Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information for

Controlling the Local Arrangements of π-Stacked Polycyclic Aromatic Hydrocarbons through Substituent Effects

Steven E. Wheeler

Department of Chemistry, Texas A&M University, College Station, TX 77843

Email: wheeler@chem.tamu.edu

Figure S1. Comparison of B97-D/TZV(2*d*,2*p*) and counterpoise-corrected df-SCS-MP2/TZVPP interaction energies, as a function of the orientation angle ϕ, for the coronene sandwich dimer.

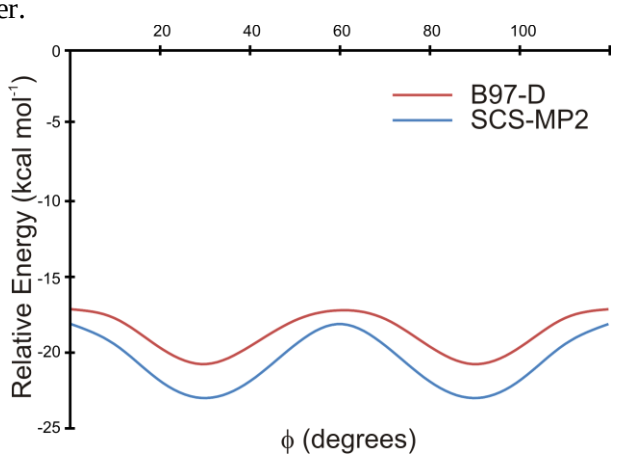

Table S1. Rigid-monomer interaction energy (E^{int}, kcal mol^{-1}) and ϕ for global minimum (ϕ_{min}), relaxed interaction energy [E^{int}(relaxed), kcal mol^{-1}] as well as the energy spanned across the full range of orientation angles (E^{span}, kcal mol^{-1}) for dimers of 1,3,5-trisubstituted benzenes.[a]

X	Y	E_{int}	E^{int}(relaxed)	ϕ_{min}	E^{span}
CCH	CCH	-6.5	-7.6	60	2.3
CCH	CH_3	-6.9	-7.8	27	0.4
CCH	CHO	-7.8	-9.3	25	1.4
CCH	CN	-7.8	-9.1	60	1.1
CCH	F	-5.7	-6.5	60	0.7
CCH	H	-4.3	-4.5	15	0.0
CCH	NH_2	-7.3	-9.1	16	0.6
CCH	NO_2	-8.4	-9.0	0	0.5
CCH	OH	-6.5	-8.3	34	1.8
CCH	OMe	-8.0	-8.8	86	1.9
CH_3	CH_3	-5.8	-7.8	55	0.6
CH_3	CHO	-7.8	-8.8	13	0.4
CH_3	CN	-8.4	-9.4	31	0.2
CH_3	F	-5.6	-6.3	82	0.1
CH_3	H	-3.3	-3.3	16	0.1
CH_3	NH_2	-5.1	-7.8	91	0.3
CH_3	NO_2	-9.6	-10.9	3	0.4
CH_3	OH	-5.2	-5.8	25	0.4
CH_3	OMe	-6.4	-6.8	95	0.4
CHO	CHO	-6.6	-8.2	60	2.8
CHO	CN	-6.1	-7.4	87	2.9
CHO	F	-6.0	-6.9	94	1.2
CHO	H	-5.1	-5.3	13	0.1
CHO	NH_2	-9.2	-13.8	116	1.5
CHO	NO_2	-5.6	-7.0	81	0.6
CHO	OH	-7.8	-12.1	64	1.9
CHO	OMe	-10.6	-13.4	116	3.4
CN	CN	-4.8	-5.7	65	3.0
CN	F	-5.8	-6.6	59	1.0
CN	H	-5.9	-6.2	-1	0.1
CN	NH_2	-10.0	-12.1	5	1.3
CN	NO_2	-4.0	-4.5	61	0.5
CN	OH	-8.8	-11.3	33	2.5
CN	OMe	-10.6	-13.3	90	2.5
F	F	-4.8	-5.4	60	0.7
F	H	-3.7	-3.8	10	0.1
F	NH_2	-5.7	-6.5	6	0.1
F	NO_2	-5.8	-6.7	0	0.1

F	OH	-5.4	-6.3	36	1.2
F	OMe	-6.8	-8.0	84	1.5
H	H	-1.8	-1.8	26	0.1
H	NH_2	-2.8	-3.0	7	0.1
H	NO_2	-6.7	-7.4	33	0.1
H	OH	-3.0	-3.0	1	0.1
H	OMe	-3.7	-3.9	60	0.1
NH_2	NH_2	-5.0	-7.1	23	0.7
NH_2	NO_2	-12.1	-15.9	-1	0.8
NH_2	OH	-5.4	-8.5	35	3.0
NH_2	OMe	-7.0	-8.4	86	3.3
NO_2	NO_2	-4.1	-6.8	31	0.8
NO_2	OH	-8.7	-11.7	116	0.6
NO_2	OMe	-11.2	-14.5	-2	1.1
OH	OH	-5.3	-6.5	61	2.6
OH	OMe	-6.8	-8.0	102	2.6
OMe	OMe	-8.0	-10.5	55	3.7

[a] B97-D/TZV(2*d*,2*p*) level of theory. Inter-ring separation of 3.8 Å.

Table S2. B97-D/TZV(2*d*,2*p*) absolute energies (hartree) for 1,3,5-trisubstituted benzene dimers as a function of the orientation angle, ϕ, along with energy at the rigid monomer and relaxed global minima.

X	Y	0	10	20	30	40	50	60	70	80
CCH	CCH	-920.98245	-920.98292	-920.98396	-920.98499	-920.98559	-920.98599	-920.98610	-920.98599	-920.98559
CCH	CH_3	-810.55635	-810.55652	-810.55684	-810.55692	-810.55660	-810.55632	-810.55628	-810.55632	-810.55660
CCH	CHO	-1032.53902	-1032.53966	-1032.54001	-1032.54001	-1032.53968	-1032.53922	-1032.53873	-1032.53827	-1032.53792
CCH	CN	-969.26246	-969.26265	-969.26311	-969.26363	-969.26397	-969.26420	-969.26428	-969.26420	-969.26397
CCH	F	-990.34166	-990.34173	-990.34198	-990.34233	-990.34256	-990.34273	-990.34282	-990.34273	-990.34256
CCH	H	-692.64418	-692.64416	-692.64416	-692.64419	-692.64416	-692.64416	-692.64418	-692.64416	-692.64416
CCH	NH_2	-858.68628	-858.68629	-858.68633	-858.68620	-858.68584	-858.68550	-858.68543	-858.68550	-858.68584
CCH	NO_2	-1306.05878	-1306.05866	-1306.05840	-1306.05818	-1306.05801	-1306.05797	-1306.05795	-1306.05797	-1306.05801
CCH	OH	-918.28712	-918.28792	-918.28873	-918.28923	-918.28915	-918.28878	-918.28829	-918.28768	-918.28714
CCH	OMe	-1036.14240	-1036.14158	-1036.14115	-1036.14119	-1036.14149	-1036.14209	-1036.14292	-1036.14360	-1036.14406
CH_3	CH_3	-700.12462	-700.12456	-700.12493	-700.12528	-700.12536	-700.12540	-700.12540	-700.12541	-700.12543
CH_3	CHO	-922.11006	-922.11021	-922.11008	-922.10992	-922.10977	-922.10971	-922.10971	-922.10975	-922.10975
CH_3	CN	-858.83506	-858.83516	-858.83530	-858.83542	-858.83535	-858.83524	-858.83517	-858.83518	-858.83532
CH_3	F	-879.91285	-879.91278	-879.91286	-879.91285	-879.91284	-879.91274	-879.91281	-879.91274	-879.91289
CH_3	H	-582.21277	-582.21271	-582.21276	-582.21279	-582.21274	-582.21273	-582.21269	-582.21279	-582.21276
CH_3	NH_2	-748.25269	-748.25273	-748.25297	-748.25302	-748.25291	-748.25273	-748.25259	-748.25267	-748.25285
CH_3	NO_2	-1195.63100	-1195.63090	-1195.63061	-1195.63043	-1195.63051	-1195.63057	-1195.63066	-1195.63062	-1195.63052
CH_3	OH	-807.85684	-807.85718	-807.85739	-807.85741	-807.85719	-807.85696	-807.85684	-807.85698	-807.85697
CH_3	OMe	-925.71171	-925.71140	-925.71124	-925.71131	-925.71128	-925.71128	-925.71128	-925.71129	-925.71153
CHO	CHO	-1144.08540	-1144.08592	-1144.08704	-1144.08823	-1144.08920	-1144.08973	-1144.08993	-1144.08975	-1144.08917
CHO	CN	-1080.81054	-1080.80939	-1080.80883	-1080.80896	-1080.80970	-1080.81068	-1080.81174	-1080.81260	-1080.81321
CHO	F	-1101.89415	-1101.89364	-1101.89326	-1101.89315	-1101.89325	-1101.89358	-1101.89398	-1101.89444	-1101.89484
CHO	H	-804.19719	-804.19725	-804.19724	-804.19722	-804.19722	-804.19718	-804.19722	-804.19719	-804.19723
CHO	NH_2	-970.24116	-970.24081	-970.24048	-970.24024	-970.24010	-970.23983	-970.23931	-970.23896	-970.23901
CHO	NO_2	-1417.60521	-1417.60543	-1417.60548	-1417.60532	-1417.60515	-1417.60521	-1417.60549	-1417.60589	-1417.60618
CHO	OH	-1029.84033	-1029.84021	-1029.84066	-1029.84154	-1029.84242	-1029.84298	-1029.84312	-1029.84308	-1029.84270
CHO	OMe	-1147.70005	-1147.69905	-1147.69739	-1147.69596	-1147.69499	-1147.69468	-1147.69490	-1147.69551	-1147.69648

