

Cartesian coordinates for the optimized structures

TDI-LPP

Atom	X	Y	Z
C	-3.6954	3.1198	-2.7838
C	-3.13	2.0163	-2.2617
C	-1.7773	1.9961	-2.1455
C	-1.0876	3.1582	-2.2225
C	-1.7022	4.2809	-2.6649
C	-2.9978	4.2396	-3.0257
C	0.222	3.1853	-1.8788
C	0.8436	4.386	-1.7505
C	0.2397	5.4667	-2.2779
C	-1.0075	5.4282	-2.7691
C	-1.0739	0.8431	-2.0278
C	0.2552	0.8054	-1.8016
C	0.8753	2.003	-1.7493
C	-1.6239	-0.3381	-2.3563
C	-0.9521	-1.4886	-2.2883
C	0.3238	-1.5656	-1.8731
C	0.9377	-0.372	-1.7157
C	2.2791	-0.4001	-1.5623
C	2.8884	0.7902	-1.6964
C	2.2171	1.9393	-1.7888
C	-1.5687	6.5756	-3.2437
N	-2.9051	6.489	-3.5702
C	-3.6485	5.3308	-3.518
C	0.9858	-2.75	-1.8409
C	2.3367	-2.7026	-1.7637
C	2.9959	-1.5498	-1.5034
C	0.3692	-3.9563	-1.974
C	1.1106	-5.0238	-2.3317
C	2.4477	-4.9659	-2.3458
C	3.0501	-3.8233	-1.9932
C	4.3891	-3.8022	-2.0108
C	5.0247	-2.6791	-1.6551
C	4.3396	-1.5776	-1.2894
C	3.1861	-6.0764	-2.6174
N	4.4125	-6.1047	-1.9665
C	5.0902	-4.9356	-2.2872

C	1.9493	4.6375	-1.0014
C	5.0482	-0.6638	-0.575
C	-0.9093	-4.246	-1.6166
C	-3.9827	1.0872	-1.7532
C	2.8472	5.6019	-1.2779
C	3.8873	5.8735	-0.4735
C	4.0974	5.245	0.7019
C	3.2002	4.2725	0.9673
C	2.1784	3.9711	0.1479
C	-3.6857	0.4187	-0.6207
C	-4.549	-0.421	-0.0249
C	-5.7801	-0.6846	-0.5109
C	-6.05	-0.0484	-1.6701
C	-5.2026	0.8148	-2.2538
C	-1.4862	-3.6474	-0.5553
C	-2.7005	-3.9997	-0.0995
C	-3.4561	-4.9571	-0.6773
C	-2.8917	-5.5133	-1.7695
C	-1.6628	-5.1934	-2.2056
C	6.3541	-0.3952	-0.7622
C	7.0423	0.4415	0.0316
C	6.5057	1.0465	1.112
C	5.1916	0.79	1.2805
C	4.4898	-0.0194	0.4694
C	5.0957	5.6036	1.5519
C	7.2433	1.7973	1.9726
C	-4.6548	-5.3703	-0.1875
C	-6.6882	-1.4731	0.1236
C	5.1385	5.2246	2.8447
C	6.0685	5.6648	3.7098
C	7.0784	6.491	3.3677
C	7.0714	6.8126	2.0582
C	6.1212	6.4047	1.2004
C	6.8125	2.153	3.1994
C	7.5817	2.8004	4.0915
C	8.8462	3.1982	3.8419
C	9.2486	2.9027	2.5891
C	8.4938	2.2252	1.7077
C	-6.5442	-1.8931	1.3964
C	-7.488	-2.586	2.0567

C	-8.6609	-2.9661	1.5093
C	-8.7724	-2.6019	0.2156
C	-7.8433	-1.8836	-0.4373
C	-5.5165	-6.1405	-0.8812
C	-6.6715	-6.6025	-0.3735
C	-7.0692	-6.374	0.8944
C	-6.2189	-5.5804	1.5773
C	-5.0827	-5.0836	1.0582
C	7.9982	6.968	4.2498
C	9.6405	3.8147	4.7591
C	-8.2013	-6.9063	1.4295
C	-9.6352	-3.6299	2.1899
C	-8.464	-6.8767	2.7558
C	-9.5608	-7.4279	3.3007
C	-10.4735	-8.0271	2.5269
C	-10.2569	-8.0687	1.207
C	-9.1449	-7.5263	0.6847
C	-10.7485	-4.1161	1.5944
C	-11.7261	-4.7512	2.2612
C	-11.6371	-4.9281	3.5845
C	-10.5496	-4.467	4.2135
C	-9.5801	-3.8429	3.5248
C	7.8685	6.8236	5.5883
C	8.7505	7.3202	6.471
C	9.8344	7.9805	6.0469
C	10.008	8.1341	4.729
C	9.1055	7.6426	3.8644
C	9.3008	3.9232	6.064
C	10.0902	4.4983	6.9859
C	11.2732	5.0165	6.6356
C	11.6423	4.9424	5.3516
C	10.8426	4.3518	4.4487
O	-0.9818	7.6295	-3.3692
O	-4.8016	5.3334	-3.8929
O	2.7939	-6.9978	-3.2962
O	6.2278	-4.9417	-2.6988
C	-3.5145	7.6053	-4.0323
C	4.9867	-7.2221	-1.4084
C	-3.3902	7.8757	-5.3529
C	-3.9925	8.9728	-5.8445

C	-4.706	9.7803	-5.0522
C	-4.8193	9.4892	-3.751
C	-4.2279	8.4072	-3.2073
C	6.2297	-7.2137	-0.8247
C	6.836	-8.361	-0.4602
C	6.231	-9.545	-0.5194
C	4.9298	-9.5109	-0.7972
C	4.2926	-8.3821	-1.1668
C	-2.612	6.9809	-6.3166
C	-4.4473	8.2012	-1.7055
C	-3.5442	6.37	-7.377
C	-1.4387	7.7343	-6.966
C	-5.7481	7.4232	-1.4437
C	-3.2937	7.6153	-0.8767
C	2.7659	-8.5859	-1.156
C	7.0645	-5.9922	-0.396
C	2.2534	-9.6323	-2.1647
C	2.2822	-8.9716	0.2653
C	7.2423	-5.9741	1.1437
C	8.4494	-5.8964	-1.0652
H	-4.7865	3.1742	-2.9074
H	0.7157	6.4551	-2.2004
H	-2.6298	-0.4269	-2.7948
H	-1.5084	-2.3499	-2.6855
H	3.9751	0.8942	-1.8338
H	2.8536	2.8133	-1.9919
H	0.6688	-6.0244	-2.4596
H	6.1136	-2.7625	-1.5158
H	2.7787	6.1979	-2.2041
H	4.5234	6.7003	-0.8247
H	3.2497	3.6647	1.884
H	1.4773	3.1909	0.4935
H	-2.7331	0.6008	-0.0924
H	-4.1767	-0.8702	0.9084
H	-7.0149	-0.1493	-2.1896
H	-5.5527	1.2788	-3.1916
H	-0.9358	-2.8881	0.0282
H	-3.0368	-3.4484	0.7924
H	-3.3762	-6.3203	-2.34
H	-1.3038	-5.7352	-3.0975

