

### Cartesian Coordinates, Angs (B3LYP/aug-cc-pvtz)

BA1			atom	BA2		
-0.4423	-0.2219	-0.2092	CARBON	-0.4390	-0.2853	-0.0052
0.4467	-1.2628	0.0521	CARBON	0.5144	-1.3049	-0.0419
1.8062	-1.0134	0.2216	CARBON	1.8708	-1.0087	-0.0365
2.2893	0.2861	0.1373	CARBON	2.2942	0.3170	0.0055
1.4083	1.3346	-0.1184	CARBON	1.3506	1.3355	0.0417
0.0543	1.0819	-0.2916	CARBON	-0.0102	1.0382	0.0366
0.0738	-2.2776	0.1228	HYDROGEN	0.1929	-2.3397	-0.0753
2.4835	-1.8328	0.4235	HYDROGEN	2.5969	-1.8104	-0.0655
3.3446	0.4838	0.2707	HYDROGEN	3.3505	0.5510	0.0095
1.7798	2.3487	-0.1859	HYDROGEN	1.6710	2.3687	0.0741
-0.6299	1.8978	-0.4860	HYDROGEN	-0.7427	1.8310	0.0644
-1.9161	-0.4917	-0.3992	CARBON	-1.9036	-0.6503	-0.0102
-2.1141	-1.5615	-0.2763	HYDROGEN	-2.1215	-1.2761	0.8638
-2.2286	-0.2151	-1.4073	HYDROGEN	-2.1225	-1.2485	-0.9029
-2.7506	0.2804	0.4660	OXYGEN	-2.7079	0.5235	0.0089
-2.4718	0.1277	1.3745	HYDROGEN	-3.6326	0.2644	0.0102

PE1			atom	PE2		
-0.0626	-0.2916	-0.4809	CARBON	-0.0759	0.0000	-0.3656
0.4760	0.9839	-0.6667	CARBON	-0.7721	-1.1983	-0.1948
1.7773	1.2776	-0.2686	CARBON	-2.1221	-1.2013	0.1382
2.5643	0.2968	0.3225	CARBON	-2.8020	0.0000	0.3073
2.0422	-0.9793	0.5110	CARBON	-2.1221	1.2013	0.1382
0.7423	-1.2678	0.1137	CARBON	-0.7721	1.1983	-0.1948
-0.1268	1.7507	-1.1372	HYDROGEN	-0.2529	-2.1393	-0.3319
2.1755	2.2715	-0.4257	HYDROGEN	-2.6437	-2.1415	0.2609
3.5772	0.5214	0.6289	HYDROGEN	-3.8532	0.0000	0.5628
2.6500	-1.7518	0.9638	HYDROGEN	-2.6437	2.1415	0.2609
0.3484	-2.2665	0.2602	HYDROGEN	-0.2529	2.1393	-0.3319
-1.4892	-0.5966	-0.8679	CARBON	1.3976	0.0000	-0.6914
-2.4706	-0.4494	0.3035	CARBON	2.2648	0.0000	0.5642
-2.5528	0.8792	0.8022	OXYGEN	3.6317	0.0000	0.1535
-1.6826	1.1419	1.1205	HYDROGEN	4.1946	0.0000	0.9324
-1.8096	0.0682	-1.6720	HYDROGEN	1.6560	-0.8779	-1.2863
-1.5635	-1.6210	-1.2423	HYDROGEN	1.6560	0.8779	-1.2863
-3.4776	-0.7012	-0.0292	HYDROGEN	2.0410	0.8853	1.1693
-2.1989	-1.1459	1.1051	HYDROGEN	2.0410	-0.8853	1.1693