CN	CN	-1017.53091	-1017.53135	-1017.53249	-1017.53370	-1017.53480	-1017.53549	-1017.53566	-1017.53550	-1017.53478
CN	F	-1038.61747	-1038.61766	-1038.61797	-1038.61838	-1038.61875	-1038.61902	-1038.61913	-1038.61902	-1038.61873
CN	H	-740.92286	-740.92284	-740.92281	-740.92280	-740.92282	-740.92282	-740.92279	-740.92282	-740.92281
CN	NH_2	-906.96670	-906.96669	-906.96648	-906.96597	-906.96541	-906.96491	-906.96469	-906.96490	-906.96541
CN	NO_2	-1354.32710	-1354.32714	-1354.32717	-1354.32731	-1354.32760	-1354.32784	-1354.32795	-1354.32786	-1354.32764
CN	OH	-966.56658	-966.56777	-966.56879	-966.56917	-966.56901	-966.56840	-966.56759	-966.56674	-966.56592
CN	OMe	-1084.42264	-1084.42149	-1084.42079	-1084.42054	-1084.42080	-1084.42150	-1084.42240	-1084.42341	-1084.42417
F	F	-1059.69831	-1059.69833	-1059.69853	-1059.69880	-1059.69903	-1059.69927	-1059.69936	-1059.69924	-1059.69905
F	H	-762.00115	-762.00118	-762.00117	-762.00114	-762.00110	-762.00115	-762.00119	-762.00112	-762.00113
F	NH_2	-928.04173	-928.04174	-928.04175	-928.04168	-928.04163	-928.04156	-928.04152	-928.04154	-928.04160
F	NO_2	-1375.41273	-1375.41269	-1375.41270	-1375.41268	-1375.41264	-1375.41261	-1375.41264	-1375.41261	-1375.41266
F	OH	-987.64414	-987.64465	-987.64512	-987.64539	-987.64548	-987.64542	-987.64516	-987.64474	-987.64425
F	OMe	-1105.49876	-1105.49826	-1105.49790	-1105.49788	-1105.49827	-1105.49878	-1105.49935	-1105.49987	-1105.50022
H	H	-464.30172	-464.30167	-464.30159	-464.30173	-464.30166	-464.30168	-464.30172	-464.30168	-464.30164
H	NH_2	-630.34084	-630.34086	-630.34081	-630.34076	-630.34080	-630.34084	-630.34084	-630.34088	-630.34081
H	NO_2	-1077.71750	-1077.71759	-1077.71767	-1077.71772	-1077.71765	-1077.71760	-1077.71749	-1077.71757	-1077.71767
H	OH	-689.94538	-689.94529	-689.94532	-689.94522	-689.94525	-689.94524	-689.94538	-689.94535	-689.94530
H	OMe	-807.79896	-807.79891	-807.79890	-807.79883	-807.79890	-807.79889	-807.79901	-807.79894	-807.79893
NH_2	NH_2	-796.38096	-796.38128	-796.38167	-796.38163	-796.38134	-796.38082	-796.38054	-796.38085	-796.38136
NH_2	NO_2	-1243.76362	-1243.76331	-1243.76268	-1243.76231	-1243.76241	-1243.76266	-1243.76277	-1243.76266	-1243.76241
NH_2	OH	-855.98265	-855.98424	-855.98573	-855.98647	-855.98643	-855.98588	-855.98521	-855.98453	-855.98373
NH_2	OMe	-973.83770	-973.83663	-973.83630	-973.83654	-973.83735	-973.83826	-973.83921	-973.84036	-973.84133
NO_2	NO_2	-1691.12040	-1691.12075	-1691.12133	-1691.12170	-1691.12159	-1691.12131	-1691.12120	-1691.12133	-1691.12156
NO_2	OH	-1303.36247	-1303.36239	-1303.36213	-1303.36206	-1303.36219	-1303.36217	-1303.36197	-1303.36167	-1303.36155
NO_2	OMe	-1421.21905	-1421.21886	-1421.21815	-1421.21751	-1421.21730	-1421.21747	-1421.21787	-1421.21810	-1421.21817
OH	OH	-915.58646	-915.58690	-915.58787	-915.58904	-915.58996	-915.59043	-915.59065	-915.59041	-915.58995
OH	OMe	-1033.44430	-1033.44328	-1033.44224	-1033.44171	-1033.44140	-1033.44159	-1033.44207	-1033.44294	-1033.44393
OMe	OMe	-1151.29396	-1151.29554	-1151.29723	-1151.29830	-1151.29919	-1151.29971	-1151.29975	-1151.29962	-1151.29913

X	Y	90	100	110	120	E_{min}	$E_{relaxed}$
CCH	CCH	-920.98499	-920.98396	-920.98292	-920.98245	-920.98610	-920.98781
CCH	CH_3	-810.55691	-810.55684	-810.55652	-810.55635	-810.55694	-810.55835
CCH	CHO	-1032.53778	-1032.53785	-1032.53828	-1032.53902	-1032.54005	-1032.54238
CCH	CN	-969.26363	-969.26311	-969.26265	-969.26246	-969.26428	-969.26636
CCH	F	-990.34233	-990.34198	-990.34173	-990.34166	-990.34282	-990.34402
CCH	H	-692.64419	-692.64416	-692.64416	-692.64418	-692.64422	-692.64453
CCH	NH_2	-858.68620	-858.68634	-858.68630	-858.68628	-858.68640	-858.68928
CCH	NO_2	-1306.05818	-1306.05840	-1306.05866	-1306.05878	-1306.05878	-1306.05984
CCH	OH	-918.28670	-918.28639	-918.28651	-918.28712	-918.28926	-918.29222
CCH	OMe	-1036.14411	-1036.14368	-1036.14308	-1036.14240	-1036.14418	-1036.14554
CH_3	CH_3	-700.12531	-700.12489	-700.12468	-700.12462	-700.12543	-700.12857
CH_3	CHO	-922.10965	-922.10966	-922.10981	-922.11006	-922.11024	-922.11175
CH_3	CN	-858.83541	-858.83531	-858.83509	-858.83506	-858.83542	-858.83715
CH_3	F	-879.91284	-879.91285	-879.91281	-879.91285	-879.91289	-879.91396
CH_3	H	-582.21277	-582.21275	-582.21274	-582.21277	-582.21282	-582.21282
CH_3	NH_2	-748.25313	-748.25300	-748.25274	-748.25269	-748.25313	-748.25742
CH_3	NO_2	-1195.63044	-1195.63064	-1195.63090	-1195.63100	-1195.63102	-1195.63300
CH_3	OH	-807.85700	-807.85677	-807.85673	-807.85684	-807.85744	-807.85843
CH_3	OMe	-925.71173	-925.71173	-925.71177	-925.71171	-925.71179	-925.71247
CHO	CHO	-1144.08822	-1144.08702	-1144.08590	-1144.08540	-1144.08993	-1144.09241
CHO	CN	-1080.81332	-1080.81291	-1080.81189	-1080.81054	-1080.81335	-1080.81548
CHO	F	-1101.89501	-1101.89494	-1101.89466	-1101.89415	-1101.89505	-1101.89659
CHO	H	-804.19721	-804.19718	-804.19716	-804.19719	-804.19726	-804.19762
CHO	NH_2	-970.23956	-970.24046	-970.24110	-970.24116	-970.24121	-970.24850
CHO	NO_2	-1417.60610	-1417.60563	-1417.60528	-1417.60521	-1417.60618	-1417.60834
CHO	OH	-1029.84226	-1029.84157	-1029.84091	-1029.84033	-1029.84315	-1029.84999
CHO	OMe	-1147.69768	-1147.69896	-1147.69991	-1147.70005	-1147.70014	-1147.70467
CN	CN	-1017.53374	-1017.53249	-1017.53131	-1017.53091	-1017.53567	-1017.53710
CN	F	-1038.61831	-1038.61796	-1038.61767	-1038.61747	-1038.61913	-1038.62035

