1116540
H	-0.2616230	5.6336090	-1.0077100	H	-1.3973490	0.0849610	4.2886870
H	-0.1091430	5.7347120	1.4390390				
H	0.4764400	4.5229820	3.7178230				
H	1.2645380	2.5396730	4.8934090	72			
C	-0.6978590	-2.2394910	3.2489730	molecule13_conf4			
C	-0.3565620	-3.4056620	2.6115590	C	-4.7709440	0.4530520	-0.1114410
C	-0.4094300	-3.5658530	1.1750080	C	-4.4013740	1.7667480	-0.2556080
C	-0.0708340	-4.7528000	0.4593210	C	-3.0894290	2.1745360	-0.7090810
C	-0.1559840	-4.8097720	-0.9277250	C	-2.6537900	3.5217960	-0.8868590
C	-0.5902730	-3.6839430	-1.6895630	C	-1.3677340	3.8115380	-1.3278550
C	-0.7245080	-3.6420930	-3.1299950	C	-0.4319140	2.7753140	-1.6211880
C	-1.1671280	-2.5351640	-3.8100390	C	0.9246680	2.9706140	-2.0803740
N	-1.5212700	-1.3486170	-3.1703650	C	1.7810870	1.9356010	-2.3550440
C	-1.9826250	-0.2219410	-3.8514030	N	1.4163490	0.5983070	-2.2136650
C	-2.3372630	0.9384430	-3.2110140	C	2.2723700	-0.4623250	-2.5100650

C	1.8938350	-1.7744180	-2.3928050
C	0.5785580	-2.1821620	-1.9522780
C	0.1263740	-3.5287760	-1.8251670
C	-1.1610520	-3.8210610	-1.3901020
C	-2.0813890	-2.7855360	-1.0507870
C	-3.4389040	-2.9826750	-0.5901780
C	-4.2855730	-1.9477970	-0.2831110
N	-3.9102010	-0.6080010	-0.3937570
B	-2.5648010	-0.3038560	-0.8421740
C	-2.1662410	1.1515400	-0.9968560
C	-0.8609750	1.4463750	-1.4429790
B	0.0807120	0.2953710	-1.7409950
C	-0.3284250	-1.1598000	-1.6148400
C	-1.6349010	-1.4558600	-1.1719760
H	-5.7687060	0.1801120	0.2251590
H	-5.1448290	2.5232010	-0.0144680
H	-3.3397440	4.3408950	-0.6731150
H	-1.0685510	4.8521240	-1.4465860
H	1.3070730	3.9802570	-2.2075560
H	2.8011620	2.1186880	-2.6818740
H	3.2747070	-0.1905350	-2.8303860
H	2.6365920	-2.5305930	-2.6326730
H	0.8041570	-4.3462040	-2.0659690
H	-1.4687240	-4.8625330	-1.3028150
H	-3.8244010	-3.9931470	-0.4746230
H	-5.3024770	-2.1308480	0.0570670
C	-2.2708060	0.4704840	2.5115760
C	-1.8896470	1.7817040	2.3930450
C	-0.5741990	2.1863630	1.9502990
C	-0.1193990	3.5319600	1.8217800
C	1.1683340	3.8213080	1.3856940
C	2.0864640	2.7836550	1.0468750
C	3.4443610	2.9776270	0.5859950
C	4.2890790	1.9407290	0.2802880
N	3.9110950	0.6017910	0.3922820
C	4.7704460	-0.4611840	0.1130190
C	4.3984630	-1.7739960	0.2589970
C	3.0853460	-2.1787390	0.7118340
C	2.6474630	-3.5249290	0.8921430

C	1.3607260	-3.8117190	1.3330670
C	0.4263880	-2.7734370	1.6237860
C	-0.9304090	-2.9655800	2.0837380
C	-1.7849510	-1.9285790	2.3567540
N	-1.4177540	-0.5921020	2.2136910
B	-0.0819020	-0.2923320	1.7394700
C	0.3302680	1.1619180	1.6124600
C	1.6371970	1.4549820	1.1688510
B	2.5648530	0.3007480	0.8404150
C	2.1635510	-1.1537030	0.9968270
C	0.8575470	-1.4455400	1.4427900
H	-3.2729840	0.2010400	2.8343460
H	-2.6300750	2.5396020	2.6347000
H	-0.7954760	4.3509300	2.0621380
H	1.4778630	4.8621180	1.2970120
H	3.8319050	3.9871810	0.4692560
H	5.3065180	2.1214500	-0.0595480
H	5.7691810	-0.1905600	-0.2225600
H	5.1411680	-2.5321380	0.0208780
H	3.3321590	-4.3455400	0.6801840
H	1.0598840	-4.8515830	1.4538900
H	-1.3147510	-3.9742910	2.2124770
H	-2.8052190	-2.1094040	2.6842940

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C	-2.2423870	3.1303730	1.6513900
C	-3.1402860	2.1094340	1.6586700
C	-2.7262490	0.7358040	1.6492140
C	-3.7081560	-0.2830180	1.6621840
C	-3.3539840	-1.6056530	1.6622600
C	-1.9940660	-1.9961930	1.6502370
C	-1.6669310	-3.3931970	1.6564190
C	-0.3791400	-3.8287220	1.6491050
B	0.7511130	-2.8070190	1.6348840
C	2.2407470	-3.1276320	1.6554740
C	3.1386500	-2.1066880	1.6623570
C	2.7246320	-0.7330640	1.6511320

C	3.7065370	0.2857640	1.6637260
C	3.3523690	1.6084000	1.6625680
C	1.9924590	1.9989450	1.6495890
C	1.6653330	3.3959600	1.6545000
C	0.3775550	3.8315060	1.6462140
B	-0.7527230	2.8098260	1.6321910
N	-0.3700490	1.3791780	1.6204820
C	-1.3510260	0.3753510	1.6265560
C	-0.9836900	-0.9971800	1.6288700
N	0.3684420	-1.3764220	1.6219020
C	1.3494270	-0.3726020	1.6274860
C	0.9820870	0.9999270	1.6284930
H	-2.6093710	4.1563490	1.6545420
H	-4.2170520	2.2849990	1.6687830
H	-4.7535230	0.0152400	1.6683430
H	-4.1097620	-2.3868050	1.6676350
H	-2.5115200	-4.0833690	1.6592730
H	-0.1846360	-4.9006600	1.6459810
H	2.6077230	-4.1535950	1.6608030
H	4.2154100	-2.2822270	1.6735610
H	4.7519000	-0.0124840	1.6706840
H	4.1081420	2.3895580	1.6676870
H	2.5099260	4.0861330	1.6572010
H	0.1830470	4.9034440	1.6418870
C	-0.3722380	3.8291440	-1.6489630
C	-1.6606500	3.3954490	-1.6568000
C	-1.9897500	1.9989320	-1.6511150
C	-3.3501950	1.6102380	-1.6637430
C	-3.7061520	0.2880870	-1.6639990
C	-2.7256420	-0.7320840	-1.6506370
C	-3.1415680	-2.1051480	-1.6605950
C	-2.2450740	-3.1273240	-1.6526920
B	-0.7549770	-2.8086710	-1.6324280
C	0.3738750	-3.8319380	-1.6457160
C	1.6622770	-3.3982330	-1.6534300
C	1.9913450	-2.0016830	-1.6485030
C	3.3518040	-1.6129990	-1.6608190
C	3.7077630	-0.2908490	-1.6619060
C	2.7272470	0.7293350	-1.6498730

C	3.1431890	2.1023800	-1.6609370
C	2.2466960	3.1245670	-1.6545220
B	0.7566080	2.8059370	-1.6346160
N	0.3719300	1.3758960	-1.6218750
C	-0.9807410	0.9985340	-1.6294920
C	-1.3499440	-0.3734700	-1.6273590
N	-0.3703430	-1.3786330	-1.6208050
C	0.9823440	-1.0012730	-1.6280580
C	1.3515320	0.3707450	-1.6269510
H	-0.1762010	4.9008110	-1.6457620
H	-2.5042040	4.0868760	-1.6597360
H	-4.1048900	2.3924350	-1.6693270
H	-4.7519310	-0.0086910	-1.6706350
H	-4.2185780	-2.2791750	-1.6716310
H	-2.6134450	-4.1527890	-1.6570470
H	0.1778200	-4.9035990	-1.6416040
H	2.5058680	-4.0896240	-1.6556440
H	4.1064970	-2.3952060	-1.6654700
H	4.7535470	0.0059230	-1.6683860
H	4.2202050	2.2763890	-1.6715590
H	2.6150750	4.1500250	-1.6596550

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C	-1.3568530	3.6031780	1.6485080
C	-2.4876470	2.8484740	1.6566090
C	-2.4416650	1.4146280	1.6516880
C	-3.6539740	0.6848770	1.6578730
C	-3.6541110	-0.6842600	1.6583030
C	-2.4418430	-1.4139190	1.6526040
C	-2.4878910	-2.8479440	1.6580250
C	-1.3570480	-3.6027120	1.6493000
B	-0.0001650	-2.9088660	1.6328340
C	1.3568530	-3.6031780	1.6485080
C	2.4876470	-2.8484740	1.6566090
C	2.4416650	-1.4146280	1.6516880
C	3.6539740	-0.6848770	1.6578730
C	3.6541110	0.6842600	1.6583030