H	6.915	-0.8446	-1.5993
H	8.1056	0.5407	-0.2346
H	4.6112	1.2212	2.1107
H	3.4365	-0.2023	0.7464
H	4.3666	4.5761	3.2877
H	5.9433	5.2906	4.7372
H	7.8239	7.4807	1.6126
H	6.2468	6.7727	0.1702
H	5.8144	1.8742	3.5716
H	7.0916	2.984	5.0596
H	10.2535	3.1563	2.2191
H	8.9779	2.0434	0.7356
H	-5.6582	-1.6398	1.9987
H	-7.2247	-2.821	3.099
H	-9.6637	-2.8342	-0.3863
H	-8.0989	-1.6517	-1.4827
H	-5.325	-6.4337	-1.9253
H	-7.2483	-7.2349	-1.0654
H	-6.4104	-5.282	2.6192
H	-4.4853	-4.4727	1.7529
H	-7.7786	-6.4294	3.4909
H	-9.718	-7.3914	4.3924
H	-11.3805	-8.4737	2.9658
H	-11.0016	-8.5523	0.5517
H	-9.0822	-7.6091	-0.4104
H	-10.9311	-4.0416	0.5126
H	-12.6095	-5.1351	1.7226
H	-12.4345	-5.4476	4.1406
H	-10.4568	-4.6057	5.3044
H	-8.7459	-3.4985	4.1532
H	7.0117	6.3157	6.0551
H	8.5884	7.1869	7.5545
H	10.5675	8.3834	6.7646
H	10.9007	8.6673	4.3595
H	9.3613	7.8193	2.8094
H	8.3628	3.5216	6.4744
H	9.7686	4.5493	8.0404
H	11.9237	5.4975	7.3843
H	12.6095	5.3739	5.0413
H	11.2472	4.3625	3.4261

H	-3.9192	9.2255	-6.9142
H	-5.202	10.6728	-5.4693
H	-5.4235	10.1693	-3.127
H	7.858	-8.3721	-0.0498
H	6.7325	-10.4714	-0.1947
H	4.3926	-10.4629	-0.6628
H	-2.158	6.112	-5.7808
H	-4.5945	9.2211	-1.2605
H	-2.993	5.6566	-8.0316
H	-4.3774	5.8073	-6.8962
H	-3.9926	7.1425	-8.0404
H	-0.8291	7.052	-7.6019
H	-0.7616	8.1616	-6.1912
H	-1.7801	8.5686	-7.6178
H	-5.9936	7.4031	-0.3572
H	-6.6139	7.8846	-1.9712
H	-5.6686	6.3663	-1.7779
H	-3.5024	7.7105	0.2139
H	-2.3389	8.1552	-1.0672
H	-3.1482	6.5286	-1.0537
H	2.2109	-7.63	-1.2675
H	6.5082	-5.0376	-0.5116
H	1.1431	-9.5882	-2.2475
H	2.6719	-9.4847	-3.1839
H	2.5088	-10.6728	-1.8668
H	1.1687	-8.9958	0.3191
H	2.633	-8.2327	1.0231
H	2.6262	-9.9757	0.5961
H	7.7324	-5.0314	1.4817
H	6.2573	-6.038	1.6624
H	7.8749	-6.8032	1.5289
H	8.913	-4.9022	-0.8698
H	8.4024	-6.0337	-2.1673
H	9.162	-6.6597	-0.6826

TDI-[6]CPP

Atom	X	Y	Z
C	-1.3426	3.0286	1.9388
C	-1.3845	4.3742	1.9093
C	-0.6196	5.1157	1.1035

C	0.1697	4.5032	0.1917
C	0.2966	3.1948	0.1994
C	-0.417	2.4675	1.099
C	0.7257	5.2148	-0.7918
C	1.5992	4.5806	-1.6393
C	1.8049	3.2219	-1.6806
C	0.9369	2.5776	-0.846
C	0.599	1.2697	-1.0832
C	0.288	0.5498	0.022
C	-0.1147	1.1379	1.1684
C	0.3943	-0.7918	-0.0174
C	0.4469	-1.5007	1.1148
C	0.2349	-0.9197	2.3009
C	-0.1363	0.3726	2.2791
C	0.6928	0.6268	-2.2705
C	0.3662	-0.6748	-2.316
C	0.2401	-1.3786	-1.1885
C	-0.2191	-2.638	-1.1755
C	0.1892	-3.4111	-0.1086
C	0.7145	-2.8253	1.0204
C	0.012	-4.7737	-0.1932
C	0.4202	-5.4931	0.8655
C	1.0499	-4.8887	1.8933
C	1.3373	-3.5736	1.9886
C	-0.9682	-3.1335	-2.223
C	-1.0602	-4.4646	-2.2607
C	-0.5832	-5.2619	-1.3074
C	-0.7646	-6.5937	-1.4919
N	-0.2751	-7.3036	-0.3924
C	0.3012	-6.8429	0.7714
C	-0.7972	6.4667	1.2282
N	-0.1978	7.192	0.1979
C	0.5318	6.5715	-0.8513
O	-1.2479	-7.1746	-2.442
O	0.7276	-7.6385	1.5812
O	1.0317	7.2371	-1.756
O	-1.4059	7.0656	2.1018
C	-0.4796	-8.643	-0.2022
C	-0.1818	8.572	0.3507
C	-1.5307	-9.0299	0.4491

C	-1.6848	-10.3384	0.4344
C	-0.8819	-11.1906	-0.1573
C	0.3622	-10.8559	-0.6277
C	0.4208	-9.5195	-0.8195
C	0.9829	9.0406	0.9867
C	0.9465	10.3711	0.9787
C	0.0432	11.2045	0.5067
C	-1.1109	10.7073	0.0332
C	-1.2034	9.3728	-0.0512
C	1.7206	-9.0242	-1.3598
C	-2.6411	-8.3426	1.1439
C	-3.2651	-6.9779	0.5215
C	-1.9891	-8.0353	2.6341
C	2.6663	-8.4562	-0.4787
C	1.5729	-7.9445	-2.6286
C	-2.5859	8.9258	-0.6322
C	-2.5199	9.1101	-2.0346
C	-3.8978	9.8254	-0.1795
C	2.1117	8.3202	1.6562
C	2.7644	8.9188	2.9439
C	3.2017	7.8705	0.7547
C	-10.5969	1.0939	2.0209
C	-11.1992	1.1255	0.8153
C	-10.8888	-1.0948	0.5425
C	-10.2617	-1.1162	1.7196
C	-9.8653	0.0121	2.333
C	-8.7154	0.1718	3.0534
C	-7.7679	-0.7746	2.9366
C	-6.4614	-0.5281	3.1201
C	-6.0295	0.6978	3.5078
C	-7.0078	1.5354	3.9271
C	-8.3132	1.2808	3.7081
C	-4.7547	1.1723	3.3463
C	-4.2113	2.2225	3.9886
C	-3.0463	2.7559	3.6201
C	-2.3596	2.3611	2.5307
C	-2.8713	1.2596	1.9526
C	-4.0263	0.6892	2.3315
C	-3.5588	-2.2617	-4.7222
C	-2.5275	-2.8663	-4.112