CN	H	-740.92285	-740.92285	-740.92280	-740.92286	-740.92286	-740.92347
CN	NH_2	-906.96599	-906.96649	-906.96668	-906.96670	-906.96672	-906.97019
CN	NO_2	-1354.32732	-1354.32713	-1354.32709	-1354.32710	-1354.32795	-1354.32875
CN	OH	-966.56539	-966.56517	-966.56559	-966.56658	-966.56919	-966.57307
CN	OMe	-1084.42452	-1084.42419	-1084.42362	-1084.42264	-1084.42452	-1084.42879
F	F	-1059.69877	-1059.69849	-1059.69833	-1059.69831	-1059.69936	-1059.70026
F	H	-762.00109	-762.00116	-762.00118	-762.00115	-762.00118	-762.00140
F	NH_2	-928.04167	-928.04174	-928.04172	-928.04173	-928.04175	-928.04303
F	NO_2	-1375.41262	-1375.41265	-1375.41271	-1375.41273	-1375.41273	-1375.41415
F	OH	-987.64389	-987.64362	-987.64372	-987.64414	-987.64552	-987.64703
F	OMe	-1105.50017	-1105.49993	-1105.49942	-1105.49876	-1105.50026	-1105.50217
H	H	-464.30173	-464.30164	-464.30168	-464.30172	-464.30181	-464.30180
H	NH_2	-630.34076	-630.34081	-630.34084	-630.34084	-630.34087	-630.34114
H	NO_2	-1077.71770	-1077.71766	-1077.71763	-1077.71750	-1077.71772	-1077.71886
H	OH	-689.94527	-689.94525	-689.94530	-689.94538	-689.94538	-689.94546
H	OMe	-807.79896	-807.79888	-807.79893	-807.79896	-807.79901	-807.79935
NH_2	NH_2	-796.38164	-796.38166	-796.38123	-796.38096	-796.38169	-796.38495
NH_2	NO_2	-1243.76232	-1243.76270	-1243.76332	-1243.76362	-1243.76363	-1243.76974
NH_2	OH	-855.98272	-855.98202	-855.98192	-855.98265	-855.98656	-855.99145
NH_2	OMe	-973.84149	-973.84080	-973.83938	-973.83770	-973.84156	-973.84379
NO_2	NO_2	-1691.12161	-1691.12134	-1691.12069	-1691.12040	-1691.12171	-1691.12598
NO_2	OH	-1303.36170	-1303.36205	-1303.36242	-1303.36247	-1303.36253	-1303.36737
NO_2	OMe	-1421.21826	-1421.21860	-1421.21891	-1421.21905	-1421.21905	-1421.22426
OH	OH	-915.58914	-915.58792	-915.58691	-915.58646	-915.59066	-915.59255
OH	OMe	-1033.44487	-1033.44544	-1033.44524	-1033.44430	-1033.44545	-1033.44748
OMe	OMe	-1151.29832	-1151.29722	-1151.29549	-1151.29396	-1151.29986	-1151.30388

Table S3. B97-D/TZV(2*d*,2*p*) absolute energies (hartree) for substituted coronene dimers as a function of the orientation angle, ϕ, along with energy at the rigid monomer global minima.

X	Y	0	10	20	30	40	50	60
H	H	-1842.954407	-1842.95540	-1842.95851	-1842.96022	-1842.95833	-1842.95560	-1842.95452
CHO	CHO	-3202.471888	-3202.47663	-3202.48334	-3202.48564	-3202.48303	-3202.47661	-3202.47214
OMe	OMe	-3216.93665	-3216.94997	-3216.95747	-3216.95950	-3216.95747	-3216.94974	-3216.93663
CHO	OMe	-3209.71925	-3209.72802	-3209.73625	-3209.74103	-3209.74351	-3209.74680	-3209.74981
CN	CN	-2949.426273	-2949.42956	-2949.43538	-2949.43864	-2949.43542	-2949.42954	-2949.42637
CN	NH_2	-2728.309267	-2728.31409	-2728.32103	-2728.32470	-2728.32660	-2728.32525	-2728.32419
NH2	NH_2	-2507.109762	-2507.11388	-2507.11528	-2507.11328	-2507.11176	-2507.10943	-2507.10982

70	80	90	100	110	120	E_{min}	ϕ_{min}	Monomer
-1842.95540	-1842.95832	-1842.96022	-1842.95851	-1842.95540	-1842.95441	-1842.96022	30	-921.46358
-3202.47661	-3202.48333	-3202.48635	-3202.48332	-3202.47615	-3202.47189	-3202.48635	90	-1601.21808
-3216.94996	-3216.95795	-3216.95951	-3216.95796	-3216.94996	-3216.93665	-3216.95951	90	-1608.45300
-3209.74680	-3209.74351	-3209.74037	-3209.73626	-3209.72803	-3209.71925	-3209.74981	60	-1604.84284
-2949.42954	-2949.43542	-2949.43864	-2949.43538	-2949.42627	-2949.42627	-2949.43864	30	-1474.69867
-2728.32525	-2728.32660	-2728.32470	-2728.32103	-2728.31409	-2728.30927	-2728.32661	41	-1364.13574
-2507.10943	-2507.11176	-2507.11328	-2507.11528	-2507.11388	-2507.10976	-2507.11529	19	-1253.53398

Table S4. B97-D/TZV(2*d*,2*p*) absolute energies (hartree) for substituted HBC dimers as a function of the orientation angle, ϕ, along with energy at the rigid monomer global minima.

X	Y	0	10	20	30	40	50	60
H	H	-3221.56866	-3221.57352	-3221.57889	-3221.57912	-3221.57887	-3221.57352	-3221.56881
CHO	CHO	-4581.15637	-4581.16598	-4581.17498	-4581.17377	-4581.17475	-4581.16655	-4581.15856
OMe	OMe	-4595.55347	-4595.57319	-4595.58034	-4595.58040	-4595.58011	-4595.57214	-4595.55341
CHO	OMe	-4588.36479	-4588.37802	-4588.38620	-4588.38516	-4588.38870	-4588.39221	-4588.39429
CN	CN	-4328.04878	-4328.05635	-4328.06425	-4328.06500	-4328.06423	-4328.05635	-4328.04891
CN	NH_2	-4106.91923	-4106.92777	-4106.93508	-4106.93759	-4106.94179	-4106.94041	-4106.93508
NH2	NH_2	-3885.73451	-3885.74103	-3885.74284	-3885.73991	-3885.74283	-3885.74101	-3885.73458

70	80	90	100	110	120	E_{min}	ϕ_{min}	Monomer
-3221.57352	-3221.57888	-3221.57902	-3221.57889	-3221.57353	-3221.56866	-3221.57912	30	-1610.75645
-4581.16649	-4581.17474	-4581.17523	-4581.17510	-4581.16687	-4581.15637	-4581.17525	93	-2290.54622
-4595.57321	-4595.58091	-4595.58037	-4595.58010	-4595.57215	-4595.55347	-4595.58169	84	-2297.74728
-4588.39191	-4588.38959	-4588.38603	-4588.38583	-4588.37818	-4588.36479	-4588.39429	60	-2294.15103
-4328.05636	-4328.06425	-4328.06491	-4328.06426	-4328.05633	-4328.04878	-4328.06500	30	-2163.99656
-4106.94043	-4106.94181	-4106.93737	-4106.93509	-4106.92777	-4106.91923	-4106.94201	77	-2053.42816
-3885.74100	-3885.74283	-3885.73981	-3885.74282	-3885.74102	-3885.73451	-3885.74287	19	-1942.83358

Cartesian Coordinates for Substituted Benzenes

```
18
BF2
C       -1.394673     -0.000002      0.000000
C       -0.709210     -1.228181      0.000000
C        0.697108     -1.206836      0.000000
C        1.418982     -0.000002      0.000000
C        0.697055      1.206818      0.000000
C       -0.709261      1.228202      0.000000
H       -2.482066     -0.000032      0.000000
H        1.239745      2.148887      0.000000
B       -1.483909      2.581929      0.000000
H        1.239652     -2.148994      0.000000
B       -1.483806     -2.581946      0.000000
B        2.978519      0.000353      0.000000
F       -2.821109      2.623292      0.000000
F       -0.837957      3.754066      0.000000
F        3.676620      1.141920      0.000000
F        3.677359     -1.140720      0.000000
F       -0.837740     -3.754029      0.000000
F       -2.821005     -2.623343      0.000000

18
CCH
C       -1.403446      0.000000      0.000000
C       -0.704503      1.220199      0.000000
C        0.701718      1.215354      0.000000
C        1.409018     -0.000000      0.000000
C        0.701717     -1.215354      0.000000
C       -0.704504     -1.220198      0.000000
H       -2.488021      0.000000      0.000000
H        1.243982     -2.154636      0.000000
H        1.243983      2.154635      0.000000
C       -1.418134     -2.456818      0.000000
C       -2.022879     -3.506111      0.000000
H       -2.555575     -4.430470      0.000000
C       -1.418132      2.456819      0.000000
C       -2.022877      3.506112      0.000000
H       -2.555573      4.430472      0.000000
C        2.836766     -0.000001      0.000000
C        4.047846     -0.000001      0.000000
H        5.114716     -0.000002      0.000000

21
CF3
C       -1.399554      0.000000     -0.000005
C       -0.695994     -1.205501     -0.002683
C        0.699773     -1.212049      0.002687
C        1.391994      0.000000     -0.000005
C        0.699774      1.212048      0.002687
C       -0.695993      1.205501     -0.002683
H       -2.483284      0.000000     -0.011077
H        1.241658      2.150597     -0.006300
H        1.241657     -2.150599     -0.006300
C       -1.454026      2.518337      0.049190
C        2.907857     -0.000000      0.054784
C       -1.454028     -2.518336      0.049190
F       -1.675009      2.898225      1.338860
F       -0.770724      3.525912     -0.552196
F       -2.667103      2.431036     -0.554628
F        3.439949      1.094875     -0.546796
F        3.344859     -0.000001      1.345298
F        3.439949     -1.094876     -0.546796
F       -1.675010     -2.898225      1.338860
F       -0.770726     -3.525912     -0.552196
F       -2.667104     -2.431035     -0.554628

24
CH2OH
C       -1.395572     -0.003687      0.000000
C       -0.691167     -1.219320      0.000000
C        0.700978     -1.206757      0.000000
C        1.401547      0.011091      0.000000
C        0.694593      1.210444      0.000000
C       -0.710379      1.208229      0.000000
H       -2.481872     -0.004000      0.000000
H        1.237471      2.151364      0.000000
H        1.244400     -2.147364      0.000000
C       -1.419987      2.545409      0.000000
C        2.914383     -0.042959      0.000000
C       -1.494396     -2.502449      0.000000
H       -1.099042      3.115810      0.888538
H       -1.099042      3.115810     -0.888538
H       -2.148849     -2.509703     -0.888538
H       -2.148849     -2.509703      0.888538
H        3.247892     -0.606106     -0.888538
H        3.247892     -0.606106      0.888538
O        3.479507      1.273382      0.000000
H        4.436878      1.170726      0.000000
```