C	2.4418430	1.4139190	1.6526040
C	2.4878910	2.8479440	1.6580250
C	1.3570480	3.6027120	1.6493000
B	0.0001650	2.9088660	1.6328340
N	-0.0000210	1.4267960	1.6264310
C	-1.2072990	0.7109750	1.6348590
C	-1.2072990	-0.7106150	1.6351140
N	0.0000210	-1.4267960	1.6264310
C	1.2072990	-0.7109750	1.6348590
C	1.2072990	0.7106150	1.6351140
H	-1.4470070	4.6891240	1.6496040
H	-3.4825700	3.2958610	1.6629520
H	-4.5864400	1.2432240	1.6539000
H	-4.5866010	-1.2426100	1.6541190
H	-3.4827070	-3.2954970	1.6643210
H	-1.4476200	-4.6886840	1.6515930
H	1.4470070	-4.6891240	1.6496040
H	3.4825700	-3.2958610	1.6629520
H	4.5864400	-1.2432240	1.6539000
H	4.5866010	1.2426100	1.6541190
H	3.4827070	3.2954970	1.6643210
H	1.4476200	4.6886840	1.6515930
C	3.6029760	1.3569980	-1.6495300
C	2.8483440	2.4878270	-1.6585140
C	1.4144560	2.4415860	-1.6527940
C	0.6846050	3.6538420	-1.6586500
C	-0.6845410	3.6540470	-1.6584870
C	-1.4142760	2.4418340	-1.6522270
C	-2.8483090	2.4877500	-1.6556570
C	-3.6029310	1.3568350	-1.6468750
B	-2.9088620	0.0000560	-1.6324870
C	-3.6029760	-1.3569980	-1.6495300
C	-2.8483440	-2.4878270	-1.6585140
C	-1.4144560	-2.4415860	-1.6527940
C	-0.6846050	-3.6538420	-1.6586500
C	0.6845410	-3.6540470	-1.6584870
C	1.4142760	-2.4418340	-1.6522270
C	2.8483090	-2.4877500	-1.6556570
C	3.6029310	-1.3568350	-1.6468750

B	2.9088620	-0.0000560	-1.6324870
N	1.4268420	-0.0000620	-1.6267960
C	0.7108760	1.2072800	-1.6356650
C	-0.7107010	1.2074080	-1.6349310
N	-1.4268420	0.0000620	-1.6267960
C	-0.7108760	-1.2072800	-1.6356650
C	0.7107010	-1.2074080	-1.6349310
H	4.6889470	1.4472200	-1.6514760
H	3.2957850	3.4827360	-1.6649100
H	1.2429710	4.5863250	-1.6544670
H	-1.2428380	4.5865400	-1.6542180
H	-3.2957860	3.4825980	-1.6606120
H	-4.6888910	1.4472760	-1.6472860
H	-4.6889470	-1.4472200	-1.6514760
H	-3.2957850	-3.4827360	-1.6649100
H	-1.2429710	-4.5863250	-1.6544670
H	1.2428380	-4.5865400	-1.6542180
H	3.2957860	-3.4825980	-1.6606120
H	4.6888910	-1.4472760	-1.6472860

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C	-0.1505650	3.5277330	-1.8429430
C	1.1227520	3.7706850	-1.4324980
C	2.0248690	2.7092620	-1.0900480
C	3.3259220	3.0269810	-0.6311840
C	4.2108310	2.0434180	-0.2798660
C	3.8584050	0.6750470	-0.3770910
C	4.8248010	-0.3253200	-0.0240440
C	4.5493820	-1.6537330	-0.1138630
B	3.1736000	-2.0952290	-0.6013340
C	2.7143470	-3.5382430	-0.7788860
C	1.4601590	-3.7809200	-1.2451330
C	0.5516110	-2.7189220	-1.5689980
C	-0.7460610	-3.0355630	-2.0353040
C	-1.6484170	-2.0519280	-2.3387140
C	-1.3088730	-0.6850480	-2.2013450
C	-2.2892270	0.3146770	-2.5161000

C	-2.0163420	1.6422130	-2.4126170
B	-0.6306520	2.0860630	-1.9612700
N	0.3432250	1.0214920	-1.6254260
C	1.6359820	1.3450700	-1.1875450
C	2.5596860	0.3225930	-0.8391340
N	2.2085110	-1.0300460	-0.9599890
C	0.9236280	-1.3541340	-1.4214050
C	-0.0088270	-0.3330190	-1.7461660
H	-0.7998810	4.3708330	-2.0756110
H	1.5140250	4.7843820	-1.3305830
H	3.5997930	4.0766340	-0.5571650
H	5.2076700	2.2907410	0.0772640
H	5.7933960	0.0428330	0.3184190
H	5.3204310	-2.3718500	0.1647640
H	3.3624380	-4.3829610	-0.5457660
H	1.0825480	-4.7944280	-1.3889690
H	-1.0133280	-4.0849900	-2.1295750
H	-2.6520970	-2.2978370	-2.6731370
H	-3.2662820	-0.0519940	-2.8312170
H	-2.8003560	2.3594860	-2.6509810
C	-4.8502810	0.6332350	0.0063230
C	-4.3739030	1.8898700	0.2160620
C	-3.0429370	2.1250860	0.6959880
C	-2.5974150	3.4567800	0.8771650
C	-1.3321400	3.7219570	1.3265490
C	-0.4276480	2.6750400	1.6261140
C	0.8908130	2.9981640	2.0916250
C	1.8037570	2.0369630	2.3909040
B	1.4197820	0.5718720	2.2254730
C	2.3163460	-0.6215890	2.5252090
C	1.8244070	-1.8785720	2.3629040
C	0.4799440	-2.1151530	1.9197130
C	0.0189250	-3.4463450	1.7876490
C	-1.2523620	-3.7132820	1.3552960
C	-2.1449030	-2.6669180	1.0201500
C	-3.4567950	-2.9900000	0.5386070
C	-4.3474920	-2.0275980	0.1762180
B	-3.9531800	-0.5605820	0.3130840
N	-2.5934190	-0.2726900	0.8248300

C	-2.1584660	1.0501970	0.9906670
C	-0.8448240	1.3270150	1.4553190
N	0.0455630	0.2824790	1.7492530
C	-0.3975050	-1.0415710	1.6043960
C	-1.7142140	-1.3174530	1.1484340
H	-5.8672880	0.5101520	-0.3656450
H	-4.9779160	2.7775900	0.0211270
H	-3.2869040	4.2638520	0.6420030
H	-0.9890090	4.7453550	1.4547280
H	1.1197370	4.0610280	2.1822490
H	2.7944450	2.3365570	2.7288620
H	3.3474190	-0.4986100	2.8517420
H	2.4289080	-2.7650910	2.5564820
H	0.7085180	-4.2513810	2.0261170
H	-1.6013710	-4.7374230	1.2475240
H	-3.6948420	-4.0529460	0.4713010
H	-5.3292010	-2.3292430	-0.1888200

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C	1.7409900	-2.2216040	2.3324040
C	2.2316000	-0.9641960	2.4902890
C	1.4343270	0.1984880	2.2226930
C	1.9963360	1.4823010	2.4180810
C	1.2669560	2.6154230	2.1761040
C	-0.0702890	2.5403240	1.7200250
C	-0.7967400	3.7533660	1.4770980
C	-2.0776650	3.7440910	1.0208720
B	-2.7638910	2.4071930	0.7627630
C	-4.1939180	2.2231160	0.2646090
C	-4.6836360	0.9639870	0.1069910
C	-3.8937570	-0.1991350	0.3955770
C	-4.4653310	-1.4837160	0.2257870
C	-3.7501180	-2.6167160	0.5052200
C	-2.4122470	-2.5405940	0.9626830
C	-1.6971500	-3.7521360	1.2413840
C	-0.4054530	-3.7419280	1.6646670
B	0.3040690	-2.4069220	1.8598310

N	-0.4782660	-1.1811080	1.5805010
C	0.0920180	0.0890370	1.7645550
C	-0.6607960	1.2647030	1.5053740
N	-1.9838120	1.1799180	1.0436880
C	-2.5523100	-0.0888050	0.8573720
C	-1.8061830	-1.2651310	1.1339680
H	2.3916460	-3.0700040	2.5406310
H	3.2547120	-0.7789660	2.8179980
H	3.0282340	1.5444280	2.7508200
H	1.7047790	3.5999910	2.3153160
H	-0.2574400	4.6813030	1.6713920
H	-2.5831480	4.6942820	0.8488960
H	-4.8377880	3.0715710	0.0333000
H	-5.7007380	0.7785430	-0.2428960
H	-5.4912800	-1.5441410	-0.1295170
H	-4.1916990	-3.6019160	0.3769710
H	-2.2454060	-4.6816230	1.0802530
H	0.0972270	-4.6912040	1.8465690
C	0.4078620	-3.7425060	-1.6641800
C	1.6994180	-3.7518320	-1.2404470
C	2.4137900	-2.5398050	-0.9620260
C	3.7516140	-2.6150140	-0.5042730
C	4.4661370	-1.4815030	-0.2251420
C	3.8938300	-0.1973120	-0.3954180
C	4.6830120	0.9663610	-0.1071270
C	4.1925460	2.2251500	-0.2650860
B	2.7624170	2.4082550	-0.7633050
C	2.0753800	3.7446730	-1.0217160
C	0.7944430	3.7530590	-1.4779270
C	0.0687190	2.5395210	-1.7205500
C	-1.2685760	2.6136960	-2.1766270
C	-1.9972480	1.4800700	-2.4183840
C	-1.4344290	0.1966430	-2.2227580
C	-2.2309080	-0.9665820	-2.4904040
C	-1.7395110	-2.2236570	-2.3323350
B	-0.3025420	-2.4079930	-1.8594940
N	0.4790120	-1.1816410	-1.5802670
C	1.8069470	-1.2647470	-1.1336770
C	2.5523520	-0.0879050	-0.8573060

N	1.9830710	1.1804390	-1.0439290
C	0.6600160	1.2643070	-1.5056100
C	-0.0920840	0.0881180	-1.7645430
H	-0.0942720	-4.6921360	-1.8457430
H	2.2481010	-4.6809730	-1.0787630
H	4.1936930	-3.5999280	-0.3755510
H	5.4920760	-1.5412050	0.1303140
H	5.7002220	0.7816170	0.2428140
H	4.8359000	3.0740550	-0.0339880
H	2.5802750	4.6952190	-0.8499780
H	0.2545810	4.6806220	-1.6724470
H	-1.7070030	3.5979650	-2.3160610
H	-3.0291780	1.5414780	-2.7511650
H	-3.2540460	-0.7820270	-2.8184150
H	-2.3894200	-3.0725320	-2.5409640