C	-1.8412	-2.4534	-3.0445
C	-2.3867	-1.2974	-2.6445
C	-3.4342	-0.6763	-3.1885
C	-4.1722	-1.1934	-4.2018
C	-7.6714	-0.9109	-4.9474
C	-6.4141	-1.4001	-5.0249
C	-5.4155	-0.7048	-4.4427
C	-5.7324	0.5636	-4.0304
C	-7.0057	1.0101	-3.9334
C	-8.0347	0.2019	-4.2247
C	-11.1777	0.0945	-0.0465
C	-9.1961	0.3863	-3.4942
C	-9.5792	1.5061	-2.8473
C	-10.4941	1.4359	-1.8387
C	-10.9889	0.2489	-1.3767
C	-10.819	-0.7756	-2.226
C	-10.0207	-0.6663	-3.3058
C	10.1533	-1.0523	3.415
C	10.937	-0.8843	2.3444
C	10.3923	1.3613	2.1813
C	9.5008	1.1711	3.169
C	9.2386	-0.0687	3.6659
C	8.06	-0.2818	4.2875
C	6.9861	0.5539	4.2365
C	5.7568	0.0425	4.3972
C	5.5517	-1.2628	4.6654
C	6.6156	-1.8512	5.2653
C	7.8655	-1.3687	5.0677
C	4.4383	-1.8786	4.1732
C	3.9814	-3.1306	4.5469
C	2.9026	-3.6587	3.9299
C	2.2991	-3.0762	2.8652
C	2.8924	-1.948	2.4316
C	3.833	-1.2865	3.0942
C	4.5565	0.8814	-2.3818
C	3.377	1.3924	-1.9354
C	2.8288	2.5627	-2.2919
C	3.565	3.108	-3.2531
C	4.7514	2.6912	-3.6818
C	5.3076	1.5739	-3.2474

C	8.9073	1.7084	-3.5619
C	7.6092	2.054	-3.6853
C	6.5822	1.2251	-3.511
C	7.0031	-0.0581	-3.422
C	8.2915	-0.4267	-3.1714
C	9.2705	0.4939	-3.0824
C	11.023	0.2743	1.6665
C	10.3206	0.3054	-2.2062
C	10.6245	-0.8549	-1.5996
C	11.1953	-0.9208	-0.3971
C	11.2465	0.2241	0.3211
C	11.3043	1.3747	-0.4056
C	10.9303	1.3911	-1.6932
H	-2.1882	4.885	2.4523
H	2.2209	5.2303	-2.2388
H	0.1705	-1.4141	3.2884
H	-0.425	0.7539	3.2759
H	1.0096	1.0301	-3.2536
H	0.3061	-1.1546	-3.3099
H	1.5518	-5.4976	2.6406
H	-1.6397	-4.9733	-3.0401
H	-2.5436	-11.0715	0.732
H	-1.2414	-12.2911	-0.2006
H	1.1706	-11.5682	-1.007
H	1.7915	10.9856	1.3545
H	0.1892	12.2911	0.5337
H	-2.0395	11.5089	-0.2023
H	2.3624	-9.9109	-1.9276
H	-3.5765	-9.0365	1.2732
H	-3.8124	-7.5323	-0.266
H	-2.5904	-6.0565	0.0622
H	-3.9506	-6.6025	1.3373
H	-2.5657	-7.6233	3.5572
H	-1.6863	-9.0349	2.9761
H	-0.9778	-7.5542	2.5804
H	3.0535	-9.4001	0.1311
H	2.3391	-7.6245	0.0832
H	3.5545	-8.2863	-0.9013
H	2.6219	-7.5941	-2.5374
H	1.2821	-8.4541	-3.6255

H	1.0831	-7.1058	-2.3085
H	-2.7223	7.9525	-0.248
H	-1.984	8.1686	-2.4866
H	-1.7922	10.4294	-2.4112
H	-3.3697	9.1321	-2.5206
H	-3.7843	10.8488	-0.3896
H	-4.9116	9.8499	-0.562
H	-3.7578	9.6857	0.9205
H	1.4916	7.3988	1.8773
H	3.6938	9.4405	2.6406
H	3.3895	8.0908	3.4135
H	1.9438	9.3337	3.5694
H	3.5211	8.7525	0.1654
H	4.0184	7.5062	1.3872
H	2.8344	6.9327	0.3623
H	-10.5162	2.0558	2.5618
H	-11.6058	2.1108	0.52
H	-10.9582	-2.0435	-0.0107
H	-9.8225	-2.0924	1.9799
H	-7.9486	-1.768	2.493
H	-5.7233	-1.2962	2.8128
H	-6.7269	2.5467	4.2958
H	-9.0147	2.1011	3.9024
H	-4.6979	2.7274	4.8501
H	-2.7182	3.6482	4.1618
H	-2.4727	0.8078	1.0374
H	-4.4213	-0.0632	1.6304
H	-3.9723	-2.7554	-5.6167
H	-2.2695	-3.7893	-4.6351
H	-1.9989	-0.8145	-1.7345
H	-3.7515	0.1993	-2.5757
H	-8.4453	-1.5742	-5.3741
H	-6.1568	-2.362	-5.495
H	-4.9621	1.2805	-3.6975
H	-7.0782	2.0035	-3.5114
H	-9.0818	2.4773	-2.9761
H	-10.5274	2.3741	-1.2628
H	-11.2026	-1.7705	-1.9756
H	-9.8725	-1.6405	-3.7737
H	10.0941	-2.0984	3.7493

H	11.4915	-1.7404	1.9516
H	10.3367	2.3634	1.6819
H	8.8424	2.0184	3.4389
H	7.0152	1.5754	3.8321
H	4.9402	0.7342	4.1227
H	6.5131	-2.8904	5.6167
H	8.7264	-2.0028	5.353
H	4.5081	-3.7069	5.3311
H	2.6347	-4.6546	4.2814
H	2.6481	-1.4425	1.4875
H	4.1378	-0.3297	2.6249
H	4.8675	-0.0126	-1.8166
H	2.9533	0.8529	-1.0608
H	3.2589	4.0673	-3.7247
H	5.2519	3.2978	-4.471
H	9.6009	2.571	-3.6297
H	7.4398	3.1391	-3.8171
H	6.2011	-0.8031	-3.2978
H	8.4838	-1.4274	-2.7886
H	10.2161	-1.8144	-1.9707
H	11.2624	-1.9144	0.0689
H	11.6058	2.3396	0.0579
H	10.8571	2.4233	-2.085

TDI-[9]CPP

Atom	X	Y	Z
C	16.3408	6.2294	5.3236
C	16.4457	7.5732	4.9823
H	17.1166	8.114	5.3818
C	15.5672	8.125	4.0573
H	15.6364	9.0434	3.826
C	14.583	7.3329	3.4768
C	14.4814	5.9892	3.8149
H	13.8089	5.4491	3.4172
C	15.36	5.4374	4.7399
H	15.289	4.5196	4.9731
O	21.307	6.2139	5.2503
O	22.7417	2.672	7.7127
N	22.1517	4.4363	6.4017
O	7.9013	4.6521	12.3505