O	-2.842534	2.376650	0.000000
H	-3.232317	3.257086	0.000000
O	-0.636972	-3.650032	0.000000
H	-1.204560	-4.427811	0.000000

21
CH3

C	-1.390656	0.000000	0.000007
C	-0.705080	1.221236	-0.001437
C	0.695327	1.204343	0.001431
C	1.410162	0.000000	0.000007
C	0.695327	-1.204343	0.001431
C	-0.705080	-1.221236	-0.001437
H	-2.479729	-0.000000	0.014497
H	1.239848	-2.147499	0.017036
H	1.239848	2.147499	0.017036
C	-1.460879	-2.530344	-0.023533
C	2.921804	0.000000	-0.020541
C	-1.460880	2.530344	-0.023533
H	-2.433465	-2.434571	0.473012
H	-1.647705	-2.855157	-1.056876
H	-0.892153	-3.324448	0.474064
H	-2.433465	2.434571	0.473012
H	-1.647705	2.855157	-1.056876
H	-0.892154	3.324448	0.474064
H	3.324646	0.889878	0.476943
H	3.297571	0.000001	-1.053500
H	3.324647	-0.889877	0.476943

18
CHO

C	-1.398738	-0.003462	0.000000
C	-0.693076	-1.221271	0.000000
C	0.702367	-1.209611	0.000000
C	1.404190	0.010414	0.000000
C	0.696370	1.213073	0.000000
C	-0.711113	1.210858	0.000000
H	-2.486704	-0.026551	0.000000
H	1.220358	2.166824	0.000000
H	1.266346	-2.140273	0.000000
C	-1.475739	2.488642	0.000000
O	-0.970062	3.592993	0.000000
H	-2.583470	2.357789	0.000000
C	-1.417358	-2.522348	0.000000
O	-2.626592	-2.636595	0.000000
H	-0.750169	-3.416245	0.000000
C	2.893096	0.033705	0.000000
O	3.596653	-0.956398	0.000000
H	3.333640	1.058457	0.000000

15
CN

C	-1.407045	0.000000	0.000000
C	-0.700097	-1.212603	0.000000
C	0.703523	-1.218537	0.000000
C	1.400193	0.000000	0.000000
C	0.703522	1.218536	0.000000
C	-0.700097	1.212603	0.000000
H	-2.491490	-0.000000	0.000000
H	1.245745	2.157693	0.000000
H	1.245745	-2.157694	0.000000
C	-1.416838	2.454033	0.000000
N	-1.997718	3.460148	0.000000
C	-1.416837	-2.454034	0.000000
N	-1.997717	-3.460149	0.000000
C	2.833674	-0.000000	0.000000
N	3.995435	0.000001	0.000000

27
COCH3

C	-1.395147	-0.002711	0.000000
C	-0.701864	1.221086	0.000000
C	0.695226	1.209588	0.000000
C	1.408424	-0.002711	0.000000
C	0.699921	-1.206877	0.000000
C	-0.706560	-1.218375	0.000000
H	-2.479610	0.030690	0.000000
H	1.213226	-2.162750	0.000000
H	1.266383	2.132059	0.000000
C	-1.419492	-2.547836	0.000000
O	-0.788627	-3.593925	0.000000
C	-1.496745	2.503234	0.000000
O	-2.718118	2.479933	0.000000
C	2.916236	0.044602	0.000000
O	3.506743	1.113992	0.000000
C	-2.939722	-2.540501	0.000000
H	-3.320375	-2.009194	0.881752
H	-3.320375	-2.009194	-0.881752
H	-3.303224	-3.570061	0.000000
C	-0.730278	3.816124	0.000000

H	-0.079826	3.880125	0.881752
H	-0.079826	3.880125	-0.881752
H	-1.440151	4.645706	0.000000
C	3.669999	-1.275623	0.000000
H	3.400200	-1.870931	0.881752
H	3.400200	-1.870931	-0.881752
H	4.743374	-1.075645	0.000000

30
COOCH3

C	-1.398834	-0.000556	0.000000
C	-0.700988	1.215260	0.000000
C	0.698935	1.211704	0.000000
C	1.402940	-0.000556	0.000000
C	0.699899	-1.211148	0.000000
C	-0.701952	-1.214704	0.000000
H	-2.482194	0.017263	0.000000
H	1.226147	-2.158275	0.000000
H	1.256048	2.141012	0.000000
C	-1.393974	-2.545152	0.000000
O	-0.818008	-3.615320	0.000000
O	-2.746308	-2.416904	0.000000
C	2.901154	0.065360	0.000000
O	3.539962	1.099245	0.000000
O	3.466254	-1.169921	0.000000
C	-1.507180	2.479793	0.000000
O	-2.721955	2.516075	0.000000
O	-0.719946	3.586824	0.000000
C	-3.480975	-3.666231	0.000000
H	-3.232265	-4.249848	0.892241
H	-4.534013	-3.379005	0.000000
H	-3.232265	-4.249848	-0.892241
C	-1.434563	4.847728	0.000000
H	-2.064343	4.924148	0.892241
H	-0.659298	5.616072	0.000000
H	-2.064343	4.924148	-0.892241
C	4.915536	-1.181497	0.000000
H	5.193311	-2.237068	0.000000
H	5.296609	-0.674300	-0.892241
H	5.296609	-0.674300	0.892241

21
COOH

C	-1.399499	-0.000867	0.000000
C	-0.700395	1.214853	0.000000
C	0.698998	1.212434	0.000000
C	1.402292	-0.000867	0.000000
C	0.700500	-1.211567	0.000000
C	-0.701897	-1.213986	0.000000
H	-2.483108	0.017397	0.000000
H	1.226487	-2.159133	0.000000
H	1.256621	2.141736	0.000000
C	-1.395077	-2.540293	0.000000
O	-0.828684	-3.613765	0.000000
O	-2.755740	-2.423316	0.000000
H	-3.104753	-3.329445	0.000000
C	2.897496	0.061974	0.000000
O	3.543955	1.089221	0.000000
O	3.476524	-1.174883	0.000000
H	4.435762	-1.024073	0.000000
C	-1.502419	2.478319	0.000000
O	-2.715271	2.524544	0.000000
O	-0.720783	3.598199	0.000000
H	-1.331008	4.353518	0.000000

12
F

C	-1.414664	0.000000	0.000000
C	-0.684962	-1.186390	0.000000
C	0.707332	-1.225135	0.000000
C	1.369924	0.000000	0.000000
C	0.707332	1.225135	0.000000
C	-0.684962	1.186389	0.000000
H	-2.497984	0.000000	0.000000
H	1.248993	2.163319	0.000000
H	1.248992	-2.163318	0.000000
F	-1.361304	2.357848	0.000000
F	-1.361304	-2.357848	0.000000
F	2.722608	0.000000	0.000000

36
NCH3_2

C	0.702628	1.216898	0.009697
C	1.413999	-0.000155	0.019415
C	0.702629	-1.216898	-0.009737
C	-0.707088	-1.224623	-0.009799
C	-1.405080	0.000154	-0.019333
C	-0.707089	1.224623	0.009758
H	1.241675	2.150321	-0.003684
H	-2.482464	0.000439	-0.054977

H	1.241675	-2.149987	-0.038023
N	-1.406890	2.436037	0.044044
N	2.812748	-0.000505	0.063255
N	-1.406889	-2.436430	0.005137
C	-0.684888	3.669968	-0.234439
H	-1.379424	4.512152	-0.171753
H	0.102885	3.831660	0.512044
H	-0.213533	3.671849	-1.233647
C	3.522412	-1.236953	-0.235068
H	4.598556	-1.057848	-0.161451
H	3.263565	-2.014742	0.494323
H	3.295245	-1.626122	-1.243799
C	-2.830447	-2.426848	-0.302784
H	-3.213768	-3.449630	-0.252138
H	-3.379657	-1.828427	0.434935
H	-3.047052	-2.015523	-1.305026
C	-2.830447	2.431373	-0.263991
H	-3.047052	2.036106	-1.272674
H	-3.379657	1.821248	0.464078
H	-3.213769	3.453216	-0.197018
C	3.522412	1.240550	-0.215285
H	3.295246	1.645777	-1.217673
H	3.263565	2.006592	0.526434
H	4.598556	1.060292	-0.144537
C	-0.684888	-3.665756	-0.293016
H	-0.213532	-3.651680	-1.292126
H	0.102885	-3.839349	0.450790
H	-1.379424	-4.508834	-0.243787

18
NH2

C	-1.403439	0.000026	-0.001975
C	-0.701384	-1.214879	-0.001481
C	0.701701	-1.215424	-0.002470
C	1.402807	0.000020	0.001975
C	0.701740	1.215403	0.001482
C	-0.701425	1.214853	0.002469
H	-2.491639	0.000046	0.010801
H	1.245861	2.157759	0.016939
H	1.245750	-2.157866	0.009923
N	-1.402317	2.428953	0.070076
H	-2.337974	2.383128	-0.311011
H	-0.894279	3.216399	-0.310188
N	-1.402543	-2.429038	0.062179
H	-0.894091	-3.215732	-0.319097
H	-2.337571	-2.382088	-0.320305
N	2.804718	-0.000242	0.069088
H	3.232726	0.834132	-0.309609
H	3.232514	-0.832776	-0.313866