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molelcule15_nested1

C	-0.6932670	1.2530220	-1.7461790
C	-1.2625390	-0.0798810	-1.8627570
C	-0.5368320	-1.3215030	-2.1314820
C	0.8311000	-1.6029450	-1.7209900
C	1.8460130	-0.6397480	-1.3073340
C	1.8600170	0.7763850	-1.6690450
C	0.7093480	1.6180340	-1.9555440
C	-1.6128730	2.3402120	-1.5413940
C	0.9694620	2.9821630	-2.3359980
C	3.1517130	1.4154860	-1.6815740
C	3.0215480	-1.1608050	-0.6667780
C	1.2272230	-2.9883090	-1.7128230
C	-1.2958870	-2.4106790	-2.6875210
C	-2.6970180	-0.1816680	-1.8071570
C	3.3495840	2.6951050	-2.2622890
C	2.2806700	3.4500630	-2.6173940
C	-0.0377100	3.9842860	-2.3086320
C	-1.2603010	3.6913300	-1.8017970
C	-2.9711280	2.1214660	-1.1955970
C	-3.5066320	0.8846370	-1.3397950

C	-3.3939470	-1.3126690	-2.3085740
C	-2.7067460	-2.3487600	-2.8493510
C	0.4912770	-3.9823830	-2.4074240
C	-0.7160360	-3.6821680	-2.9463100
C	3.1868280	-2.5451780	-0.3938180
C	2.3597800	-3.4392130	-0.9876060
C	4.1828840	-0.3709900	-0.4482040
C	4.2835160	0.8404810	-1.0467280
H	2.4004780	4.4588950	-3.0058190
H	0.2287900	4.9967870	-2.6031360
H	-2.0154340	4.4591510	-1.6554800
H	-3.5803010	2.9762050	-0.9149850
H	-4.5658840	0.7010120	-1.1833220
H	-4.4807600	-1.2981120	-2.2891190
H	-3.2170540	-3.1978280	-3.2982570
H	0.9037190	-4.9875920	-2.4601090
H	-1.3142700	-4.4333670	-3.4568340
H	4.0516620	-2.8629800	0.1819390
H	2.5378750	-4.5099710	-0.9206950
H	5.2082090	1.4124860	-1.0203030
H	4.3660830	3.0729240	-2.3481270
H	5.0168300	-0.8115170	0.0913210
C	-1.4601640	1.2720820	1.8292690
C	-2.0536640	-0.0486050	1.7026610
C	-1.3521530	-1.2952140	1.3955590
C	0.0188500	-1.6081600	1.7756780
C	1.0523020	-0.6731340	2.2051680
C	1.0848620	0.7498930	1.8778630
C	-0.0537770	1.6148120	1.6099990
C	-2.3562860	2.3744990	2.0673750
C	0.2290330	2.9789810	1.2557950
C	2.3824650	1.3736800	1.8869950
C	2.2204400	-1.2273070	2.8351890
C	0.3884060	-3.0001050	1.7561840
C	-2.1392790	-2.3625390	0.8420650
C	-3.4892310	-0.1319440	1.7921110
C	2.6012140	2.6524340	1.3140280
C	1.5442540	3.4255320	0.9646110
C	-0.7542970	4.0019010	1.3242570

C	-1.9762990	3.7245580	1.8408980
C	-3.7179740	2.1756150	2.4163840
C	-4.2759580	0.9482590	2.2705030
C	-4.2139530	-1.2542520	1.3104880
C	-3.5541930	-2.2881230	0.7337830
C	-0.3707200	-3.9637130	1.0450030
C	-1.5823970	-3.6322020	0.5365230
C	2.3633790	-2.6212560	3.0749610
C	1.5161430	-3.4872120	2.4661140
C	3.3858970	-0.4536290	3.0873830
C	3.5002280	0.7750240	2.5249870
H	1.6772820	4.4287170	0.5695270
H	-0.4686900	5.0127020	1.0455850
H	-2.7131870	4.5062090	2.0108840
H	-4.3140090	3.0412220	2.6967870
H	-5.3398910	0.7851110	2.4273930
H	-5.3002770	-1.2288880	1.3591860
H	-4.0839930	-3.1240500	0.2850810
H	0.0290030	-4.9703110	0.9503810
H	-2.1954560	-4.3558280	0.0065300
H	3.2341370	-2.9690080	3.6259390
H	1.6808150	-4.5618750	2.4977270
H	4.4312000	1.3352690	2.5660050
H	3.6231430	3.0096390	1.2190090
H	4.2169510	-0.9188660	3.6124620

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molecule15_nested2

C	0.5322210	-1.8178540	1.6321680
C	0.3457340	-0.3816010	1.8426550
C	1.0863920	0.6979530	1.2083720
C	2.1533240	0.5636620	0.2155010
C	3.0983380	-0.5436340	0.1252410
C	3.0196070	-1.8345960	0.8123830
C	1.7934980	-2.4698260	1.2978110
C	-0.5845360	-2.6662780	1.9510430
C	1.8520200	-3.8963240	1.5125460
C	4.2248820	-2.6237580	0.8565830

C	4.2715620	-0.3205190	-0.6857510
C	2.3873230	1.7010410	-0.6344980
C	0.6568480	2.0417860	1.5000320
C	-0.7552230	-0.0047040	2.6922890
C	4.2505890	-3.9545640	1.3558930
C	3.0825130	-4.5997450	1.5911690
C	0.6844190	-4.6814630	1.6936150
C	-0.5202330	-4.0798240	1.8436820
C	-1.7741810	-2.1727790	2.5506640
C	-1.8020400	-0.9042860	3.0230380
C	-0.9317770	1.3271760	3.1462250
C	-0.2358530	2.3319090	2.5629930
C	1.7294640	2.9459130	-0.4465910
C	0.9845330	3.1428990	0.6665770
C	4.3571880	0.7505210	-1.6118140
C	3.4045230	1.7133580	-1.6236590
C	5.4339370	-1.1275540	-0.5750990
C	5.4401760	-2.2006280	0.2521760
H	3.0582830	-5.6563620	1.8482420
H	0.7903920	-5.7629810	1.7421050
H	-1.4299390	-4.6535140	2.0020880
H	-2.6009820	-2.8592970	2.7101920
H	-2.6481290	-0.5283400	3.5911070
H	-1.7113730	1.5269520	3.8761180
H	-0.4330980	3.3728950	2.8041630
H	1.9182400	3.7470120	-1.1558040
H	0.5591090	4.1146040	0.9007610
H	5.2218850	0.7976860	-2.2701050
H	3.4586840	2.5618260	-2.3010920
H	6.3254450	-2.8203470	0.3737810
H	5.2072010	-4.4673130	1.4224010
H	6.3120500	-0.8511500	-1.1544340
C	-1.9466150	-1.3024770	-0.9450390
C	-3.0194950	-0.5772760	-0.2763850
C	-2.9774660	0.8260510	0.1456790
C	-2.2250070	1.9030030	-0.4851620
C	-1.3696120	1.7949410	-1.6710940
C	-0.6188490	0.6153780	-2.0814280
C	-0.7436550	-0.7414220	-1.5543330

C	-2.0632390	-2.7387740	-0.9871830
C	0.3314610	-1.6524160	-1.8362410
C	0.3885780	0.8071670	-3.0944780
C	-1.1368070	3.0093700	-2.4115780
C	-2.4335350	3.2333000	0.0313100
C	-3.8617910	1.1937660	1.2238260
C	-4.1640960	-1.3446690	0.1457230
C	1.4360920	-0.1259860	-3.3082070
C	1.4683760	-1.2806210	-2.6027240
C	0.2514590	-3.0417560	-1.5524530
C	-0.9515240	-3.5815180	-1.2461860
C	-3.2836510	-3.4043850	-0.7085390
C	-4.3314070	-2.7127080	-0.1977100
C	-5.1229480	-0.8448960	1.0674400
C	-4.9069780	0.3450830	1.6771570
C	-3.1260420	3.4760860	1.2447840
C	-3.8278530	2.4758590	1.8290560
C	-1.5445140	4.2847840	-1.9371160
C	-2.0693430	4.3993670	-0.6937970
C	-0.3410720	3.0415760	-3.5876600
C	0.4398920	1.9769170	-3.8938120
H	2.2820800	-1.9924440	-2.7083160
H	1.1304960	-3.6593310	-1.7130440
H	-1.0866690	-4.6561080	-1.1609020
H	-3.3338290	-4.4794590	-0.8661360
H	-5.2635090	-3.2056320	0.0687240
H	-5.9638590	-1.4790840	1.3382240
H	-5.5614230	0.7065520	2.4671440
H	-3.1533770	4.4916020	1.6333150
H	-4.4447980	2.6521080	2.7073100
H	-1.3333600	5.1590640	-2.5484350
H	-2.2904840	5.3707470	-0.2572570
H	1.1553900	2.0123180	-4.7123040
H	2.2185710	0.1294680	-4.0169890
H	-0.2857670	3.9689890	-4.1530610