C	17.0622	4.4852	7.0748
C	17.3524	5.522	6.1944
C	18.663	5.7556	5.8021
H	18.8608	6.4636	5.2002
C	19.6888	4.9524	6.2901
C	19.4013	3.9156	7.1705
C	18.088	3.682	7.5628
C	17.8011	2.6453	8.44
C	18.8242	1.8421	8.928
C	20.1375	2.0757	8.5357
H	20.8385	1.5275	8.8693
C	20.425	3.1125	7.6553
C	15.6507	11.896	16.915
C	14.8399	11.6735	18.0218
H	13.8999	11.5811	17.9114
C	15.3998	11.589	19.2914
H	14.845	11.4383	20.0473
C	16.7734	11.7269	19.454
C	17.587	11.9472	18.3472
H	18.5249	12.0415	18.4594
C	17.0236	12.0339	17.0809
H	17.5798	12.1843	16.3235
C	9.7659	3.9023	11.349
C	10.4752	5.097	11.4351
H	10.1049	5.8357	11.9029
C	11.7242	5.206	10.8354
C	12.2633	4.1248	10.1528
C	11.5568	2.9323	10.0667
C	10.3079	2.821	10.6657
C	9.5984	1.6286	10.5803
C	10.1403	0.5451	9.8977
H	9.6562	-0.2693	9.838
C	11.3893	0.6563	9.298
C	12.0965	1.8488	9.3809
C	20.1479	-0.4183	16.915
C	21.0255	-0.6474	15.8592
H	21.9452	-0.8119	16.0355
C	20.5593	-0.6363	14.5514
H	21.1582	-0.793	13.8319
C	19.2135	-0.396	14.2963

C	18.3366	-0.1646	15.3489
H	17.4171	-0.001	15.1748
C	18.8021	-0.1758	16.6598
H	18.2041	-0.0198	17.3784
C	7.1231	5.3929	-5.2917
H	6.2161	5.113	-5.312
C	8.0709	4.7455	-6.0764
C	9.3973	5.1549	-6.0445
H	10.0447	4.7131	-6.5804
C	9.7787	6.2139	-5.2279
H	10.6863	6.4945	-5.2055
C	8.8337	6.8613	-4.4433
C	7.5045	6.4519	-4.4752
H	6.8577	6.8944	-3.9371
O	7.6404	0.2959	11.2501
C	11.7924	-0.287	8.105
C	11.0945	-1.4884	8.07
H	10.5653	-1.7519	8.8143
C	11.1751	-2.3071	6.9504
H	10.6978	-3.1287	6.927
C	11.9487	-1.9222	5.8627
C	12.6473	-0.7208	5.8946
H	13.1759	-0.4575	5.1521
C	12.566	0.0979	7.0174
H	13.0434	0.9194	7.0395
C	9.5066	-3.2082	-2.2775
C	8.6396	-3.1592	-1.193
H	7.7067	-3.0488	-1.3349
C	9.1368	-3.2682	0.0989
H	8.5453	-3.234	0.8418
C	10.5037	-3.4284	0.3062
C	11.3707	-3.4796	-0.7783
H	12.3027	-3.5883	-0.6359
C	10.8708	-3.3683	-2.0701
H	11.4641	-3.403	-2.8126
C	17.3603	11.015	20.9372
C	16.846	9.8492	21.4891
H	15.9636	9.5685	21.2708
C	17.6163	9.0928	22.363
H	17.2637	8.2951	22.7417

C	18.9066	9.5021	22.6852
C	19.4244	10.6679	22.1302
H	20.3038	10.9466	22.3503
C	18.6512	11.4243	21.2562
H	19.0037	12.2201	20.8794
C	13.4845	8.7946	12.5387
C	12.3072	8.9192	11.8115
H	11.8891	9.7689	11.7261
C	11.7397	7.8024	11.2086
H	10.9346	7.8895	10.7102
C	12.3497	6.5609	11.333
C	13.5271	6.4341	12.0603
H	13.9447	5.5855	12.1446
C	14.0945	7.551	12.6631
H	14.8992	7.465	13.1605
C	23.4923	4.9702	6.2742
C	24.1741	5.8201	7.1354
C	25.5246	6.0782	6.9344
H	25.9913	6.6607	7.5222
C	26.194	5.4841	5.8691
H	27.1171	5.6614	5.7306
C	25.5122	4.6343	5.0078
H	25.969	4.228	4.2806
C	24.161	4.3762	5.212
C	13.8109	1.9778	9.3171
C	14.6413	0.8699	9.2087
H	14.3238	0.0115	9.4625
C	15.9354	1.0167	8.7239
H	16.5038	0.2592	8.6491
C	16.4011	2.2737	8.3507
C	15.5677	3.3817	8.4601
C	14.2738	3.2349	8.9439
C	13.4434	4.3428	9.0524
C	13.9064	5.5998	8.6792
H	13.3385	6.3569	8.754
C	15.2032	5.7467	8.1944
H	15.5185	6.6047	7.9406
C	16.0336	4.6365	8.0859
C	21.1539	0.8743	20.8766
C	22.106	0.5695	19.9133

H	23.0257	0.7428	20.0816
C	21.7166	0.0133	18.7013
H	22.3678	-0.1946	18.041
C	20.3722	-0.2403	18.4525
C	19.42	0.0645	19.4158
H	18.4998	-0.1077	19.2481
C	19.8095	0.6207	20.6278
H	19.1576	0.8297	21.2887
C	23.2813	6.3318	8.2901
H	22.385	5.8915	8.2364
C	17.8515	0.8499	12.5005
H	17.2379	1.1639	13.1562
C	18.8058	-0.1001	12.8418
C	19.702	-0.5584	11.8817
H	20.3558	-1.207	12.115
C	19.6431	-0.0645	10.5835
H	20.2561	-0.3781	9.929
C	18.6881	0.8855	10.2453
C	17.7927	1.3438	11.2023
H	17.1382	1.9928	10.9702
C	20.8839	5.74	23.5145
C	21.5648	6.75	22.8415
H	22.3976	6.5654	22.4246
C	21.0223	8.0271	22.7777
H	21.4861	8.7179	22.3186
C	19.8017	8.2963	23.3869
C	19.1236	7.2862	24.06
H	18.2899	7.4708	24.4765
C	19.6661	6.0092	24.1238
H	19.2014	5.3183	24.5825
C	22.2629	4.1048	22.363
H	22.8638	4.8037	22.1372
C	21.3054	4.3028	23.3519
C	20.4252	3.2794	23.6836
H	19.7721	3.4152	24.3599
C	20.5005	2.0579	23.0233
H	19.8971	1.3593	23.2495
C	21.4552	1.8599	22.0345
C	22.3354	2.8833	21.7028
H	22.9888	2.7477	21.0268