27
NHCH3

C	-1.405865	0.004260	-0.006240
C	-0.691747	1.223876	-0.004694
C	0.706660	1.215353	-0.007775
C	1.405775	-0.012844	0.006284
C	0.699226	-1.219661	0.004689
C	-0.714049	-1.210984	0.007737
H	-2.491122	0.027276	-0.003423
H	1.221917	-2.170969	0.016056
H	1.269190	2.143727	-0.005955
N	-1.384271	-2.434386	0.057769
H	-0.829755	-3.204091	-0.286588
N	-1.416489	2.416249	0.032836
H	-2.357632	2.318857	-0.318275
N	2.800439	0.018880	0.054449
H	3.189385	0.880603	-0.298636
C	-2.792662	-2.522446	-0.295383
H	-3.084989	-3.576973	-0.305161
H	-3.403986	-2.008269	0.457034
H	-3.019044	-2.076273	-1.279895
C	-0.785824	3.677944	-0.322725
H	-1.552802	4.458274	-0.342957
H	-0.040727	3.954645	0.433910
H	-0.278615	3.645246	-1.303160
C	3.580490	-1.160144	-0.288271
H	4.639892	-0.886170	-0.301869
H	3.441700	-1.939391	0.471821
H	3.306177	-1.588713	-1.268405

21
NHOH

C	-1.406727	0.007805	-0.003405
C	-0.684288	1.214103	-0.002557
C	0.710134	1.214349	-0.004253
C	1.393587	-0.014434	0.003408
C	0.696599	-1.222168	0.002595
C	-0.709305	-1.199655	0.004212
H	-2.490817	0.009819	-0.028533
H	1.236881	-2.162147	-0.017922

H	1.254027	2.152114	-0.030055
N	-1.375285	-2.447648	0.098703
H	-0.862680	-3.161000	-0.413835
N	-1.432483	2.415141	0.084935
H	-2.304381	2.326249	-0.431031
N	2.807429	0.033297	0.096755
H	3.168586	0.831186	-0.420223
O	-2.693277	-2.436542	-0.494804
H	-3.253592	-2.664364	0.258247
O	-0.761351	3.549117	-0.509338
H	-0.681691	4.150669	0.242148
O	3.456430	-1.116787	-0.491110
H	3.934362	-1.484153	0.263585

15
NO

C	0.714592	-1.210903	0.000000
C	-0.693003	-1.209200	0.000000
C	-1.405968	-0.013403	0.000000
C	-0.700696	1.204758	0.000000
C	0.691376	1.224306	0.000000
C	1.393699	0.004442	0.000000
H	1.263065	-2.149885	0.000000
H	1.230322	2.168789	0.000000
H	-2.493388	-0.018905	0.000000
N	-1.345924	2.522380	0.000000
O	-2.559678	2.495779	0.000000
N	2.857406	-0.095584	0.000000
O	3.441247	0.968856	0.000000
N	-1.511482	-2.426794	0.000000
O	-0.881569	-3.464635	0.000000

18
NO2

C	-1.409078	-0.000000	0.000000
C	-0.687804	-1.191311	0.000000
C	0.704539	-1.220297	0.000000
C	1.375608	-0.000000	0.000000
C	0.704539	1.220297	0.000000
C	-0.687804	1.191312	0.000000
H	-2.491884	-0.000000	0.000000
H	1.245942	2.158035	0.000000
H	1.245942	-2.158035	0.000000
N	2.877623	-0.000001	0.000000
O	3.435381	-1.091610	0.000000
O	3.435380	1.091610	0.000000
N	-1.438811	-2.492095	0.000000
O	-0.772328	-3.520931	0.000000
O	-2.663052	-2.429321	0.000000
N	-1.438812	2.492094	0.000000
O	-2.663053	2.429322	0.000000
O	-0.772328	3.520931	0.000000

24
OCF3

C	-1.410190	-0.002147	0.000000
C	-0.687011	1.194231	0.000000
C	0.703236	1.222334	0.000000
C	1.377740	-0.002147	0.000000
C	0.706954	-1.220187	0.000000
C	-0.690728	-1.192085	0.000000
H	-2.490546	0.029427	0.000000
H	1.219789	-2.171589	0.000000
H	1.270758	2.142163	0.000000
O	2.767831	0.139263	0.000000
O	-1.504520	2.327381	0.000000
O	-1.263311	-2.466643	0.000000
C	3.599118	-0.943495	0.000000
C	-0.982468	3.588674	0.000000
C	-2.616649	-2.645180	0.000000
F	-0.219167	3.839392	1.092685
F	-0.219167	3.839392	-1.092685
F	-2.016548	4.437593	0.000000
F	-3.215427	-2.109500	1.092685
F	-3.215427	-2.109500	-1.092685
F	-2.834794	-3.965179	0.000000
F	4.851343	-0.472414	0.000000
F	3.434595	-1.729891	-1.092685
F	3.434595	-1.729891	1.092685

15
OH

C	-1.407741	0.000668	0.000000
C	-0.694483	-1.204216	0.000000
C	0.703292	-1.219472	0.000000
C	1.390123	0.000668	0.000000
C	0.704448	1.218805	0.000000
C	-0.695640	1.203547	0.000000
H	-2.494260	-0.013601	0.000000
H	1.235352	2.166894	0.000000

H	1.258909	-2.153292	0.000000
O	2.762066	-0.061610	0.000000
H	3.111181	0.838566	0.000000
O	-1.434388	-2.361213	0.000000
H	-0.829371	-3.113645	0.000000
O	-1.327677	2.422824	0.000000
H	-2.281810	2.275079	0.000000

24
OMe

C	0.716776	-1.214201	0.000000
C	-0.692358	-1.208221	0.000000
C	-1.409917	-0.013645	0.000000
C	-0.700171	1.203710	0.000000
C	0.693141	1.227847	0.000000
C	1.392529	0.004511	0.000000
H	1.231601	-2.166560	0.000000
H	1.260496	2.149878	0.000000
H	-2.492096	0.016682	0.000000
O	-1.487701	2.325434	0.000000
O	-1.270034	-2.451104	0.000000
O	2.757736	0.125671	0.000000
C	-0.824724	3.591352	0.000000
H	-0.197641	3.708578	0.895866
H	-0.197641	3.708578	-0.895866
H	-1.617763	4.343560	0.000000
C	-2.697839	-2.509907	0.000000
H	-3.112902	-2.025451	0.895866
H	-3.112902	-2.025451	-0.895866
H	-2.952752	-3.572804	0.000000
C	3.522564	-1.081443	0.000000
H	3.310542	-1.683127	0.895866
H	3.310542	-1.683127	-0.895866
H	4.570515	-0.770756	0.000000

24
SCH3

C	0.713403	-1.210868	0.000000
C	-0.695807	-1.213408	0.000000
C	-1.405344	-0.012391	0.000000
C	-0.702939	1.209291	0.000000
C	0.691942	1.223260	0.000000
C	1.398746	0.004117	0.000000
H	1.247731	-2.154059	0.000000
H	1.241604	2.157596	0.000000
H	-2.489335	-0.003537	0.000000
C	-0.473776	4.030937	0.000000
H	0.150463	3.988669	0.898009
H	0.150463	3.988669	-0.898009
H	-1.052199	4.959232	0.000000
C	-3.254006	-2.425771	0.000000
H	-3.529520	-1.864029	0.898009
H	-3.529520	-1.864029	-0.898009
H	-3.768721	-3.390848	0.000000
C	3.727783	-1.605167	0.000000
H	3.379057	-2.124640	0.898009
H	3.379057	-2.124640	-0.898009
H	4.820920	-1.568384	0.000000
S	-1.707252	2.683035	0.000000
S	-1.469951	-2.820041	0.000000
S	3.177203	0.137006	0.000000

15
SH

C	-1.404980	0.000654	0.000000
C	-0.697498	-1.209410	0.000000
C	0.701924	-1.217076	0.000000
C	1.396129	0.000654	0.000000
C	0.703056	1.216422	0.000000
C	-0.698630	1.208756	0.000000
H	-2.491009	0.000631	0.000000
H	1.246050	2.156961	0.000000
H	1.244958	-2.157593	0.000000
S	3.181272	-0.071291	0.000000
S	-1.652376	-2.719418	0.000000
S	-1.528896	2.790708	0.000000
H	3.387572	1.260618	0.000000
H	-2.785514	2.303415	0.000000
H	-0.602059	-3.564034	0.000000

21
SiF3

C	-1.396598	-0.000000	0.000005
C	-0.706345	-1.223426	-0.002641
C	0.698298	-1.209490	0.000005
C	1.412693	-0.000000	0.000005
C	0.698298	1.209487	0.002621
C	-0.706345	1.223429	0.000005
H	-2.484200	-0.000023	0.021496
H	1.242078	2.151342	0.026150

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H        1.242078     -2.151394      0.021496
Si       3.268333      0.000012     -0.010802
Si      -1.634155      2.830466     -0.010802
Si      -1.634155     -2.830436     -0.016924
F       -1.928659      3.343788     -1.500404
F       -0.785433      3.971904      0.726851
F       -3.048409      2.665378      0.724025
F       -3.048409     -2.666937      0.718258
F       -1.928659     -3.340535     -1.507632
F       -0.785433     -3.973467      0.718258
F        3.832488     -1.307313      0.724025
F        3.860134      0.001623     -1.500404
F        3.832488      1.305744      0.726850