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molecule16_nested

C	1.7317410	-0.2430870	1.8861320	H	2.4005160	-3.7581860	4.7887410
C	1.3264540	1.1396440	1.8858560	H	-4.7781680	1.7726680	1.2752680
C	0.2432090	1.7328620	2.6808890	H	-1.8178400	-4.7528640	3.3365120
C	-1.1399830	1.3271750	2.6811410	H	4.7781680	-1.7726680	1.2752680
C	-1.7317410	0.2430870	1.8861320	H	1.8178400	4.7528640	3.3365120
C	-1.3264540	-1.1396440	1.8858560	H	4.0963260	-3.0166400	3.3410060
C	-0.2432090	-1.7328620	2.6808890	H	-3.0620560	-4.0723600	1.2703340
C	1.1399830	-1.3271750	2.6811410	H	-4.0963260	3.0166400	3.3410060
C	2.9915850	-0.5488100	1.2736200	H	3.0620560	4.0723600	1.2703340
C	3.5857470	0.3418720	0.3415800	C	1.7328620	-0.2432090	-2.6808890
C	3.2021490	1.6476070	0.3403460	C	1.3271750	1.1399830	-2.6811410
C	2.2209510	2.0769840	1.2720000	C	0.2430870	1.7317410	-1.8861320
C	0.5575130	2.9876790	3.3053630	C	-1.1396440	1.3264540	-1.8858560
C	-0.3429760	3.5949960	4.2197750	C	-1.7328620	0.2432090	-2.6808890
C	-1.6514890	3.2108470	4.2205500	C	-1.3271750	-1.1399830	-2.6811410
C	-2.0818120	2.2131450	3.3065870	C	-0.2430870	-1.7317410	-1.8861320
C	-2.9915850	0.5488100	1.2736200	C	1.1396440	-1.3264540	-1.8858560
C	-3.5857470	-0.3418720	0.3415800	C	2.9876790	-0.5575130	-3.3053630
C	-3.2021490	-1.6476070	0.3403460	C	3.5949960	0.3429760	-4.2197750
C	-2.2209510	-2.0769840	1.2720000	C	3.2108470	1.6514890	-4.2205500
C	-0.5575130	-2.9876790	3.3053630	C	2.2131450	2.0818120	-3.3065870
C	0.3429760	-3.5949960	4.2197750	C	0.5488100	2.9915850	-1.2736200
C	1.6514890	-3.2108470	4.2205500	C	-0.3418720	3.5857470	-0.3415800
C	2.0818120	-2.2131450	3.3065870	C	-1.6476070	3.2021490	-0.3403460
C	-3.8097960	1.6166610	1.7445320	C	-2.0769840	2.2209510	-1.2720000
C	-1.6476070	-3.7921760	2.8558270	C	-2.9876790	0.5575130	-3.3053630
C	3.8097960	-1.6166610	1.7445320	C	-3.5949960	-0.3429760	-4.2197750
C	1.6476070	3.7921760	2.8558270	C	-3.2108470	-1.6514890	-4.2205500
C	3.4343390	-2.3008280	2.8590170	C	-2.2131450	-2.0818120	-3.3065870
C	-2.3322800	-3.4181790	1.7411500	C	-0.5488100	-2.9915850	-1.2736200
C	-3.4343390	2.3008280	2.8590170	C	0.3418720	-3.5857470	-0.3415800
C	2.3322800	3.4181790	1.7411500	C	1.6476070	-3.2021490	-0.3403460
H	4.4297620	-0.0034280	-0.2487430	C	2.0769840	-2.2209510	-1.2720000
H	3.7253770	2.3933580	-0.2512590	C	-3.7921760	1.6476070	-2.8558270
H	-0.0081950	4.4606890	4.7871940	C	-1.6166610	-3.8097960	-1.7445320
H	-2.4005160	3.7581860	4.7887410	C	3.7921760	-1.6476070	-2.8558270
H	-4.4297620	0.0034280	-0.2487430	C	1.6166610	3.8097960	-1.7445320
H	-3.7253770	-2.3933580	-0.2512590	C	3.4181790	-2.3322800	-1.7411500
H	0.0081950	-4.4606890	4.7871940	C	-2.3008280	-3.4343390	-2.8590170

C	-3.4181790	2.3322800	-1.7411500
C	2.3008280	3.4343390	-2.8590170
H	4.4606890	0.0081950	-4.7871940
H	3.7581860	2.4005160	-4.7887410
H	0.0034280	4.4297620	0.2487430
H	-2.3933580	3.7253770	0.2512590
H	-4.4606890	-0.0081950	-4.7871940
H	-3.7581860	-2.4005160	-4.7887410
H	-0.0034280	-4.4297620	0.2487430
H	2.3933580	-3.7253770	0.2512590
H	-4.7528640	1.8178400	-3.3365120
H	-1.7726680	-4.7781680	-1.2752680
H	4.7528640	-1.8178400	-3.3365120
H	1.7726680	4.7781680	-1.2752680
H	4.0723600	-3.0620560	-1.2703340
H	-3.0166400	-4.0963260	-3.3410060
H	-4.0723600	3.0620560	-1.2703340
H	3.0166400	4.0963260	-3.3410060

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molecule16_edge-to-edge

C	2.4372690	-1.5935550	0.9855920
C	1.7611280	-1.2212900	-0.2288580
C	2.3793560	-0.7478810	-1.4729980
C	3.2577370	0.3885300	-1.5987330
C	3.7629110	1.2339580	-0.5071260
C	4.5038760	0.7785190	0.6400010
C	4.8400770	-0.6126850	0.9698440
C	3.8923390	-1.6763380	1.1645990
C	1.6540360	-2.2207650	2.0107520
C	0.2362340	-2.1261370	2.0041360
C	-0.3991610	-1.8229830	0.8366040
C	0.3726830	-1.5680250	-0.3266470
C	1.8186090	-1.2777460	-2.6843310
C	2.3846640	-0.9678620	-3.9488700
C	3.1908460	0.1252900	-4.0674520
C	3.4660220	0.9131930	-2.9185310
C	3.7552870	2.6479360	-0.7599270

C	4.0976910	3.5735110	0.2614190
C	4.8236890	3.1396680	1.3321890
C	5.1980960	1.7719470	1.4079850
C	6.1831650	-0.8337110	1.4238290
C	6.6565510	-2.1479870	1.6816900
C	5.7509940	-3.1452330	1.9021000
C	4.3628830	-2.8520980	1.8395260
C	3.6587040	3.1665700	-2.0861260
C	6.9895690	0.2417960	1.9067730
C	2.2249940	-3.1855410	2.8956870
C	0.5411260	-1.9117760	-2.7012330
C	3.4958540	-3.6209960	2.6739590
C	6.4265000	1.4703260	2.0710660
C	3.7062520	2.3030280	-3.1373210
C	-0.2272970	-1.8838330	-1.5801140
H	-0.3186260	-2.4697570	2.8742900
H	-1.4769340	-1.9093730	0.7389120
H	2.0299400	-1.5044750	-4.8259980
H	3.5013240	0.4954230	-5.0421350
H	3.9257910	4.6332500	0.0872550
H	5.2555020	3.8413140	2.0425130
H	7.7167010	-2.2958020	1.8750830
H	6.0636910	-4.1169320	2.2782630
H	3.6887370	4.2440020	-2.2284820
H	7.9896810	0.0198240	2.2717940
H	1.5813980	-3.6585050	3.6338140
H	0.1480080	-2.2701160	-3.6494830
H	3.9110420	-4.4690160	3.2136820
H	6.9475360	2.2721920	2.5889510
H	3.7965810	2.6582560	-4.1612900
H	-1.2640200	-2.1988160	-1.5962310
C	-3.8928880	1.6771040	1.1631710
C	-4.8402400	0.6129570	0.9693150
C	-4.5036700	-0.7783440	0.6402150
C	-3.7628630	-1.2342350	-0.5068380
C	-3.2575160	-0.3893110	-1.5987560
C	-2.3789840	0.7470480	-1.4733740
C	-1.7611730	1.2212350	-0.2293220
C	-2.4377730	1.5944670	0.9845740

C	-4.3638580	2.8533780	1.8369100	H	-7.9892910	-0.0196920	2.2725490
C	-5.7520760	3.1460500	1.8992250				
C	-6.6572270	2.1481570	1.6800370				
C	-6.1833420	0.8338340	1.4233740	96			
C	-5.1974570	-1.7715070	1.4089370	molecule16_up-down_edge-to-edge			
C	-4.8229300	-3.1392220	1.3336690	C	2.3722550	1.1065020	-0.3259880
C	-4.0973510	-3.5734900	0.2628030	C	3.6200820	1.7528310	-0.0158340
C	-3.7552180	-2.6483210	-0.7590170	C	4.9639160	1.3196660	-0.4208430
C	-3.4656140	-0.9145820	-2.9183610	C	5.5478540	0.0387490	-0.1247450
C	-3.1899480	-0.1273280	-4.0676000	C	4.8814060	-1.1061340	0.5090880
C	-2.3833880	0.9655830	-3.9493810	C	3.6955200	-1.7545370	0.0147680
C	-1.8176330	1.2759740	-2.6848390	C	2.8574830	-1.3239000	-1.1127810
C	-0.3727010	1.5678180	-0.3267800	C	2.2069510	-0.0436630	-1.2223000
C	0.3987030	1.8235310	0.8366030	C	1.1681510	1.8112080	0.0079870
C	-0.2371680	2.1278230	2.0035850	C	1.1830320	2.8923490	0.9280510
C	-1.6549650	2.2226190	2.0094710	C	2.3636870	3.5296190	1.1766040
C	-3.7061410	-2.3044360	-3.1365720	C	3.5502110	3.0717520	0.5449240
C	0.2278270	1.8827890	-1.5801960	C	5.8497900	2.3606420	-0.8589180
C	-3.4971180	3.6233900	2.6706340	C	7.1502540	2.0552060	-1.3425990
C	-6.4256880	-1.4698310	2.0723080	C	7.7144460	0.8568780	-1.0137400
C	-2.2262750	3.1883060	2.8931920	C	6.9741670	-0.0705150	-0.2337640
C	-0.5401090	1.9098840	-2.7016660	C	5.6502820	-1.8042360	1.4998330
C	-3.6587760	-3.1675300	-2.0849970	C	5.0851710	-2.8805060	2.2356860
C	-6.9892110	-0.2415910	1.9073860	C	3.9908940	-3.5217950	1.7323550
H	-6.0651420	4.1180240	2.2743760	C	3.4215890	-3.0728550	0.5114160
H	-7.7174100	2.2957090	1.8734470	C	2.4105650	-2.3699860	-1.9873120
H	-5.2544340	-3.8405820	2.0444670	C	1.6342670	-2.0758910	-3.1397020
H	-3.9254740	-4.6332930	0.0890080	C	0.9706440	-0.8855540	-3.2013740
H	-3.5003040	-0.4978620	-5.0421730	C	1.1113480	0.0500900	-2.1440110
H	-2.0282380	1.5016230	-4.8266840	C	7.0672500	-1.6472230	1.5872960
H	1.4765400	1.9094990	0.7392700	C	2.4559870	-3.7417890	-1.5914140
H	0.3173440	2.4721170	2.8736950	C	-0.0260760	1.6538070	-0.7549910
H	-3.7965280	-2.6601200	-4.1603790	C	5.5861570	3.7333640	-0.5648070
H	1.2644950	2.1979070	-1.5960440	C	0.0145960	0.9315910	-1.9055960
H	-3.9125620	4.4719180	3.2093610	C	2.7725530	-4.0494250	-0.3035610
H	-6.9462890	-2.2715370	2.5908740	C	7.7149510	-0.9466750	0.6160420
H	-1.5829480	3.6620620	3.6310460	C	4.5639010	4.0418460	0.2795880
H	-0.1465580	2.2674810	-3.6500210	H	0.2342550	3.2945700	1.2704070
H	-3.6890200	-4.2450170	-2.2268960	H	2.3930420	4.4690690	1.7248320