PE3			atom	PE4		
-0.0802	-0.0068	0.3784	CARBON	-0.0360	-0.3153	-0.4240
-0.7723	1.1932	0.2006	CARBON	0.4237	0.9996	-0.5206
-2.1198	1.1982	-0.1417	CARBON	1.7227	1.3294	-0.1512
-2.8013	-0.0019	-0.3135	CARBON	2.5876	0.3481	0.3220
-2.1255	-1.2044	-0.1381	CARBON	2.1436	-0.9656	0.4212
-0.7777	-1.2039	0.2042	CARBON	0.8432	-1.2909	0.0499
-0.2517	2.1332	0.3383	HYDROGEN	-0.2455	1.7692	-0.8813
-2.6382	2.1394	-0.2701	HYDROGEN	2.0601	2.3544	-0.2340
-3.8506	0.0002	-0.5767	HYDROGEN	3.5996	0.6042	0.6065
-2.6481	-2.1436	-0.2636	HYDROGEN	2.8099	-1.7384	0.7818
-0.2623	-2.1464	0.3456	HYDROGEN	0.5091	-2.3192	0.1233
1.3927	-0.0064	0.7062	CARBON	-1.4533	-0.6762	-0.7997
2.2676	0.0038	-0.5541	CARBON	-2.4668	-0.4818	0.3258
3.6594	0.0688	-0.2595	OXYGEN	-2.6198	0.9162	0.5671
3.9239	-0.7399	0.1886	HYDROGEN	-3.1552	1.0445	1.3544
1.6499	0.8672	1.3077	HYDROGEN	-1.7819	-0.0797	-1.6535
1.6408	-0.8905	1.3006	HYDROGEN	-1.4958	-1.7239	-1.1060
2.0394	-0.8693	-1.1749	HYDROGEN	-3.4249	-0.9225	0.0275
2.0516	0.8916	-1.1482	HYDROGEN	-2.1219	-0.9943	1.2302

atom	PE5		
CARBON	-0.0039	-0.3542	-0.4089
CARBON	0.8326	-1.1434	0.3839
CARBON	2.0963	-0.6998	0.7547
CARBON	2.5488	0.5466	0.3345
CARBON	1.7287	1.3407	-0.4586
CARBON	0.4647	0.8916	-0.8258
HYDROGEN	0.4928	-2.1189	0.7114
HYDROGEN	2.7292	-1.3286	1.3673
HYDROGEN	3.5332	0.8935	0.6195
HYDROGEN	2.0724	2.3109	-0.7927
HYDROGEN	-0.1656	1.5181	-1.4444
CARBON	-1.3854	-0.8361	-0.7777
CARBON	-2.4441	-0.6051	0.3090
OXYGEN	-2.6909	0.7682	0.5883
HYDROGEN	-3.0921	1.1781	-0.1837
HYDROGEN	-1.7168	-0.3503	-1.7001
HYDROGEN	-1.3595	-1.9097	-0.9856
HYDROGEN	-3.3722	-1.1123	0.0216
HYDROGEN	-2.1100	-1.0368	1.2525

PEA1			atom	PEA2		
-0.0625	0.0000	-0.3815	CARBON	-0.0585	0.0034	0.3662
-0.7584	-1.1981	-0.2048	CARBON	-0.7553	1.2016	0.1969
-2.1057	-1.2011	0.1388	CARBON	-2.1056	1.2056	-0.1356
-2.7847	0.0000	0.3130	CARBON	-2.7862	0.0049	-0.3050
-2.1057	1.2011	0.1388	CARBON	-2.1063	-1.1966	-0.1369
-0.7584	1.1981	-0.2048	CARBON	-0.7561	-1.1944	0.1952
-0.2408	-2.1397	-0.3441	HYDROGEN	-0.2362	2.1428	0.3337
-2.6260	-2.1415	0.2662	HYDROGEN	-2.6267	2.1463	-0.2578
-3.8338	0.0000	0.5772	HYDROGEN	-3.8376	0.0054	-0.5601
-2.6260	2.1415	0.2662	HYDROGEN	-2.6282	-2.1367	-0.2598
-0.2408	2.1397	-0.3441	HYDROGEN	-0.2369	-2.1356	0.3304
1.4105	0.0000	-0.7052	CARBON	1.4153	-0.0018	0.6893
2.3011	0.0000	0.5565	CARBON	2.2986	-0.0105	-0.5650
3.7416	0.0000	0.3194	NITROGEN	3.7153	-0.0551	-0.1954
4.0284	-0.8153	-0.2085	HYDROGEN	4.3023	-0.1526	-1.0141
1.6592	-0.8780	-1.3074	HYDROGEN	1.6635	0.8796	1.2877
1.6592	0.8780	-1.3074	HYDROGEN	1.6702	-0.8747	1.2925
2.0579	0.8733	1.1653	HYDROGEN	2.0768	-0.9052	-1.1502
2.0579	-0.8733	1.1653	HYDROGEN	2.0330	0.8509	-1.1925
4.0284	0.8152	-0.2087	HYDROGEN	3.9959	0.7994	0.2712