21
SiH3
C       -1.392580     -0.000000      0.000006
C       -0.710002     -1.229759     -0.001788
C        0.696290     -1.206009      0.000006
C        1.420005     -0.000000      0.000006
C        0.696290      1.206008      0.001764
C       -0.710002      1.229760      0.000006
H       -2.482501     -0.000013      0.017522
H        1.241238      2.149888      0.020658
H        1.241238     -2.149915      0.017522
H       -2.968255      2.698040      0.659926
H       -1.912425      3.314499     -1.425884
H       -0.853277      3.919123      0.661707
H       -2.968255     -2.698999      0.655991
H       -1.912425     -3.312416     -1.430716
H       -0.853277     -3.920083      0.655991
H        3.820698     -1.221565      0.659925
H        3.826652      0.001040     -1.425884
H        3.820698      1.220602      0.661706
Si       3.309616      0.000019     -0.025465
Si      -1.654791      2.866221     -0.025465
Si      -1.654791     -2.866181     -0.029645
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Cartesian Coordinates for Substituted Coronenes

36
H
C -1.248060 -3.537925 0.000000
C -0.000000 -2.852249 0.000000
C -0.000000 -1.426623 0.000000
C -1.235479 -0.713347 0.000000
C -2.470027 -1.426165 0.000000
C -2.439770 -2.849909 0.000000
C 1.235479 -0.713347 0.000000
C -1.235479 0.713347 -0.000000
C 0.000000 1.426623 -0.000000
C 1.235479 0.713347 -0.000000
C 0.000000 2.852249 -0.000000
C -1.248060 3.537925 -0.000000
C -2.439770 2.849909 -0.000000
C -2.470027 1.426165 -0.000000
C -3.687856 0.688039 -0.000000
C -3.687856 -0.688039 0.000000
H -4.627481 -1.235884 0.000000
H -4.627481 1.235884 -0.000000
H -1.243203 -4.625586 0.000000
H -3.383982 -3.389834 0.000000
H -1.243203 4.625586 -0.000000
H -3.383982 3.389834 -0.000000
C 1.248060 -3.537925 0.000000
C 2.439770 -2.849909 0.000000
C 2.470027 -1.426165 0.000000
H 1.243203 -4.625586 0.000000
H 3.383982 -3.389834 0.000000
C 3.687856 -0.688039 0.000000
C 3.687856 0.688039 -0.000000
C 2.470027 1.426165 -0.000000
H 4.627481 -1.235884 0.000000
H 4.627481 1.235884 -0.000000
C 1.248060 3.537925 -0.000000
H 1.243203 4.625586 -0.000000
C 2.439770 2.849909 -0.000000
H 3.383982 3.389834 -0.000000