H	7.7358510	2.8453300	-1.8073460
H	8.7668240	0.6580170	-1.2042500
H	5.6362070	-3.2845600	3.0819460
H	3.6385550	-4.4576540	2.1605790
H	1.4339780	-2.8704740	-3.8549820
H	0.2201590	-0.6987800	-3.9659480
H	7.6099420	-2.2167180	2.3380480
H	2.0850760	-4.4957680	-2.2819400
H	-0.9016200	2.2275000	-0.4750840
H	6.2992620	4.4843290	-0.8966140
H	-0.8271270	0.9134090	-2.5934460
H	2.6486690	-5.0553600	0.0902860
H	8.8001460	-0.9438550	0.5436940
H	4.4307450	5.0489300	0.6682600
C	-4.9639400	-1.3196280	0.4210680
C	-5.5478360	-0.0387240	0.1248160
C	-4.8813820	1.1060790	-0.5091690
C	-3.6954720	1.7545430	-0.0149550
C	-2.8573690	1.3239710	1.1125660
C	-2.2069040	0.0437170	1.2221670
C	-2.3722870	-1.1065370	0.3259600
C	-3.6201520	-1.7529000	0.0160560
C	-5.8498360	-2.3605090	0.8593350
C	-7.1502740	-2.0549640	1.3430070
C	-7.7144340	-0.8566670	1.0139860
C	-6.9741450	0.0705940	0.2338650
C	-5.6502890	1.8040880	-1.4999530
C	-5.0852170	2.8803130	-2.2359150
C	-3.9909730	3.5216890	-1.7326430
C	-3.4216210	3.0728510	-0.5116840
C	-2.4103490	2.3701230	1.9869780
C	-1.6340360	2.0760620	3.1393660
C	-0.9704970	0.8856780	3.2011310
C	-1.1112720	-0.0500350	2.1438380
C	-1.1682220	-1.8112770	-0.0080640
C	-1.1832080	-2.8925580	-0.9279500
C	-2.3638950	-3.5298900	-1.1762290
C	-3.5503430	-3.0719220	-0.5445000
C	-2.4557720	3.7418870	1.5909940

C	0.0260760	-1.6538280	0.7548110
C	-5.5862500	-3.7332890	0.5654490
C	-7.0672610	1.6470840	-1.5873750
C	-4.5640370	-4.0419470	-0.2789300
C	-0.0145380	-0.9315660	1.9053900
C	-2.7725420	4.0494840	0.3031830
C	-7.7149430	0.9466610	-0.6160200
H	-7.7358850	-2.8450020	1.8078820
H	-8.7668030	-0.6577460	1.2044840
H	-5.6362780	3.2842670	-3.0822070
H	-3.6386550	4.4575250	-2.1609380
H	-1.4336980	2.8706820	3.8545940
H	-0.2200070	0.6989240	3.9657040
H	-0.2344810	-3.2948700	-1.2703460
H	-2.3932900	-4.4694500	-1.7242640
H	-2.0847230	4.4959170	2.2813900
H	0.9016540	-2.2274750	0.4748780
H	-6.2993700	-4.4841730	0.8974080
H	-7.6099620	2.2165040	-2.3381770
H	-4.4309190	-5.0491010	-0.6674330
H	0.8272320	-0.9133500	2.5931830
H	-2.6490270	5.0554920	-0.0905970
H	-8.8001350	0.9438710	-0.5436280

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C	2.7926870	-1.1697600	-1.6670540
C	2.1066890	0.0984810	-1.8020500
C	3.8179240	-1.5627310	-0.7049160
C	3.5894450	-1.5393720	0.7173530
C	2.5351280	-0.8230940	1.4317740
C	2.4127560	0.6100370	1.4905390
C	3.3852980	1.5294370	0.9031140
C	3.7392100	1.6882100	-0.4878860
C	2.8155010	1.3428150	-1.5604300
C	1.5718690	1.1517720	2.5172040
C	1.9093470	2.3759900	3.1649620
C	3.1397730	2.9239770	2.9397260

C	3.9052470	2.5085630	1.8091000	H	1.2821480	3.2520280	-3.9820960
C	4.7805020	2.6285230	-0.8048640	H	6.4594340	3.7832510	-0.0577800
C	4.8188590	3.2860360	-2.0683970	H	5.5781190	3.8014610	2.2730710
C	3.6968160	3.2646040	-2.8465580	C	-3.7338070	-1.2336170	-1.1051820
C	2.6449410	2.3450460	-2.5663220	C	-4.4705740	0.0059700	-0.9628110
C	0.9685580	0.1457630	-2.6784820	C	-2.4649590	-1.6247350	-0.5087620
C	0.4628580	-1.0348880	-3.2910970	C	-2.2813840	-1.5953960	0.9223500
C	1.2996080	-2.1076500	-3.3997720	C	-2.9894750	-0.7731270	1.8983580
C	2.5387110	-2.1245990	-2.7012710	C	-2.9405730	0.6662400	1.9341700
C	4.8658260	-2.4150560	-1.1948340	C	-2.2227940	1.5035740	0.9767290
C	5.8397750	-2.9474030	-0.3045340	C	-2.4796980	1.6311040	-0.4372600
C	5.5284790	-3.0418620	1.0230150	C	-3.7718490	1.2731140	-1.0075910
C	4.3000430	-2.5069970	1.4994490	C	-3.3098810	1.3054480	3.1643860
C	0.5798620	0.3455400	3.1380780	C	-2.6738830	2.5147490	3.5760460
C	0.7242440	-1.0105160	3.1087530	C	-1.5986620	2.9740330	2.8690180
C	1.8356310	-1.5772490	2.4289870	C	-1.3567310	2.4852390	1.5523910
C	2.4006590	-2.7713620	2.9663980	C	-1.6850570	2.5701990	-1.1744120
C	3.6857210	-3.1032880	2.6412650	C	-2.2201880	3.2521160	-2.3060240
C	4.7732650	-3.0269970	-2.4793730	C	-3.5738890	3.2396110	-2.4930690
C	3.5665350	-3.0204000	-3.1190320	C	-4.3841320	2.2907990	-1.8023760
C	0.5487450	1.3675860	-3.2759110	C	-5.8613970	-0.0018920	-1.3260210
C	1.4472090	2.3930130	-3.3348570	C	-6.4964300	-1.2017940	-1.7581710
C	5.5925270	3.1884180	0.2208120	C	-5.7069340	-2.2203360	-2.2136440
C	5.1115960	3.1948050	1.4997010	C	-4.2986180	-2.1878270	-2.0059510
H	1.2527000	2.7469870	3.9474560	C	-1.6350690	-2.5151240	-1.2670990
H	3.5216340	3.7374320	3.5527280	C	-0.4945680	-3.1254200	-0.6722510
H	5.6513510	3.9490060	-2.2920150	C	-0.4743560	-3.2602670	0.6849620
H	3.5911490	3.9222100	-3.7068060	C	-1.4875530	-2.6483470	1.4739170
H	-0.4730660	-0.9871370	-3.8402150	C	-4.1078850	0.6149980	4.1176210
H	1.0666730	-2.9383280	-4.0629100	C	-4.1718730	-0.7500190	4.0753410
H	6.7075920	-3.4581300	-0.7158910	C	-3.4252510	-1.4487930	3.0871350
H	6.1379590	-3.6349080	1.7016760	C	-2.8879050	-2.7222440	3.4414620
H	-0.1637130	0.8185690	3.7727270	C	-1.8175570	-3.2059940	2.7430420
H	0.0993990	-1.6499300	3.7246690	C	-2.1051710	-3.0979400	-2.4797200
H	1.8560300	-3.2989040	3.7462360	C	-3.4467450	-3.0665960	-2.7375690
H	4.2191030	-3.8940500	3.1640400	C	-6.5443890	1.2123940	-1.6229530
H	5.5974690	-3.6449660	-2.8279460	C	-5.7974200	2.3015880	-1.9747020
H	3.3823860	-3.6466570	-3.9893310	C	-0.4971350	3.1134820	-0.6096110
H	-0.3743970	1.3859630	-3.8479960	C	-0.3753950	3.1279500	0.7484250

H	-2.9637050	2.9597810	4.5252020
H	-0.9772720	3.7851130	3.2403050
H	-1.5749290	3.9255770	-2.8648190
H	-4.0558990	3.9171460	-3.1946190
H	-7.5706090	-1.2002090	-1.9281210
H	-6.1281700	-3.0532260	-2.7729050
H	0.2206320	-3.6442640	-1.3032780
H	0.2523670	-3.9032990	1.1747800
H	-4.5146290	1.1695380	4.9606480
H	-4.6315930	-1.3151450	4.8833230
H	-3.2346770	-3.2002600	4.3547400
H	-1.2568190	-4.0717730	3.0883580
H	-1.4305770	-3.7262690	-3.0555690
H	-3.8888160	-3.6849840	-3.5158960
H	-7.6195840	1.1891060	-1.7847600
H	-6.2556280	3.1722480	-2.4393330
H	0.1813240	3.6762660	-1.2427480
H	0.4006980	3.7095480	1.2384830

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C	2.3098110	-0.8579340	0.8555410
C	2.2394280	-1.0530700	-0.5890630
C	3.0970590	0.1045160	1.5880930
C	3.4718800	1.3734330	0.9871560
C	4.0681730	1.6364780	-0.3129140
C	5.2261110	0.8914120	-0.7494570
C	5.5726700	-0.4978230	-0.4713370
C	4.7357290	-1.5872790	-0.8922030
C	3.3639170	-1.4710290	-1.3782580
C	6.2395960	1.6381520	-1.4246890
C	7.6135250	1.2873920	-1.2600030
C	7.9584690	0.1967060	-0.5117750
C	6.9572140	-0.7789080	-0.2246580
C	5.3787970	-2.8370970	-1.1586610
C	4.9226560	-3.6635830	-2.2308020
C	3.9263810	-3.2113830	-3.0509330
C	3.0890970	-2.1401830	-2.6130770