C	11.6206	-2.7499	4.5166
C	12.4907	-2.4139	3.4832
H	13.324	-2.003	3.6794
C	12.1371	-2.6787	2.1658
H	12.7298	-2.4483	1.4603
C	10.9163	-3.2771	1.8819
C	10.0496	-3.6131	2.9122
H	9.2137	-4.0238	2.7181
C	10.3997	-3.3483	4.2327
H	9.808	-3.5785	4.9371
C	9.5529	7.6822	-3.1419
C	9.0218	7.5332	-1.866
H	8.1427	7.1902	-1.7563
C	9.7757	7.8869	-0.756
H	9.4117	7.7859	0.1173
C	11.06	8.3919	-0.9186
C	11.5933	8.541	-2.1913
H	12.4708	8.8842	-2.304
C	10.8372	8.1873	-3.3045
H	11.2018	8.2885	-4.1776
C	13.4277	7.6511	2.421
C	13.8502	8.5655	1.4641
H	14.7355	8.9091	1.4917
C	12.976	8.9815	0.4657
H	13.2636	9.6072	-0.1882
C	11.6792	8.4787	0.4242
C	11.2595	7.5621	1.3811
H	10.3731	7.2203	1.3525
C	12.1337	7.1483	2.3795
H	11.8449	6.5222	3.0324
C	8.1568	-0.7676	-5.5118
C	7.2339	-1.4506	-4.7271
H	6.3046	-1.2786	-4.827
C	7.6707	-2.385	-3.7926
H	7.0395	-2.8506	-3.2572
C	9.0283	-2.6364	-3.6458
C	9.9512	-1.9534	-4.4305
H	10.8803	-2.126	-4.3297
C	9.5137	-1.0212	-5.3619
H	10.1454	-0.5541	-5.8995

C	15.1428	11.302	15.4637
C	15.9127	10.6078	14.5387
H	16.8614	10.6592	14.573
C	15.2972	9.8358	13.5594
H	15.8227	9.3617	12.9259
C	13.9091	9.7602	13.5052
C	13.1386	10.4543	14.4334
H	12.1919	10.4019	14.3961
C	13.7575	11.2241	15.4095
H	13.2306	11.6994	16.0433
C	21.7832	3.355	7.2598
C	23.6024	3.375	4.2519
H	22.6386	3.1673	4.4212
C	6.3687	2.3538	12.4175
C	5.2873	2.4673	11.5499
C	3.9989	2.5852	12.0603
H	3.2606	2.6624	11.4688
C	3.7927	2.5919	13.435
H	2.9131	2.6721	13.7828
C	4.8749	2.4784	14.2995
H	4.734	2.4819	15.2401
C	6.1626	2.3583	13.7923
C	21.0547	5.1882	5.9105
C	6.6504	2.6297	-5.5692
H	6.008	3.1163	-5.0632
C	6.6869	1.2437	-5.4927
H	6.0733	0.7808	-4.9354
C	7.6253	0.5317	-6.2327
C	8.5244	1.2103	-7.0493
H	9.1664	0.7239	-7.5538
C	8.488	2.5963	-7.1258
H	9.1012	3.0594	-7.6817
C	7.5496	3.3083	-6.3858
N	7.6242	2.5096	11.7349
C	8.4223	3.682	11.7668
C	7.5139	2.5007	14.5738
H	8.2652	2.6395	13.9305
C	23.8685	3.7955	2.842
H	24.8042	3.6043	2.6163
H	23.7001	4.7552	2.7488

H	23.28	3.2986	2.236
C	23.1236	7.8357	8.0668
H	24.0072	8.2549	8.0174
H	22.6177	8.2263	8.8109
H	22.6401	7.9927	7.2279
C	23.9164	6.0159	9.6361
H	23.781	5.0695	9.8471
H	23.4995	6.5688	10.3306
H	24.8759	6.2096	9.5973
C	5.3222	2.6364	10.0029
H	6.2502	2.4837	9.6635
C	7.4809	3.6264	15.5722
H	6.685	4.1781	15.42
H	8.2845	4.1786	15.4698
H	7.4528	3.2582	16.4808
C	24.5034	2.1581	4.3731
H	25.1628	2.1646	3.6492
H	23.9618	1.3427	4.3148
H	24.9667	2.1794	5.2374
C	4.8832	4.0336	9.684
H	3.9884	4.1872	10.0555
H	4.8574	4.1541	8.7121
H	5.5134	4.672	10.0768
C	4.4223	1.5574	9.5213
H	4.8214	0.6853	9.7251
H	4.3	1.6429	8.5536
H	3.5546	1.6322	9.9697
C	8.2728	1.3994	11.097
C	7.6907	1.1814	15.2978
H	6.8293	0.8941	15.6693
H	8.3387	1.2908	16.0236
H	8.0152	0.5045	14.6679

TDI-2Ph-TDI

Atom	X	Y	Z
N	-3.2595	7.383	0.3711
C	-4.1673	6.7874	-0.4745
C	-3.9424	5.4696	-0.7305
C	-2.9064	4.7903	-0.1975
C	-2.0435	5.4246	0.6161

C	-2.1807	6.7424	0.939
C	-2.7244	3.4709	-0.4609
C	-1.6894	2.7832	0.0796
C	-0.9608	4.7569	1.0402
C	-2.5649	0.7555	-0.8056
C	-1.7141	1.4288	-0.0026
C	-0.9873	0.6611	0.8279
O	-1.4283	7.3594	1.6631
O	-5.0882	7.43	-0.9313
O	-4.9534	-7.2532	-1.8825
O	-1.3781	-7.4391	0.8204
C	-2.1178	-6.7512	0.1492
C	-1.9946	-5.4027	-0.0117
C	-3.8545	-5.3128	-1.4071
C	-4.0603	-6.6555	-1.3212
N	-3.1665	-7.3348	-0.5258
C	-4.0724	-9.1559	0.6142
C	-4.218	-10.4889	0.7177
C	-3.6412	-11.3185	-0.1611
C	-2.9057	-10.8171	-1.1616
C	-2.7348	-9.4905	-1.3017
C	-3.3264	-8.6731	-0.4033
C	-4.109	9.0352	1.7808
C	-4.273	10.3429	2.0491
C	-3.7847	11.2842	1.2315
C	-3.1208	10.922	0.1264
C	-2.9347	9.6256	-0.1798
C	-3.4365	8.6935	0.6599
C	-0.9844	-0.673	0.7556
C	-1.7002	-1.3536	-0.1569
C	-2.5549	-0.6032	-0.8851
C	-0.9368	-4.776	0.5225
C	-1.6658	-2.7092	-0.2252
C	-2.679	-3.3419	-0.8663
C	-2.8455	-4.6863	-0.7679
C	-3.54	-2.6098	-1.61
C	-4.687	-4.5882	-2.1655
C	-3.4386	-1.2617	-1.6632
C	-4.2365	-0.5081	-2.4387
C	-4.2503	0.8243	-2.3554