48
CHO_6
C 1.256652 -3.558987 0.000027
C -0.000000 -2.863863 0.000035
C 0.003441 -1.430365 0.000063
C 1.240315 -0.712162 0.000071
C 2.480003 -1.432134 0.000067
C 2.439593 -2.845639 0.000042
C -1.236908 -0.718050 0.000083
C 1.236908 0.718050 0.000083
C -0.003441 1.430365 0.000063
C -1.240315 0.712162 0.000071
C 0.000000 2.863863 0.000035
C 1.244330 3.535576 0.000034
C 2.453538 2.867717 0.000093
C 2.480110 1.431908 0.000104
C 3.683965 0.689982 0.000082
C 3.710153 -0.691128 0.000069
H 4.645506 1.189390 0.000048
H 3.353063 -3.428292 0.000036
H 1.292119 4.617932 0.000018
C -1.244330 -3.535576 0.000034
C -2.453538 -2.867717 0.000093
C -2.480110 -1.431908 0.000104
H -1.292119 -4.617932 0.000018
C -3.683965 -0.689982 0.000082
C -3.710153 0.691128 0.000069
C -2.480003 1.432134 0.000067
H -4.645506 -1.189390 0.000048
C -1.256652 3.558987 0.000027
C -2.439593 2.845639 0.000042
H -3.353063 3.428292 0.000036
C 5.056075 -1.346235 0.000058
O 6.104545 -0.727538 0.000081
H 5.073090 -2.453631 0.000138
C -3.693633 -3.705907 0.000238
O -3.681950 -4.923248 -0.000603
H -4.661532 -3.167456 0.001211
C -1.362605 5.052124 -0.000038
O -2.422870 5.650403 -0.000424
H -0.412456 5.621317 -0.000052
C 1.362605 -5.052124 -0.000038
O 2.422870 -5.650403 -0.000424
H 0.412456 -5.621317 -0.000052
C 3.693633 3.705907 0.000238
O 3.681950 4.923248 -0.000603
H 4.661532 3.167456 0.001211
C -5.056075 1.346235 0.000058
O -6.104545 0.727538 0.000081

```
H      -5.073090      2.453631      0.000138

60
OMe_6
C       1.257723      3.539091      0.000000
C       0.000000      2.849498      0.000000
C       0.010846      1.428767      0.000000
C       1.242771      0.704991      0.000000
C       2.467737      1.424749      0.000000
C       2.451523      2.845625      0.000000
C      -1.231925      0.723776      0.000000
C       1.231925     -0.723776      0.000000
C      -0.010846     -1.428767      0.000000
C      -1.242771     -0.704991      0.000000
C      -0.000000     -2.849498      0.000000
C       1.238621     -3.545894      0.000000
C       2.436081     -2.858765      0.000000
C       2.467738     -1.424749      0.000000
C       3.690145     -0.700270      0.000000
C       3.693805      0.680325      0.000000
H       4.617015     -1.257476      0.000000
H       3.397514      3.369714      0.000000
H       1.219502     -4.627190      0.000000
C      -1.238621      3.545894      0.000000
C      -2.436081      2.858765      0.000000
C      -2.467738      1.424749      0.000000
H      -1.219502      4.627190      0.000000
C      -3.690145      0.700270      0.000000
C      -3.693805     -0.680325      0.000000
C      -2.467737     -1.424749      0.000000
H      -4.617015      1.257476      0.000000
C      -1.257723     -3.539091      0.000000
C      -2.451523     -2.845625      0.000000
H      -3.397514     -3.369714      0.000000
C       6.086884      0.755532      0.000000
H       6.853494      1.534459      0.000000
H       6.191564      0.126114      0.895408
H       6.191564      0.126114     -0.895408
C       3.697752     -4.893630      0.000000
H       4.755628     -5.168071      0.000000
H       3.204999     -5.298994      0.895408
H       3.204999     -5.298994     -0.895408
C      -2.389132     -5.649162      0.000000
H      -2.097867     -6.702530      0.000000
H      -2.986564     -5.425109      0.895408
H      -2.986564     -5.425109     -0.895408
C      -6.086884     -0.755532      0.000000
H      -6.853494     -1.534459      0.000000
H      -6.191564     -0.126114      0.895408
H      -6.191564     -0.126114     -0.895408
C      -3.697752      4.893630      0.000000
H      -4.755628      5.168071      0.000000
H      -3.204999      5.298994      0.895408
H      -3.204999      5.298994     -0.895408
C       2.389132      5.649162      0.000000
H       2.097867      6.702530      0.000000
H       2.986564      5.425109      0.895408
H       2.986564      5.425109     -0.895408
O       1.168659      4.907259      0.000000
O       4.834141      1.441541      0.000000
O       3.665482     -3.465718      0.000000
O      -1.168659     -4.907259      0.000000
O      -4.834141     -1.441541      0.000000
O      -3.665482      3.465718      0.000000

54
CHO_3_OMe_3
C      -1.257390      3.550003     -0.000077
C      -0.000000      2.852722     -0.000040
C      -0.006714      1.426192     -0.000012
C      -1.243653      0.709183     -0.000004
C      -2.480983      1.432160     -0.000005
C      -2.448389      2.855685     -0.000063
C       1.235969      0.722555     -0.000003
C      -1.231767     -0.718910     -0.000008
C       0.007752     -1.431535     -0.000002
C       1.238486     -0.707279     -0.000005
C       0.000156     -2.864629     -0.000007
C      -1.248931     -3.548166     -0.000059
C      -2.445781     -2.863941     -0.000068
C      -2.470437     -1.426305     -0.000030
C      -3.675714     -0.705054     -0.000010
C      -3.708800      0.683115      0.000024
H      -4.621281     -1.235698     -0.000003
H      -3.375847      3.408520     -0.000119
H      -1.263711     -4.627783     -0.000111
C       1.227251      3.535852     -0.000024
C       2.445981      2.870427      0.000012
C       2.480753      1.432476     -0.000004
H       1.240552      4.620084     -0.000024
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C	3.697322	0.692570	-0.000044
C	3.703183	-0.686053	-0.000047
C	2.470565	-1.426209	-0.000019
H	4.639707	1.219603	-0.000091
C	1.262888	-3.553355	0.000019
C	2.448521	-2.830663	-0.000002
H	3.380770	-3.384416	0.000007
C	-3.719232	-4.893419	0.000212
H	-4.781058	-5.147471	-0.000012
H	-3.233794	-5.301480	-0.896863
H	-3.234278	-5.301057	0.897741
C	6.097495	-0.774183	0.000109
H	6.848472	-1.566679	0.000013
H	6.208043	-0.149954	-0.897100
H	6.207942	-0.150268	0.897549
C	-2.378600	5.667379	0.000173
H	-2.067977	6.714048	-0.000015
H	-2.974572	5.450708	-0.896911
H	-2.974025	5.450871	0.897660
O	-1.164755	4.905557	-0.000131
O	-3.666054	-3.461310	-0.000118
O	4.830700	-1.444175	-0.000083
C	3.672335	3.709050	0.000107
O	3.676714	4.929555	0.000052
H	4.642266	3.168372	0.000476
C	1.376125	-5.034736	0.000103
O	2.431006	-5.648648	-0.000104
H	0.423006	-5.604572	0.000255
C	-5.048433	1.325600	0.000136
O	-6.107404	0.718772	-0.000229
H	-5.065638	2.435992	0.000274

42
CN_6

C	-1.249237	3.546479	0.000000
C	0.009203	2.852596	0.000000
C	-0.000000	1.427788	0.000000
C	-1.236501	0.713894	0.000000
C	-2.465819	1.434268	0.000000
C	-2.444978	2.850188	0.000000
C	1.236501	0.713894	0.000000
C	-1.236501	-0.713894	0.000000
C	-0.000000	-1.427788	0.000000
C	1.236501	-0.713894	0.000000
C	-0.009203	-2.852596	0.000000
C	-1.245846	-3.542507	0.000000
C	-2.446722	-2.855110	0.000000
C	-2.475022	-1.418328	0.000000
C	-3.690824	-0.692319	0.000000
C	-3.695959	0.691369	0.000000
H	-4.633252	-1.230952	0.000000
H	-3.382662	3.397038	0.000000
H	-1.250590	-4.627990	0.000000
C	1.245846	3.542507	0.000000
C	2.446722	2.855110	0.000000
C	2.475022	1.418328	0.000000
H	1.250590	4.627990	0.000000
C	3.690824	0.692319	0.000000
C	3.695959	-0.691369	0.000000
C	2.465819	-1.434268	0.000000
H	4.633252	1.230952	0.000000
C	1.249237	-3.546479	0.000000
C	2.444978	-2.850188	0.000000
H	3.382662	-3.397038	0.000000
C	3.674385	3.590131	0.000000
N	4.685144	4.164445	0.000000
C	1.271952	-4.977176	0.000000
N	1.263943	-6.139676	0.000000
C	-4.946337	1.387046	0.000000
N	-5.949087	1.975231	0.000000
C	-1.271952	4.977176	0.000000
N	-1.263943	6.139676	0.000000
C	4.946337	-1.387046	0.000000
N	5.949087	-1.975231	0.000000
C	-3.674385	-3.590131	0.000000
N	-4.685144	-4.164445	0.000000

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CN_3_NH2_3

C	2.443479	2.887578	0.041599
C	2.466942	1.446616	0.012664
C	1.231013	0.725788	0.015119
C	-0.014118	1.425085	0.011330
C	-0.000000	2.852882	-0.002073
C	1.225841	3.549897	0.021514
C	1.241219	-0.700315	0.011330
C	-1.244057	0.703194	0.015119
C	-1.227100	-0.724769	0.011330
C	0.013045	-1.428982	0.015119
C	-2.470668	-1.426441	-0.002073

C	-3.687221	-0.713339	0.021514
C	-3.722456	0.672325	0.041599
C	-2.486278	1.413126	0.012664
C	-2.457705	2.823811	-0.029560
C	-1.265206	3.532492	-0.032289
H	-3.380786	3.390618	-0.087817
H	1.213491	4.636812	0.033812
H	-4.622342	-1.267492	0.033812
C	3.674345	0.716529	-0.029560
C	3.691831	-0.670545	-0.032289
C	2.470668	-1.426441	-0.002073
H	4.626755	1.232537	-0.087817
C	2.461380	-2.836558	0.021514
C	1.278977	-3.559904	0.041599
C	0.019335	-2.859743	0.012664
H	3.408851	-3.369320	0.033812
C	-2.426624	-2.861947	-0.032289
C	-1.216640	-3.540341	-0.029560
H	-1.245969	-4.623156	-0.087817
C	4.949398	-1.348250	-0.070718
N	5.964267	-1.917491	-0.094866
C	-3.642318	-3.612180	-0.070718
N	-4.642729	-4.206461	-0.094866
C	-1.307081	4.960430	-0.070718
N	-1.321537	6.123952	-0.094866
N	3.626624	3.610429	0.025924
H	4.419738	3.196673	0.492692
H	3.526266	4.592886	0.238391
N	-4.940036	1.335534	0.025924
H	-4.978269	2.229269	0.492692
H	-5.740689	0.757393	0.238391
N	1.313412	-4.945963	0.025924
H	0.558531	-5.425942	0.492692
H	2.214423	-5.350279	0.238391

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NH2_6

C	-1.253024	3.556330	-0.004757
C	-0.000000	2.856175	-0.004112
C	-0.011794	1.429590	0.012308
C	-1.243959	0.704581	0.012308
C	-2.473520	1.428087	-0.004112
C	-2.439612	2.844740	-0.015890
C	1.232165	0.725009	0.012308
C	-1.232165	-0.725009	0.012308
C	0.011794	-1.429590	0.012308
C	1.243959	-0.704581	0.012308
C	-0.000000	-2.856175	-0.004112
C	-1.243811	-3.535136	-0.015890
C	-2.453360	-2.863316	-0.004757
C	-2.473520	-1.428087	-0.004112