C	0.9337330	-1.2751670	-1.1374590
C	-0.1613810	-1.6212260	-0.2946320
C	0.0929840	-1.9524930	1.0034330
C	1.3315560	-1.5821040	1.6035270
C	3.0537610	0.0469070	3.0240920
C	3.3043960	1.2078000	3.8122440
C	3.2409970	2.4318190	3.2085710
C	3.2279760	2.5312160	1.7872460
C	5.8870100	2.8079110	-2.1547550
C	4.6660550	3.3938830	-1.9673620
C	3.8595150	2.9377590	-0.8856440
C	3.1239000	3.9361900	-0.1826520
C	2.9560490	3.7828870	1.1645170
C	2.4260740	-1.0434320	3.6893190
C	1.5108180	-1.7868330	2.9985090
C	0.7711260	-1.4850080	-2.5348190
C	1.8379570	-1.9409170	-3.2607960
C	6.6229300	-3.1368380	-0.5376910
C	7.3909880	-2.1212110	-0.0364070
H	8.3689430	1.9435100	-1.6866670
H	8.9988260	-0.0400190	-0.3011370
H	5.4700730	-4.5766770	-2.4531650
H	3.6615560	-3.7385240	-3.9647470
H	-1.1384840	-1.7812960	-0.7377590
H	-0.6703580	-2.4026870	1.6299250
H	3.3320330	1.1124810	4.8953240
H	3.1946800	3.3492370	3.7912690
H	6.6356910	3.2636890	-2.7993700
H	4.4063890	4.3257070	-2.4645090
H	2.9079740	4.8809440	-0.6757430
H	2.6118800	4.6052780	1.7875840
H	2.5164040	-1.1244270	4.7702220
H	0.8366970	-2.4688170	3.5118880
H	-0.2333370	-1.4769870	-2.9517930
H	1.7072400	-2.3096240	-4.2761090
H	7.0131780	-4.1500140	-0.6079770
H	8.4073500	-2.3046930	0.3051840
C	-5.2384950	-0.6311550	-0.7939580
C	-4.0633530	-1.4623930	-0.6779260

C	-5.5825960	0.5678010	-0.0377580	H	-6.7061970	-2.1677600	-3.4960950
C	-4.7679410	1.7505140	-0.0779180	H	-8.3957600	1.9356010	1.4168710
C	-3.4165530	1.8368320	-0.6244130	H	-7.0455540	4.0089140	1.1663440
C	-2.2571690	1.1894860	-0.0770720	H	0.1081740	2.4538040	-2.2419860
C	-2.2628930	0.5045570	1.2113100	H	-1.8901690	3.6656940	-3.1089300
C	-3.0205860	-0.6624000	1.5978980	H	-3.8311090	4.8595350	-2.2405580
C	-3.4207700	-1.6527390	0.6130480	H	-5.5785260	5.0834690	-0.4639290
C	-0.9772320	1.6102080	-0.5673420	H	-8.9976330	0.0193830	0.0696310
C	0.1552810	1.6557440	0.2954590	H	-8.4069720	-1.3427800	-1.9420680
C	-0.0389210	1.5086630	1.6370600	H	-2.9121140	-4.3701260	-2.1700730
C	-1.2508200	0.9364530	2.1224230	H	-2.5377990	-4.9543500	0.2281050
C	-2.9184120	-1.1003450	2.9635100	H	-2.3080560	-0.5932920	4.9835140
C	-3.1431370	-2.4630470	3.3156040	H	-0.6750780	1.1182990	4.1983690
C	-3.1093420	-3.4058130	2.3274890				
C	-3.1512120	-3.0123980	0.9587490				
C	-3.8707520	-2.4841320	-1.6699670				
C	-4.7105370	-2.5497440	-2.8184740	108			
C	-5.9385320	-1.9521890	-2.7557960	molecule17_up-down_edge-to-edge			
C	-6.2711880	-1.1131350	-1.6554990	C	2.9763340	-0.7863890	0.1305450
C	-6.9585460	0.7197810	0.3363730	C	2.2837730	-0.9232740	-1.1480350
C	-7.3917900	1.9021790	0.9994120	C	3.8302800	0.2989590	0.5475610
C	-6.6479680	3.0427330	0.8627380	C	3.8113340	1.5998410	-0.1107660
C	-5.4270570	3.0025350	0.1338950	C	4.0158420	1.9176920	-1.5107850
C	-0.8767940	2.2988430	-1.8076790	C	5.0313110	1.2244740	-2.2766450
C	-1.9751900	2.9621860	-2.2832420	C	5.3783780	-0.1898080	-2.2822450
C	-3.1974010	2.8997740	-1.5573200	C	4.3858180	-1.1927560	-2.5695820
C	-4.0558310	4.0414100	-1.5599580	C	2.9379750	-1.0787080	-2.4172150
C	-5.0186300	4.1604870	-0.5963650	C	5.8586140	2.0505400	-3.0975780
C	-7.9642190	-0.1106290	-0.2432760	C	7.2167550	1.6857770	-3.3353910
C	-7.6403280	-0.8644020	-1.3365630	C	7.6940770	0.4824740	-2.8974920
C	-3.1127760	-3.6550650	-1.3758580	C	6.7540340	-0.5231010	-2.5243240
C	-2.9020310	-3.9719730	-0.0638180	C	4.8281360	-2.3419780	-3.2961070
C	-2.2611770	-0.2977330	3.9377990	C	3.9678310	-2.9553060	-4.2570220
C	-1.3715750	0.6467610	3.5087800	C	2.7245710	-2.4348480	-4.4854430
H	1.1114040	1.9756440	-0.1049760	C	2.1502890	-1.5613280	-3.5126290
H	0.7536030	1.7229930	2.3470550	C	0.9056910	-1.3069950	-1.0749750
H	-3.1268100	-2.7444770	4.3660360	C	0.3850870	-1.9209960	0.1015240
H	-3.0433790	-4.4667740	2.5585030	C	1.2469090	-2.2801770	1.0967710
H	-4.4645310	-3.2490080	-3.6142850	C	2.5493900	-1.6993790	1.1472170
				C	4.3352510	0.2673310	1.8928720

C	4.6025370	1.4730940	2.6055680	C	-4.8413550	0.4849210	1.6069640
C	4.1150750	2.6491670	2.1108690	C	-4.6872350	-0.9595860	1.6557490
C	3.6632900	2.7239310	0.7611990	C	-1.5150540	1.4930280	3.0013660
C	5.3430600	3.2683640	-3.6254240	C	-2.0421710	2.3764660	3.9911250
C	4.1668410	3.7810460	-3.1549870	C	-3.2265250	3.0122010	3.7428650
C	3.6223210	3.2247490	-1.9618610	C	-4.0988410	2.5229010	2.7239780
C	2.9847530	4.1420010	-1.0782020	C	-6.1751120	1.0089930	1.7078820
C	3.1230510	3.9440930	0.2662880	C	-7.2858270	0.1421290	1.9261860
C	4.2581560	-0.9245490	2.6656900	C	-7.0399780	-1.1185160	2.3926460
C	3.3310790	-1.8684690	2.3224530	C	-5.7203340	-1.6570720	2.3528190
C	0.1136270	-1.3456620	-2.2538580	C	-3.4395610	-3.0884290	1.6798660
C	0.7318500	-1.4582680	-3.4681490	C	-2.7113440	-4.0987640	0.9880550
C	6.1887300	-2.7489690	-3.2128660	C	-2.6069440	-4.0022320	-0.3710390
C	7.1375300	-1.8734570	-2.7608400	C	-3.0177480	-2.8142800	-1.0385380
H	7.8612540	2.3991740	-3.8443840	C	-3.5493220	-0.4604310	-2.4385080
H	8.7381560	0.2067300	-3.0260420	C	-3.4316380	0.6751980	-3.2868910
H	4.3638050	-3.7674880	-4.8625510	C	-2.5588200	1.6686900	-2.9399680
H	2.0959510	-2.8023290	-5.2933830	C	-1.8481820	1.5858340	-1.7115680
H	-0.6562700	-2.2210570	0.1185620	C	-0.1032410	1.3172120	2.9649750
H	0.9225040	-2.9016050	1.9280450	C	0.5161220	1.2203490	1.7500010
H	5.0118330	1.4080600	3.6110820	C	-0.2688740	1.2301390	0.5652920
H	4.0967440	3.5550540	2.7124500	C	0.2818880	1.8214000	-0.6085370
H	5.9270740	3.7953530	-4.3770210	C	-0.5472750	2.1672460	-1.6353120
H	3.7724810	4.7238110	-3.5269940	C	-3.7389050	-1.7242250	-3.0722360
H	2.5976120	5.0776580	-1.4743170	C	-3.3081040	-2.8526830	-2.4337670
H	2.8602150	4.7210240	0.9805600	C	-4.2402300	-3.5279250	2.7736640
H	4.7777350	-0.9684720	3.6202770	C	-5.4323300	-2.8962680	2.9935650
H	3.0852640	-2.6846920	2.9983860	C	-6.3911410	2.3929270	1.9629750
H	-0.9613270	-1.4538750	-2.1622440	C	-5.3842120	3.1079240	2.5507330
H	0.1570830	-1.6680590	-4.3677460	H	-1.4076580	2.6659660	4.8256770
H	6.4695780	-3.7162720	-3.6243910	H	-3.5655150	3.8415300	4.3597280
H	8.1952430	-2.1245930	-2.7958250	H	-8.2897580	0.5603460	1.9276630
C	-3.2371880	-1.6155260	-0.2901170	H	-7.8379400	-1.7370190	2.7979400
C	-3.6470070	-1.7966560	1.0858710	H	-2.4566450	-5.0190370	1.5085190
C	-3.1568830	-0.3788130	-1.0593550	H	-2.2704870	-4.8445980	-0.9712890
C	-2.3228460	0.7288570	-0.6670030	H	-3.8745120	0.6390590	-4.2798330
C	-1.6589310	0.8951870	0.6236180	H	-2.2833300	2.4449900	-3.6505350
C	-2.3190780	1.0878910	1.8855050	H	0.4739590	1.4722540	3.8739840
C	-3.7507620	1.3472860	1.9900790	H	1.5951030	1.2906620	1.6646350