PEA3			atom	PEA4		
-0.0720	-0.2220	-0.5005	CARBON	-0.0767	-0.2092	-0.5143
0.5055	1.0463	-0.5890	CARBON	0.5311	1.0443	-0.6074
1.8069	1.2733	-0.1512	CARBON	1.8414	1.2412	-0.1809
2.5560	0.2318	0.3837	CARBON	2.5695	0.1826	0.3481
1.9950	-1.0383	0.4750	CARBON	1.9788	-1.0739	0.4444
0.6953	-1.2599	0.0363	CARBON	0.6707	-1.2645	0.0173
-0.0706	1.8619	-1.0074	HYDROGEN	-0.0240	1.8740	-1.0276
2.2355	2.2638	-0.2319	HYDROGEN	2.2927	2.2211	-0.2661
3.5692	0.4057	0.7211	HYDROGEN	3.5890	0.3323	0.6774
2.5726	-1.8579	0.8826	HYDROGEN	2.5396	-1.9068	0.8482
0.2713	-2.2548	0.1050	HYDROGEN	0.2236	-2.2487	0.0918
-1.4955	-0.4656	-0.9439	CARBON	-1.5098	-0.4197	-0.9345
-2.5026	-0.4772	0.2151	CARBON	-2.5057	-0.4327	0.2485
-2.5922	0.8376	0.8522	NITROGEN	-2.6252	0.7999	1.0192
-3.3070	0.8447	1.5684	HYDROGEN	-1.7332	1.0728	1.4135
-1.7986	0.3046	-1.6548	HYDROGEN	-1.8087	0.3625	-1.6370
-1.5575	-1.4283	-1.4569	HYDROGEN	-1.6015	-1.3722	-1.4644
-3.4887	-0.7205	-0.1856	HYDROGEN	-3.4962	-0.6856	-0.1358
-2.2308	-1.2830	0.9111	HYDROGEN	-2.2270	-1.2325	0.9381
-1.7169	1.0811	1.3005	HYDROGEN	-2.9440	1.5662	0.4387

atom	<b>PEA5</b>		
CARBON	-0.0462	-0.2931	-0.4367
CARBON	0.4358	1.0130	-0.5375
CARBON	1.7376	1.3256	-0.1622
CARBON	2.5842	0.3344	0.3224
CARBON	2.1190	-0.9718	0.4259
CARBON	0.8165	-1.2789	0.0480
HYDROGEN	-0.2174	1.7926	-0.9057
HYDROGEN	2.0908	2.3450	-0.2483
HYDROGEN	3.5981	0.5766	0.6123
HYDROGEN	2.7708	-1.7529	0.7952
HYDROGEN	0.4659	-2.3015	0.1256
CARBON	-1.4654	-0.6419	-0.8133
CARBON	-2.4799	-0.4941	0.3332
NITROGEN	-2.7017	0.9113	0.6778
HYDROGEN	-3.2514	1.3773	-0.0339
HYDROGEN	-1.7941	-0.0189	-1.6501
HYDROGEN	-1.5024	-1.6759	-1.1640
HYDROGEN	-3.4014	-1.0189	0.0463
HYDROGEN	-2.0908	-0.9983	1.2197
HYDROGEN	-3.2043	1.0009	1.5509