C	-3.4633	1.4898	-1.4936
C	-4.7822	4.8265	-1.5521
C	-3.5887	2.8185	-1.2713
C	-4.5975	3.5296	-1.8123
C	-4.5224	-3.2662	-2.2582
C	-0.7076	-3.4558	0.3804
C	-0.718	3.4664	0.7367
C	2.5755	-3.4106	1.8695
C	1.2624	-3.6235	1.7009
C	0.5626	-3.0805	0.688
C	1.2642	-2.2185	-0.0748
C	2.5868	-2.0263	0.088
C	2.6491	3.3223	2.0238
C	1.326	3.5299	1.9577
C	0.567	3.0711	0.9453
C	1.2269	2.2788	0.0763
C	2.5567	2.0801	0.1442
N	11.2847	-7.3829	0.3711
C	12.1924	-6.7873	-0.4746
C	11.9675	-5.4696	-0.7307
C	10.9315	-4.7903	-0.1977
C	10.0687	-5.4245	0.6161
C	10.2059	-6.7423	0.939
C	10.7495	-3.4708	-0.4611
C	9.7146	-2.7831	0.0794
C	8.986	-4.7568	1.0401
C	10.5901	-0.7555	-0.806
C	9.7392	-1.4288	-0.0029
C	9.0125	-0.661	0.8276
O	9.4536	-7.3592	1.6632
O	13.1134	-7.43	-0.9315
O	12.9784	7.2531	-1.8835
O	9.4034	7.4392	0.8196
C	10.143	6.7512	0.1484
C	10.0197	5.4028	-0.0124
C	11.8796	5.3128	-1.4079
C	12.0854	6.6555	-1.3221
N	11.1916	7.3348	-0.5266
C	12.0977	9.156	0.6131
C	12.2433	10.489	0.7165

C	11.6663	11.3186	-0.1623
C	10.9307	10.8171	-1.1626
C	10.7598	9.4904	-1.3026
C	11.3515	8.6731	-0.4043
C	12.1343	-9.0351	1.7808
C	12.2983	-10.3427	2.0492
C	11.8099	-11.284	1.2316
C	11.146	-10.9219	0.1266
C	10.9598	-9.6256	-0.1796
C	11.4617	-8.6934	0.6599
C	9.0096	0.6731	0.7552
C	9.7254	1.3537	-0.1574
C	10.58	0.6032	-0.8855
C	8.962	4.7761	0.5219
C	9.6909	2.7092	-0.2258
C	10.7041	3.3419	-0.8669
C	10.8706	4.6863	-0.7686
C	11.565	2.6098	-1.6106
C	12.7121	4.5881	-2.1663
C	11.4637	1.2616	-1.6638
C	12.2615	0.508	-2.4393
C	12.2753	-0.8244	-2.3559
C	11.4884	-1.4898	-1.494
C	12.8073	-4.8265	-1.5524
C	11.6137	-2.8185	-1.2717
C	12.6225	-3.5297	-1.8126
C	12.5474	3.2662	-2.2589
C	8.7328	3.4558	0.38
C	8.7432	-3.4663	0.7366
C	5.4498	3.4108	1.8692
C	6.7629	3.6236	1.7005
C	7.4626	3.0806	0.6876
C	6.761	2.2185	-0.0751
C	5.4384	2.0263	0.0878
C	5.3761	-3.3222	2.0239
C	6.6993	-3.5297	1.9577
C	7.4582	-3.071	0.9452
C	6.7983	-2.2787	0.0763
C	5.4684	-2.0801	0.1442
C	3.3445	2.6567	1.078

C	4.7055	2.663	1.0275
C	3.3198	-2.6629	1.0277
C	4.6807	-2.6566	1.0782
C	-4.7507	-8.2496	1.6371
C	-6.2806	-8.3962	1.582
C	-4.2094	-8.5046	3.0538
C	-1.8844	-8.9655	-2.4545
C	-2.4929	-9.3437	-3.8153
C	-0.4282	-9.4451	-2.3338
C	-4.6911	7.9997	2.7383
C	-6.2235	8.1089	2.809
C	-4.0531	8.1064	4.1336
C	-2.1623	9.2626	-1.4446
C	-2.8747	9.7804	-2.7052
C	-0.7106	9.7653	-1.3702
C	12.7761	8.2498	1.6359
C	14.306	8.3963	1.5807
C	12.235	8.5048	3.0527
C	9.9092	8.9654	-2.4553
C	10.5175	9.3435	-3.8162
C	8.4531	9.445	-2.3344
C	12.7164	-7.9994	2.7383
C	14.2489	-8.1087	2.8089
C	12.0786	-8.1061	4.1335
C	10.1873	-9.2626	-1.4444
C	10.8997	-9.7805	-2.7051
C	8.7357	-9.7653	-1.3699
H	-0.1947	5.3584	1.5494
H	-0.4054	1.0819	1.6628
H	-4.8182	-10.9259	1.5316
H	-3.7708	-12.4093	-0.0611
H	-2.4403	-11.5204	-1.8705
H	-4.8164	10.6665	2.9512
H	-3.9279	12.3521	1.4672
H	-2.7263	11.7151	-0.5286
H	-0.4016	-1.1721	1.5446
H	-0.1751	-5.4218	0.9828
H	-5.5312	-5.0371	-2.7161
H	-4.9593	-0.9151	-3.1599
H	-4.9806	1.3071	-3.0204

H	-5.6478	5.3228	-2.023
H	-5.3709	3.1088	-2.4698
H	-5.2888	-2.783	-2.8797
H	2.9956	-3.9799	2.7108
H	0.7791	-4.295	2.4324
H	0.7937	-1.7374	-0.9505
H	3.049	-1.3694	-0.6648
H	3.1193	3.8046	2.8928
H	0.8877	4.1257	2.7774
H	0.713	1.8729	-0.8127
H	2.9736	1.5016	-0.6943
H	8.22	-5.3583	1.5494
H	8.4306	-1.0818	1.6626
H	12.8435	10.9261	1.5303
H	11.7959	12.4094	-0.0624
H	10.4652	11.5203	-1.8715
H	12.8418	-10.6662	2.9513
H	11.9532	-12.352	1.4675
H	10.7515	-11.7151	-0.5283
H	8.4269	1.1723	1.5442
H	8.2003	5.422	0.9823
H	13.5561	5.037	-2.7171
H	12.9843	0.915	-3.1605
H	13.0055	-1.3073	-3.0209
H	13.6729	-5.3228	-2.0233
H	13.3959	-3.1089	-2.4703
H	13.3138	2.7829	-2.8805
H	5.0297	3.9801	2.7105
H	7.2462	4.2952	2.432
H	7.2314	1.7374	-0.9508
H	4.9761	1.3694	-0.6649
H	4.9061	-3.8043	2.893
H	7.1376	-4.1255	2.7774
H	7.3121	-1.8729	-0.8128
H	5.0515	-1.5015	-0.6943
H	-4.5381	-7.1752	1.4143
H	-6.7765	-7.6772	2.2738
H	-6.617	-9.4159	1.8735
H	-6.6622	-8.1904	0.5553
H	-4.4453	-9.5296	3.4165