H	1.3274780	2.1017960	-0.6093620
H	-0.1890220	2.7573480	-2.4754050
H	-4.0462710	-1.7454640	-4.1152380
H	-3.2328520	-3.8057860	-2.9520900
H	-4.0033630	-4.4732840	3.2561630
H	-6.1877190	-3.3287900	3.6462240
H	-7.4012570	2.7911580	1.9001440
H	-5.5705270	4.0909780	2.9782750

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molecule18_nested

C	-2.9372030	-0.8239580	1.6185140
C	-4.3224740	-0.4570080	1.8084710
C	-5.3195560	-0.1660090	0.7910490
C	-5.1816820	0.9625640	-0.0960440
C	-4.0071570	1.8221040	-0.1099520
C	-2.6740040	1.4714900	-0.5418320
C	-2.5230050	0.4813320	-1.5915690
C	-2.6012290	-1.7238310	0.5323260
C	-3.2436180	-1.8224930	-0.7694390
C	-3.2471080	-0.7660630	-1.7615170
C	-4.8201510	-0.5308450	3.1413860
C	-6.1762730	-0.9232530	3.3628160
C	-7.0041760	-1.1691650	2.3007380
C	-6.6349280	-0.6789630	1.0110610
C	-1.7129940	-2.7877060	0.8681360
C	-0.7513130	-2.6039570	1.9028570
C	-0.8729690	-1.5631630	2.7779880
C	-2.0788070	-0.8045700	2.7672990
C	-3.5985000	-1.1222010	-3.1043040
C	-4.2999170	-2.3350920	-3.3616600
C	-4.2599420	-3.3398690	-2.4366230
C	-3.5413230	-3.1474100	-1.2213990
C	-1.6447110	2.4593360	-0.3998520
C	-0.5116240	2.4546710	-1.2637780
C	-0.5987380	1.7669230	-2.4399260
C	-1.6753000	0.8630510	-2.6715910
C	-6.3789310	1.5167070	-0.6415120

C	-6.5011570	2.9318920	-0.7955410
C	-5.5431160	3.7448730	-0.2515310
C	-4.2671390	3.2070330	0.1028010
C	-1.8972570	-4.0736980	0.2800570
C	-2.9128230	-4.2754720	-0.6145000
C	-2.5709860	-0.3522600	4.0254870
C	-3.9243140	-0.3327850	4.2318320
C	-7.6702630	-0.3912240	0.0739870
C	-7.5485720	0.7064680	-0.7341100
C	-1.8991710	3.6622510	0.3204050
C	-3.1962910	4.0676760	0.4824160
C	-1.9671380	0.4119800	-3.9913710
C	-3.0198840	-0.4335400	-4.2112590
H	-6.5069770	-1.0865410	4.3861760
H	-8.0097810	-1.5570770	2.4464440
H	0.0351940	-3.3442320	2.0216100
H	-0.1791870	-1.4496400	3.6050740
H	-4.7043310	-2.5065120	-4.3569190
H	-4.6292750	-4.3351410	-2.6744890
H	0.2980990	3.1535420	-1.0836860
H	0.1335280	1.9154530	-3.2280020
H	-7.4303230	3.3373560	-1.1893660
H	-5.6913300	4.8197870	-0.1750420
H	-1.2758280	-4.8959840	0.6273370
H	-3.1502570	-5.2690170	-0.9877340
H	-1.8779000	-0.2528490	4.8582120
H	-4.3374750	-0.2305000	5.2330800
H	-8.6157140	-0.9237230	0.1522510
H	-8.3955450	1.0696090	-1.3124720
H	-1.0715880	4.3389180	0.5162260
H	-3.4301290	5.0804870	0.8043050
H	-1.3716860	0.8032090	-4.8132500
H	-3.3156940	-0.7204810	-5.2178410
C	5.1889920	-0.9357600	-0.2195670
C	5.3353640	0.0890130	0.7849110
C	4.3602070	0.2419320	1.8520220
C	2.9607590	0.5881340	1.7398660
C	2.5730820	1.6085870	0.7855580
C	3.1928990	1.9009060	-0.4979360

C	3.2191840	0.9876020	-1.6233820	H	-0.2772760	-3.0223020	-1.4580520
C	4.0171530	-1.7933460	-0.3204240	H	4.4913430	4.6872110	-2.0508520
C	2.6819370	-1.3994350	-0.7056620	H	4.6198500	3.1007430	-3.9609900
C	2.5210450	-0.2855160	-1.6218840	H	0.2333420	0.8655790	3.8444670
C	6.6494870	0.5932530	1.0324050	H	-0.0822650	2.9342950	2.5134530
C	7.0408780	0.9482350	2.3592840	H	3.4542590	-5.1386980	0.2077260
C	6.2428740	0.5715160	3.4057920	H	1.0927520	-4.3813790	-0.0057560
C	4.8901930	0.1746870	3.1726480	H	8.3825350	-0.8845450	-1.4900770
C	4.2828570	-3.1924090	-0.2693910	H	8.6102320	0.9513390	0.1669460
C	5.5598640	-3.6815770	-0.6857930	H	4.4721580	-0.3845820	5.2245170
C	6.5097070	-2.8084510	-1.1442220	H	2.0031240	-0.4074740	4.9083030
C	6.3812580	-1.4187850	-0.8378790	H	3.0050080	5.3408360	-0.2422070
C	1.6800440	-0.5372010	-2.7446490	H	1.1652770	4.6980960	1.3278510
C	0.6117410	-1.4733720	-2.6321630	H	3.2862650	1.4041220	-5.0549020
C	0.5278540	-2.3009310	-1.5497170	H	1.3789560	-0.2041470	-4.8614070
C	1.6582430	-2.4032120	-0.6882450				
C	3.4488130	3.2826790	-0.7679780				
C	4.1534990	3.6582280	-1.9479760				
C	4.2226440	2.7866570	-2.9981520	120			
C	3.5581110	1.5301560	-2.9058030	molecule18_edge-to-edge			
C	2.1329100	0.3982100	2.8954700	C	4.9068870	1.4057640	-0.9267860
C	0.9032180	1.1061200	3.0247210	C	3.7149530	1.8645810	-0.2497980
C	0.7258970	2.2430080	2.2902660	C	3.1920220	1.3437300	1.0041870
C	1.6611030	2.5904780	1.2728510	C	2.6199590	0.0294130	1.1883110
C	3.2158740	-4.0965470	0.0051060	C	2.2071390	-0.7559700	0.0442350
C	1.9172790	-3.6817630	-0.1155320	C	2.9760650	-1.1013750	-1.1355900
C	7.5427310	-0.5920530	-0.8632690	C	4.2825150	-1.6956170	-0.9795640
C	7.6687230	0.4187820	0.0508880	C	5.9230220	0.7037170	-0.1707130
C	4.0295090	-0.1785640	4.2522380	C	5.7599660	-0.4366010	0.7083890
C	2.6713910	-0.1840910	4.0792330	C	5.1085250	-1.6273880	0.2170200
C	2.7984540	4.2993900	-0.0066230	C	3.2008450	3.1304450	-0.6588150
C	1.8021520	3.9490300	0.8631790	C	2.6668630	4.0237810	0.3194130
C	2.9982650	0.9790320	-4.0960450	C	2.7165720	3.6810870	1.6448090
C	1.9660910	0.0869570	-3.9933320	C	2.9269830	2.3169890	2.0132020
H	8.0434280	1.3361240	2.5246950	C	7.2476250	1.2106090	-0.2904640
H	6.5955390	0.6271940	4.4333390	C	7.6345560	1.8710260	-1.4946240
H	5.7135490	-4.7575710	-0.7288510	C	6.7024190	2.1728880	-2.4515890
H	7.4373670	-3.1630050	-1.5876490	C	5.3203730	2.1019170	-2.1074430
H	-0.1174460	-1.5278960	-3.4352920	C	5.5886590	-2.8744750	0.7132850
				C	6.2120000	-2.9222110	1.9951250

C	6.7087660	-1.7764600	2.5556480	H	6.1001060	-4.9250110	0.2124750
C	6.6855470	-0.5732970	1.7912410	C	-5.8671640	0.3929700	0.4506610
C	2.2540980	-1.3778240	-2.3410140	C	-5.1942010	1.5831100	-0.0120320
C	2.9263430	-1.9606460	-3.4548560	C	-4.1596130	1.6276880	-1.0357550
C	4.0812950	-2.6614080	-3.2335550	C	-2.8155000	1.1235150	-0.8824550
C	4.6564240	-2.6907490	-1.9290070	C	-2.2952950	0.8616900	0.4469880
C	1.9897510	-0.2546570	2.4433700	C	-2.8694500	0.0437070	1.4943610
C	0.9019980	-1.1724940	2.5112990	C	-3.3118220	-1.3047360	1.2142480
C	0.2794700	-1.5457110	1.3520160	C	-5.8481840	-0.7977860	-0.3733300
C	0.8852310	-1.2790430	0.0909820	C	-4.7029980	-1.4672300	-0.9548570
C	8.1535270	1.0581920	0.8024300	C	-3.5976620	-1.8512960	-0.1051770
C	7.8055120	0.3052330	1.8919110	C	-5.8132530	2.8291560	0.2971020
C	4.4321710	3.0222360	-2.7389120	C	-5.8001520	3.8817260	-0.6699520
C	3.4277780	3.5780380	-1.9941590	C	-5.2701970	3.6500530	-1.9113660
C	2.6283210	1.8864860	3.3394120	C	-4.3917960	2.5393060	-2.1067250
C	2.2110380	0.6024600	3.5596370	C	-7.1165100	-1.3807540	-0.6520920
C	0.8285430	-1.4171320	-2.3288500	C	-8.1775820	-1.2241110	0.2898860
C	0.1846420	-1.5185680	-1.1269430	C	-8.0331300	-0.3883670	1.3648050
C	5.4012810	-3.8320890	-1.4980510	C	-6.9556140	0.5467180	1.3676170
C	5.6780400	-3.9971610	-0.1669070	C	-2.9560620	-3.0854360	-0.4206940
H	2.3381060	5.0099630	0.0006420	C	-2.9651780	-3.5550040	-1.7683690
H	2.4608930	4.3969840	2.4227380	C	-3.8929840	-3.0748350	-2.6510830
H	8.6827980	2.1283680	-1.6307530	C	-4.9133970	-2.2058380	-2.1621670
H	6.9892860	2.6578830	-3.3819550	C	-2.5188000	0.3655330	2.8471370
H	6.4073630	-3.8931530	2.4456190	C	-2.8564400	-0.5271260	3.9050690
H	7.3012410	-1.8132520	3.4671900	C	-3.1121170	-1.8383120	3.6125780
H	2.4078600	-2.0267870	-4.4089690	C	-3.1538840	-2.2694650	2.2541000
H	4.5001660	-3.3053590	-4.0041710	C	-1.8690510	1.4243560	-1.9142330
H	0.4563440	-1.3909840	3.4783760	C	-0.4926880	1.6184340	-1.5941000
H	-0.6805800	-2.0489070	1.3693570	C	-0.1477280	1.8184740	-0.2874340
H	9.1152970	1.5641660	0.7525510	C	-1.0667290	1.5098270	0.7571320
H	8.4718560	0.2116740	2.7465210	C	-7.2986950	-2.1024220	-1.8692110
H	4.6947580	3.4275420	-3.7136310	C	-6.2306080	-2.3703940	-2.6836730
H	2.8772150	4.4443770	-2.3548330	C	-7.1601170	1.7962060	2.0229890
H	2.6023790	2.6273470	4.1358620	C	-6.6427920	2.9281910	1.4530790
H	1.8520820	0.2930970	4.5387010	C	-3.5546090	2.4885000	-3.2601560
H	0.2935330	-1.5645170	-3.2643450	C	-2.3262730	1.8894040	-3.1819980
H	-0.8715550	-1.7594180	-1.0760400	C	-1.5660000	1.3882770	3.1228900
H	5.6192630	-4.6142110	-2.2218950	C	-0.7638960	1.8342430	2.1094500

C	-2.7968090	-3.6141230	1.9293360
C	-2.5153570	-3.9442100	0.6306400
H	-6.3331130	4.8026840	-0.4446590
H	-5.3869050	4.3691520	-2.7190620
H	-9.0960990	-1.7857510	0.1336570
H	-8.8245530	-0.2810840	2.1032110
H	-2.3110990	-4.3817910	-2.0365440
H	-3.9946790	-3.5056020	-3.6447660
H	-2.7107120	-0.2028800	4.9332500
H	-3.1623050	-2.5881110	4.3994090
H	0.2210720	1.7930310	-2.3950380
H	0.8345250	2.1859220	-0.0157580
H	-8.3030590	-2.4249990	-2.1352050
H	-6.3609230	-2.8934350	-3.6283240
H	-7.8901420	1.8594280	2.8270130
H	-6.9587680	3.9145570	1.7864750
H	-3.8457810	3.0523260	-4.1439950
H	-1.6173750	1.9600760	-4.0042280
H	-1.3531880	1.6406760	4.1593130
H	0.1267760	2.4217690	2.3102460
H	-2.6185370	-4.3147830	2.7417230
H	-2.0778760	-4.9051480	0.3708970

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molecule18_up-down_edge-to-edge

C	4.5436080	1.2947810	-1.1248060
C	3.5487740	1.8236840	-0.2163180
C	3.1560590	1.2966860	1.0798650
C	2.5452030	-0.0059080	1.2344170
C	2.2817450	-0.8815800	0.1072870
C	3.2403170	-1.4978680	-0.7838660
C	4.4959240	-1.9624560	-0.2405840
C	5.7537070	0.7300230	-0.5723530
C	5.8962040	-0.0449090	0.6489400
C	5.2900480	-1.3455630	0.8086660
C	3.0144760	3.1009750	-0.5521290
C	2.6648480	4.0124600	0.4894890
C	2.8030690	3.6401670	1.7996800

C	2.9426200	2.2553150	2.1186240
C	6.9733950	1.1247640	-1.1926550
C	6.9705970	1.4759780	-2.5742660
C	5.7900980	1.7173530	-3.2249200
C	4.5988410	1.8348080	-2.4515210
C	5.8583760	-2.2221630	1.7827050
C	6.6393370	-1.6810070	2.8458830
C	7.2125510	-0.4473070	2.6951530
C	7.0159120	0.2682470	1.4776590
C	2.7427400	-2.1377350	-1.9669880
C	3.5244570	-3.1288640	-2.6280830
C	4.5271120	-3.7480930	-1.9304090
C	4.9265370	-3.2555620	-0.6535540
C	1.7673260	-0.2322360	2.4123620
C	0.5921270	-1.0389420	2.3521830
C	0.1015650	-1.4033930	1.1287400
C	0.9336650	-1.3191950	-0.0256060
C	8.1445110	1.2928550	-0.3908010
C	8.0965110	1.0427080	0.9543560
C	3.6333370	2.7939160	-2.8766810
C	2.9415020	3.4898550	-1.9223160
C	2.5566460	1.8133790	3.4187320
C	1.9753940	0.5834480	3.5626510
C	1.3554290	-2.0698800	-2.2892100
C	0.4680370	-1.7762470	-1.2913820
C	5.6326860	-4.0861250	0.2703100
C	5.9219200	-3.6261460	1.5271700
H	2.3508780	5.0172530	0.2167930
H	2.6331610	4.3479180	2.6078380
H	7.9254280	1.6136510	-3.0773470
H	5.7787080	2.0361930	-4.2647950
H	6.9170760	-2.3266510	3.6763510
H	7.9574120	-0.0888510	3.4024830
H	3.1772220	-3.5261700	-3.5793670
H	4.9880980	-4.6605760	-2.3028820
H	0.0059850	-1.1800410	3.2570290
H	-0.8938680	-1.8201770	1.0219480
H	9.0395040	1.6965910	-0.8589960
H	8.9432250	1.2629980	1.6005450

H	3.6244420	3.1098260	-3.9175300	C	-2.7831390	-3.5090800	1.7965650
H	2.3768350	4.3837690	-2.1783050	C	-2.1788540	-0.4641590	-3.7050150
H	2.5672430	2.5262010	4.2406390	C	-1.4496680	0.6157430	-3.2891360
H	1.5094500	0.2935650	4.5020240	C	-1.2152500	1.9963240	2.1770890
H	1.0107680	-2.4614240	-3.2436690	C	-2.3665790	2.3992080	2.7953410
H	-0.5946770	-1.9391900	-1.4242410	C	-6.4549370	2.8686920	-2.1045310
H	5.8609570	-5.1085760	-0.0226800	C	-6.1196970	3.7047210	-1.0730260
H	6.3655100	-4.2756870	2.2783340	C	-8.0361940	-1.5228460	0.3172320
C	-3.0069480	-0.8113480	-1.3966260	C	-7.6108170	-1.6182920	1.6157030
C	-2.4137780	0.4560170	-1.0292650	H	0.4928100	1.9960770	-2.0577720
C	-2.4976490	1.1011040	0.2721130	H	0.7696570	2.1581440	0.4125030
C	-3.7005940	1.6591280	0.8484100	H	-2.4998910	-4.6343210	-2.0958600
C	-4.8628490	1.8937970	0.0162010	H	-2.6891250	-3.0505710	-4.0107720
C	-5.5724810	0.9450260	-0.8161950	H	-6.3685520	-2.0338010	3.9925920
C	-5.9571000	-0.3280390	-0.2546320	H	-4.0195870	-2.8357800	4.0894610
C	-3.3229340	-1.7821480	-0.3696750	H	-7.7582700	0.9771060	-3.4855810
C	-4.0169120	-1.5642640	0.8863220	H	-8.6455250	-1.0055950	-2.2782730
C	-5.3387180	-0.9833490	0.8890150	H	-4.3693110	4.1028900	3.1949370
C	-1.4198930	0.9750960	-1.9109330	H	-5.7645170	4.9458410	1.3050720
C	-0.2948870	1.6761550	-1.3805140	H	-2.0793000	-4.9060590	0.3299000
C	-0.1437190	1.7773210	-0.0260480	H	-2.4861360	-4.1042030	2.6569150
C	-1.2623850	1.5457770	0.8251300	H	-2.1304140	-0.8084490	-4.7358230
C	-2.8740580	-3.1150480	-0.5963690	H	-0.7937820	1.1447970	-3.9770390
C	-2.7140310	-3.5801880	-1.9347860	H	-0.2428190	2.1332350	2.6435950
C	-2.8043310	-2.7072330	-2.9850760	H	-2.3400780	2.8726530	3.7746340
C	-2.7776780	-1.3055330	-2.7228820	H	-6.9927360	3.2381050	-2.9748030
C	-6.2290470	-1.4117570	1.9173400	H	-6.4013320	4.7555300	-1.0884060
C	-5.6947170	-1.8894450	3.1506590	H	-9.0337040	-1.8427590	0.0244830
C	-4.4017520	-2.3341230	3.2030840	H	-8.2653310	-1.9931650	2.3992630
C	-3.6465370	-2.3900590	1.9944060				
C	-6.3438350	1.4606050	-1.9073960				
C	-7.2847500	0.6214280	-2.5731080				
C	-7.7693740	-0.4746480	-1.9118530				
C	-7.2273770	-0.8421880	-0.6447880				
C	-3.5721260	2.4506380	2.0333410				
C	-4.4654240	3.5375520	2.2705720				
C	-5.2409730	3.9945840	1.2385340				
C	-5.4026320	3.2105180	0.0570660				
C	-2.5493320	-3.9439500	0.5195730				