H	-4.6497	-7.7885	3.785
H	-3.1029	-8.3768	3.0855
H	-1.8412	-7.8488	-2.4363
H	-2.5033	-10.4438	-3.9811
H	-1.9129	-8.8916	-4.6523
H	-3.5414	-8.9756	-3.8979
H	0.2077	-8.9982	-3.132
H	-0.3401	-10.5505	-2.4251
H	0.0079	-9.1468	-1.3525
H	-4.4763	6.9639	2.3775
H	-6.6531	7.3024	3.4466
H	-6.5575	9.0791	3.2394
H	-6.6753	8.0105	1.795
H	-4.424	7.2989	4.8055
H	-4.283	9.0759	4.6287
H	-2.9448	8.0082	4.0734
H	-2.0943	8.1531	-1.561
H	-3.9197	9.3973	-2.7578
H	-2.3489	9.444	-3.6281
H	-2.9168	10.8917	-2.7393
H	-0.1262	9.433	-2.2587
H	-0.6508	10.8758	-1.3353
H	-0.1985	9.3662	-0.4643
H	12.5635	7.1753	1.4132
H	14.802	7.6774	2.2724
H	14.6424	9.416	1.8721
H	14.6875	8.1905	0.554
H	12.4709	9.5299	3.4154
H	12.6753	7.7887	3.7839
H	11.1285	8.377	3.0846
H	9.866	7.8487	-2.4371
H	10.5279	10.4436	-3.9821
H	9.9375	8.8914	-4.6531
H	11.5661	8.9754	-3.8989
H	7.817	8.9981	-3.1326
H	8.3649	10.5504	-2.4257
H	8.0171	9.1467	-1.3531
H	12.5016	-6.9637	2.3773
H	14.6784	-7.3022	3.4463
H	14.5829	-9.0788	3.2393

H	14.7006	-8.0104	1.7948
H	12.4494	-7.2985	4.8054
H	12.3084	-9.0756	4.6288
H	10.9703	-8.0079	4.0735
H	10.1194	-8.1531	-1.5609
H	11.9447	-9.3974	-2.7578
H	10.3739	-9.4441	-3.6279
H	10.9418	-10.8918	-2.7391
H	8.1512	-9.4331	-2.2584
H	8.6759	-10.8758	-1.335
H	8.2237	-9.3662	-0.464

TDI-3Ph-TDI

Atom	X	Y	Z
O	-3.4753	3.1298	59.9464
O	-3.0405	3.4238	64.4133
N	10.5163	-1.4176	44.0144
C	2.3758	2.7562	41.9536
O	-3.1888	5.4594	40.1439
O	10.3911	-1.8032	41.7339
N	-3.4208	5.6573	42.3616
N	-3.2557	3.2846	62.2322
O	10.626	9.8247	58.3982
O	10.5504	-0.9498	46.138
C	3.0292	6.453	61.4528
C	0.4547	3.4591	40.4106
H	0.9447	3.1332	39.6679
C	6.0451	1.0669	44.8199
C	8.0101	-0.0869	43.7215
C	-1.3833	4.5309	41.4306
C	5.172	7.1849	62.4414
N	10.5996	10.3091	60.6787
C	4.5478	2.1644	40.9912
H	5.095	2.1006	40.2171
C	10.0413	-0.9759	45.1233
C	-2.6105	3.6809	63.2992
C	0.171	3.8284	45.2907
C	8.8622	9.1011	59.6535
O	10.5083	10.7199	62.9069
C	-1.6775	4.7271	43.8418

C	-0.6055	4.8475	64.3087
H	-1.0599	4.8221	65.1455
C	3.9073	1.5162	45.6568
H	4.194	1.0917	46.4571
C	6.9408	7.9174	58.6231
C	-1.1562	4.4036	63.1998
C	2.0523	2.6432	44.3335
C	6.6873	0.6088	43.6535
C	6.3123	1.7071	47.3358
C	6.1449	3.0864	47.3672
H	6.1598	3.5858	46.5564
C	5.959	3.7391	48.5806
H	5.8443	4.6813	48.6015
C	5.9374	3.0104	49.7627
C	6.1032	1.6312	49.7313
H	6.0899	1.1317	50.5421
C	6.2907	0.9784	48.5179
H	6.4038	0.0362	48.4969
C	2.4613	6.1542	62.6767
C	9.8961	-1.3134	42.7434
C	7.1631	8.4747	63.4404
H	6.8169	8.3256	64.3139
C	0.8209	3.4217	44.187
C	2.8817	2.4712	43.1409
C	0.5976	3.9003	46.7657
C	-0.208	3.1669	47.6287
H	-0.933	2.6596	47.2835
C	0.0501	3.1728	48.9938
H	-0.4999	2.6712	49.5849
C	1.1121	3.9144	49.496
C	1.9177	4.6499	48.6329
H	2.6442	5.1551	48.9781
C	1.6612	4.6418	47.2678
H	2.2111	5.1435	46.6767
C	4.3397	6.9174	61.3011
C	-0.9067	4.4464	59.4809
H	-1.4239	4.2088	58.7173
C	6.9561	8.3594	60.9402
C	-0.777	4.6734	61.8922
C	8.2432	8.9968	60.9298

C	-1.4809	4.2021	60.8356
C	2.6216	2.199	45.5731
H	2.1393	2.3588	46.3786
C	-1.136	4.2299	42.7643
C	0.9144	5.4698	60.3963
C	8.7645	9.4778	62.0491
C	6.3095	7.7748	59.8366
C	3.225	2.7016	40.9337
H	2.9306	3.0478	40.0968
C	3.8231	7.4347	58.9213
H	4.1118	7.8462	58.1158
C	4.7698	6.7506	63.6287
H	5.3598	6.8084	64.3714
C	1.2483	5.6351	62.8127
C	-2.8361	3.5359	60.8565
C	5.9106	3.7031	51.1802
C	2.2728	6.3007	60.2655
C	1.0021	3.3292	41.7549
C	-0.7813	4.0627	40.2171
H	-1.187	4.1543	39.3645
C	11.8451	11.097	60.5061
C	13.0456	10.4045	60.6316
C	14.2476	11.1027	60.6578
H	15.0675	10.6287	60.7415
C	14.2505	12.4889	60.5636
H	15.0735	12.9632	60.5793
C	13.0515	13.1791	60.4381
H	13.053	14.1275	60.3701
C	11.8481	12.4831	60.412
C	0.8087	5.4082	64.1779
H	1.3568	5.5954	64.9311
C	6.6871	0.9574	46.0229
C	4.9902	1.7376	42.2413
C	11.7942	-2.1758	44.1347
C	11.8685	-3.5563	44.2759
C	13.0987	-4.1987	44.2027
H	13.1483	-5.1432	44.3021
C	14.2561	-3.4605	43.9883
H	15.0979	-3.8991	43.9412
C	14.1833	-2.0801	43.847

H	14.974	-1.574	43.7006
C	12.9531	-1.4377	43.9203
C	2.6039	6.9165	59.0154
H	1.9876	6.9529	58.2884
C	10.2887	9.7361	59.5437
C	6.4624	7.9662	62.2688
C	-4.6321	6.2426	42.2047
C	-4.5916	7.5753	41.8124
C	-5.7655	8.2327	41.462
H	-5.7375	9.1432	41.1952
C	-6.9784	7.5552	41.4986
H	-7.7811	8.0038	41.258
C	-7.0189	6.2225	41.8909
H	-7.8481	5.7605	41.917
C	-5.8465	5.5673	42.2465
C	0.2755	4.9731	59.2926
C	8.6458	-0.1517	44.9978
C	8.067	0.3676	46.1851
H	8.5145	0.3443	47.0272
C	-1.0774	4.456	45.1076
H	-1.5565	4.7174	45.8869
C	0.4717	5.2289	61.6882
C	8.5315	-0.584	42.6388
C	5.7447	4.8077	53.5443
C	6.3441	7.2419	57.2266
C	6.1649	5.864	57.2371
H	6.1793	5.3907	58.0635
C	5.9671	5.1756	56.0497
H	5.845	4.2351	56.055
C	5.9454	5.8675	54.8415
C	6.1246	7.2454	54.831
H	6.1102	7.7187	54.0046
C	6.3224	7.9338	56.0184
H	6.4445	8.8743	56.0131
C	8.2245	9.1086	63.2783
H	8.7046	9.3612	64.0576
C	-2.7663	5.1924	41.2004
C	13.0554	0.1649	43.5437
H	12.1286	0.5406	43.5489
C	10.1214	10.2649	61.9131

C	10.626	13.0472	60.2184
H	9.9262	12.4678	60.6316
C	-5.7127	3.4665	62.3629
C	-6.929	2.8609	62.6558
H	-7.7336	3.3649	62.614
C	-6.971	1.5158	63.0063
H	-7.802	1.1032	63.205
C	-5.7951	0.7764	63.0638
H	-5.8231	-0.1424	63.3044
C	-4.5773	1.3821	62.7709
C	-4.5368	2.7271	62.4205
C	-3.3217	8.3205	41.9065
H	-2.554	7.6924	41.781
C	-3.1225	9.1341	43.2089
H	-2.2531	9.5873	43.1828
H	-3.1497	8.5301	43.9778
H	-3.836	9.8004	43.2926
C	-5.491	4.9426	61.8346
H	-4.5609	5.1852	61.5627
C	0.4924	5.124	57.8804
C	1.5004	4.3009	57.394
H	1.9855	3.742	57.9902
C	1.7978	4.2948	56.034
H	2.4883	3.7301	55.7045
C	1.0887	5.1118	55.1658
C	0.0807	5.9349	55.6522
H	-0.406	6.4938	55.056
C	-0.2182	5.9411	57.0069
H	-0.9073	6.5058	57.3417
C	1.5912	4.1863	50.9657
C	-3.2032	0.4913	62.7029
H	-2.4361	1.1195	62.8284
C	-2.9939	-0.2056	61.3901
H	-3.7439	-0.8153	61.2227
H	-2.1584	-0.716	61.4214
H	-2.9451	0.459	60.6735
C	1.6905	3.3657	53.1311
H	1.5553	2.6119	53.6908
C	1.7545	4.7302	53.6856
C	10.4946	-4.1112	44.4486

H	9.8562	-3.5666	43.9098
C	10.3763	-5.6078	44.0144
H	10.9264	-6.1643	44.6002
H	10.687	-5.7015	43.0886
H	9.4403	-5.8923	44.072
C	-6.7242	3.5616	44.004
H	-6.5846	4.1327	44.7885
H	-6.5418	2.6297	44.2393
H	-7.6536	3.6467	43.7006
C	-3.1613	-0.5498	63.9059
H	-3.1873	-0.0657	64.7585
H	-2.3365	-1.0761	63.8536
H	-3.9346	-1.1485	63.8484
C	-6.4984	5.0327	60.8304
H	-6.3411	4.3497	60.1452
H	-6.4686	5.9221	60.412
H	-7.3808	4.8929	61.2331
C	-3.2368	9.5426	40.7768
H	-3.9458	10.1963	40.9441
H	-3.35	9.1649	39.8771
H	-2.3644	9.9853	40.8343
C	10.3158	13.1829	58.4662
H	9.3939	13.4803	58.3198
H	10.4481	12.308	58.0426
H	10.9366	13.8323	58.0739
C	1.852	3.2093	51.5934
H	2.1374	2.3978	51.1854
C	-5.7077	4.0337	42.7957
H	-4.7581	3.8204	43.0259
C	10.3265	14.6476	60.6212
H	10.9459	15.2285	60.1347
H	10.4521	14.7714	61.5836
H	9.4047	14.8765	60.3806
C	12.9295	8.6364	60.9298
H	11.9952	8.2786	60.9141
C	9.9324	-4.2075	45.9811
H	9.012	-4.5456	45.9706
H	9.9503	-3.3169	46.3891
H	10.4981	-4.8176	46.4989
C	13.8026	0.7913	44.6473

H	14.7093	0.4215	44.6787
H	13.3467	0.6097	45.4946
H	13.8506	1.7588	44.5009
C	13.8581	8.1477	59.6431
H	13.4507	8.4587	58.8062
H	14.7583	8.5262	59.7268
C	13.6345	0.3434	42.0739
H	13.6764	1.2971	41.849
H	13.0522	-0.1163	41.4306
H	14.5351	-0.0424	42.0268
C	1.7127	5.4982	51.2952
H	1.8528	6.1574	50.6257
C	13.7103	8.5204	62.4623
H	14.6309	8.8472	62.3838
H	13.7209	7.5853	62.75
H	13.2235	9.0612	63.1161
C	-6.2153	5.9286	62.9697
H	-7.1683	5.7099	63.0324
H	-6.113	6.8657	62.6977
H	-5.791	5.7905	63.8431
C	1.6146	5.905	52.833
H	1.4841	6.7908	53.1521
C	-6.1857	3.1763	41.7078
H	-7.1184	3.3979	41.5038
H	-6.1271	2.2371	41.9798
H	-5.6339	3.3195	40.9128
C	6.6637	3.9494	53.6123
H	7.2089	3.7238	54.3551
C	6.686	3.3285	52.1217
H	7.3145	2.6423	51.9334
C	5.6855	5.6195	52.6029
H	5.5783	6.5428	52.8016
C	5.7788	5.1934	51.1488
H	5.7581	5.7536	50.3799
C	8.1723	8.5894	58.529
H	8.5587	8.7053	57.6712
C	3.4159	6.1778	63.817
H	3.1595	5.827	64.6643
C	0.2346	3.6899	42.9579
C	4.718	1.5133	44.4695

C	4.1625	1.973	43.3345
C	6.2619	0.8887	42.3877
C	6.8809	0.4332	41.2004
H	6.517	0.604	40.3426
C	8.0551	-0.2822	41.3783
H	8.542	-0.5726	40.6198
C	-2.9227	5.4158	43.5698
O	-3.6622	5.8128	44.6055
C	4.6787	7.3688	60.0301