C	-3.683423	-0.690396	-0.015890
C	-3.706384	0.693014	-0.004757
H	-4.637482	-1.209605	-0.065080
H	-3.366290	3.411375	-0.065080
H	-1.271192	-4.620980	-0.065080
C	1.243811	3.535136	-0.015890
C	2.453360	2.863316	-0.004757
C	2.473520	1.428087	-0.004112
H	1.271192	4.620980	-0.065080
C	3.683423	0.690396	-0.015890
C	3.706384	-0.693014	-0.004757
C	2.473520	-1.428087	-0.004112
H	4.637482	1.209605	-0.065080
C	1.253024	-3.556330	-0.004757
C	2.439612	-2.844740	-0.015890
H	3.366290	-3.411375	-0.065080
N	-4.931274	1.378387	-0.070794
H	-4.956781	2.230724	0.473510
H	-5.722413	0.792014	0.161836
N	-1.271918	4.959802	-0.070794
H	-0.546527	5.408060	0.473510
H	-2.175302	5.351762	0.161836
N	3.659355	3.581415	-0.070794
H	4.410254	3.177336	0.473510
H	3.547111	4.559748	0.161836
N	4.931274	-1.378387	-0.070794
H	4.956781	-2.230724	0.473510
H	5.722413	-0.792014	0.161836
N	1.271918	-4.959802	-0.070794
H	0.546527	-5.408060	0.473510
H	2.175302	-5.351762	0.161836
N	-3.659355	-3.581415	-0.070794
H	-4.410254	-3.177336	0.473510
H	-3.547111	-4.559748	0.161836

Cartesian Coordinates for Substituted HBCs

60
H
C -1.2332000 3.5955960 0.0000000
C -2.4969860 2.8657520 0.0000000
C -2.4882460 1.4366370 0.0000000
C -3.7302250 0.7297020 0.0000000
C -3.7302250 -0.7297030 0.0000000
C -2.4882460 -1.4366380 0.0000000
C -2.4969860 -2.8657520 0.0000000
C -1.2332000 -3.5955960 0.0000000
C 0.0000000 -2.8734500 0.0000000
C 1.2332000 -3.5955960 0.0000000
C 2.4969860 -2.8657520 0.0000000
C 2.4882460 -1.4366370 0.0000000
C 3.7302250 -0.7297020 0.0000000
C 3.7302250 0.7297030 0.0000000
C 2.4882460 1.4366380 0.0000000
C 2.4969860 2.8657520 0.0000000
C 1.2332000 3.5955960 0.0000000
C 0.0000000 2.8734500 0.0000000
C 0.0000000 1.4271440 0.0000000
C -1.2358170 0.7135590 0.0000000
C -1.2358170 -0.7135590 0.0000000
C 0.0000000 -1.4271440 0.0000000
C 1.2358170 -0.7135590 0.0000000
C 1.2358170 0.7135590 0.0000000
C -1.2019140 5.0004800 0.0000000
C 0.0000000 5.6938820 0.0000000
C 1.2019130 5.0004800 0.0000000
C -4.9311880 1.4592620 0.0000000
C -4.9307300 2.8468890 0.0000000
C -3.7292560 3.5410330 0.0000000
C -3.7292560 -3.5410330 0.0000000
C -4.9307300 -2.8468890 0.0000000
C -4.9311880 -1.4592630 0.0000000
C 1.2019140 -5.0004800 0.0000000
C 0.0000000 -5.6938820 0.0000000
C -1.2019130 -5.0004800 0.0000000
C 4.9311880 -1.4592620 0.0000000
C 4.9307300 -2.8468890 0.0000000
C 3.7292560 -3.5410330 0.0000000
C 3.7292560 3.5410330 0.0000000
C 4.9307300 2.8468890 0.0000000
C 4.9311880 1.4592630 0.0000000
H -2.1196960 5.5745040 0.0000000
H 0.0000000 6.7806640 0.0000000
H 2.1196950 5.5745050 0.0000000
H -5.8872220 0.9515610 0.0000000
H -5.8719350 3.3902310 0.0000000
H -3.7671880 4.6228190 0.0000000
H -3.7671880 -4.6228200 0.0000000
H -5.8719350 -3.3902320 0.0000000
H -5.8872220 -0.9515620 0.0000000
H 2.1196960 -5.5745040 0.0000000
H 0.0000000 -6.7806640 0.0000000
H -2.1196950 -5.5745050 0.0000000
H 5.8872220 -0.9515610 0.0000000
H 5.8719350 -3.3902310 0.0000000
H 3.7671880 -4.6228190 0.0000000
H 3.7671880 4.6228200 0.0000000
H 5.8719350 3.3902320 0.0000000
H 5.8872220 0.9515620 0.0000000

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CHO_6
C 1.235459 3.594748 0.000000
C 2.499892 2.866642 0.000000
C 2.490430 1.434823 0.000000
C 3.731170 0.727796 0.000000
C 3.732454 -0.731331 0.000000
C 2.487674 -1.439111 0.000000
C 2.495492 -2.867112 0.000000
C 1.232577 -3.597909 0.000000
C -0.002712 -2.873859 0.000000
C -1.235459 -3.594748 0.000000
C -2.499892 -2.866642 0.000000
C -2.490430 -1.434823 0.000000
C -3.731170 -0.727796 0.000000
C -3.732454 0.731331 0.000000
C -2.487674 1.439111 0.000000
C -2.495492 2.867112 0.000000
C -1.232577 3.597909 0.000000
C 0.002712 2.873859 0.000000
C 0.001504 1.428711 0.000000
C 1.238216 0.713184 0.000000
C 1.236647 -0.715569 0.000000
C -0.001504 -1.428711 0.000000
C -1.238216 -0.713184 0.000000
C -1.236647 0.715569 0.000000

C	1.204096	4.995974	0.000000
C	0.000000	5.693962	0.000000
C	-1.206036	4.995277	0.000000
C	4.929029	1.455734	0.000000
C	4.931340	2.847524	0.000000
C	3.723231	3.542584	0.000000
C	3.724665	-3.540617	0.000000
C	4.931250	-2.846846	0.000000
C	4.929307	-1.453058	0.000000
C	-1.204096	-4.995974	0.000000
C	-0.000000	-5.693962	0.000000
C	1.206036	-4.995277	0.000000
C	-4.929029	-1.455734	0.000000
C	-4.931340	-2.847524	0.000000
C	-3.723231	-3.542584	0.000000
C	-3.724665	3.540617	0.000000
C	-4.931250	2.846846	0.000000
C	-4.929307	1.453058	0.000000
H	2.119280	5.577382	0.000000
H	-2.110077	5.590988	0.000000
H	5.890423	0.954226	0.000000
H	3.786914	4.623430	0.000000
H	3.770677	-4.623951	0.000000
H	5.897208	-0.967982	0.000000
H	-2.119280	-5.577382	0.000000
H	2.110077	-5.590988	0.000000
H	-5.890423	-0.954226	0.000000
H	-3.786914	-4.623430	0.000000
H	-3.770677	4.623951	0.000000
H	-5.897208	0.967982	0.000000
C	6.209149	-3.604973	0.000000
O	7.315157	-3.099899	0.000000
H	6.082120	-4.714034	0.000000
C	6.226744	3.575163	0.000000
O	6.342348	4.785543	0.000000
H	7.123606	2.910530	0.000000
C	0.017590	7.179688	0.000000
O	-0.972802	7.885010	0.000000
H	1.041608	7.624203	0.000000
C	-6.209149	3.604973	0.000000
O	-7.315157	3.099899	0.000000
H	-6.082120	4.714034	0.000000
C	-6.226744	-3.575163	0.000000
O	-6.342348	-4.785543	0.000000
H	-7.123606	-2.910530	0.000000
C	-0.017590	-7.179688	0.000000
O	0.972802	-7.885010	0.000000
H	-1.041608	-7.624203	0.000000

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OMe_6

C	1.231942	3.592882	-0.000000
C	2.497414	2.860113	-0.000000
C	2.482325	1.434859	-0.000000
C	3.727497	0.729547	-0.000000
C	3.725637	-0.732768	-0.000000
C	2.483787	-1.432327	-0.000000
C	2.495556	-2.863333	-0.000000
C	1.228223	-3.592881	-0.000000
C	0.001462	-2.867186	-0.000000
C	-1.231942	-3.592882	0.000000
C	-2.497414	-2.860113	0.000000
C	-2.482325	-1.434859	0.000000
C	-3.727497	-0.729547	0.000000
C	-3.725637	0.732768	0.000000
C	-2.483787	1.432327	0.000000
C	-2.495556	2.863333	0.000000
C	-1.228223	3.592881	0.000000
C	-0.001462	2.867186	0.000000
C	-0.001311	1.424766	0.000000
C	1.233229	0.713519	-0.000000
C	1.234540	-0.711249	-0.000000
C	0.001311	-1.424766	-0.000000
C	-1.233229	-0.713519	0.000000
C	-1.234540	0.711249	0.000000
C	1.204641	4.991632	-0.000000
C	0.000000	5.693055	0.000000
C	-1.206349	4.999021	0.000000
C	4.925202	1.452566	-0.000000
C	4.930330	2.846528	-0.000000
C	3.726105	3.544239	-0.000000
C	3.720559	-3.539067	-0.000000
C	4.930331	-2.846527	-0.000000
C	4.932454	-1.454781	-0.000000
C	-1.204641	-4.991632	0.000000
C	0.000000	-5.693055	0.000000
C	1.206349	-4.999021	-0.000000
C	-4.925202	-1.452566	0.000000
C	-4.930330	-2.846528	0.000000
C	-3.726105	-3.544239	0.000000

C	-3.720559	3.539067	0.000000
C	-4.930331	2.846527	0.000000
C	-4.932454	1.454781	0.000000
H	2.110742	5.583811	-0.000000
H	-2.130849	5.556601	0.000000
H	5.891093	0.963950	-0.000000
H	3.746733	4.623670	-0.000000
H	3.780352	-4.619861	-0.000000
H	5.877582	-0.932931	-0.000000
H	-2.110742	-5.583811	0.000000
H	2.130849	-5.556601	-0.000000
H	-5.891093	-0.963950	0.000000
H	-3.746733	-4.623670	0.000000
H	-3.780352	4.619861	0.000000
H	-5.877582	0.932931	0.000000
C	7.322061	-2.958711	-0.000000
H	8.076038	-3.749580	-0.000000
H	7.438867	-2.332560	-0.896466
H	7.438867	-2.332560	0.896466
C	-1.098712	7.820447	0.000000
H	-0.790787	8.868844	0.000000
H	-1.699377	7.608528	-0.896466
H	-1.699377	7.608528	0.896466
C	-6.223349	-4.861736	0.000000
H	-7.285251	-5.119264	0.000000
H	-5.739490	-5.275968	-0.896466
H	-5.739490	-5.275968	0.896466
O	0.111249	7.059428	-0.000000
O	6.058019	-3.626058	-0.000000
O	-6.169268	-3.433370	0.000000
C	6.223349	4.861736	-0.000000
H	7.285251	5.119264	-0.000000
H	5.739490	5.275968	-0.896466
H	5.739490	5.275968	0.896466
C	-7.322061	2.958711	0.000000
H	-8.076038	3.749580	0.000000
H	-7.438867	2.332560	-0.896466
H	-7.438867	2.332560	0.896466
C	1.098712	-7.820447	-0.000000
H	0.790787	-8.868844	-0.000000
H	1.699377	-7.608528	-0.896466
H	1.699377	-7.608528	0.896466
O	6.169268	3.433370	-0.000000
O	-0.111249	-7.059428	0.000000
O	-6.058019	3.626058	0.000000

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CHO_3_OMe_3

C	-3.728621	-0.723041	0.000000
C	-3.728201	0.736168	0.000000
C	-2.486341	1.434473	0.000000
C	-2.500762	2.864474	0.000000
C	-1.234031	3.596410	0.000000
C	0.002026	2.870255	-0.000000
C	1.238140	3.590601	-0.000000
C	2.501642	2.860633	-0.000000
C	2.485460	1.435997	-0.000000
C	3.731087	0.733485	-0.000000
C	3.731599	-0.729502	-0.000000
C	2.484701	-1.436882	-0.000000
C	2.490482	-2.867560	-0.000000
C	1.226560	-3.596801	-0.000000
C	0.000881	-2.870470	-0.000000
C	-1.230327	-3.597960	0.000000
C	-2.497567	-2.866907	0.000000
C	-2.486727	-1.433373	0.000000
C	-1.236626	-0.713126	0.000000
C	-1.237306	0.713182	0.000000
C	0.000727	1.427512	-0.000000
C	1.236286	0.714947	-0.000000
C	1.235898	-0.714387	-0.000000
C	0.001019	-1.428129	-0.000000
C	-4.924698	-1.454145	0.000000
C	-4.929640	-2.846129	0.000000
C	-3.719962	-3.541931	0.000000
C	-3.721025	3.542228	0.000000
C	-4.933169	2.849753	0.000000
C	-4.934853	1.457637	0.000000
C	1.203022	4.991985	-0.000000
C	0.000001	5.692257	-0.000000
C	-1.207421	4.992546	0.000000
C	4.928172	1.451388	-0.000000
C	4.934542	2.847373	-0.000000
C	3.729777	3.544891	-0.000000
C	3.721676	-3.537841	-0.000000
C	4.929639	-2.846129	-0.000000
C	4.927384	-1.450617	-0.000000
C	-1.207148	-4.993617	0.000000
C	-0.001374	-5.697125	0.000000
C	1.205077	-5.002526	-0.000000

H	-5.888259	-0.955988	0.000000
H	-3.782402	-4.622808	0.000000
H	-3.776915	4.622942	0.000000
H	-5.881218	0.938182	0.000000
H	2.116221	5.577376	-0.000000
H	-2.112267	5.587060	0.000000
H	5.892042	0.959434	-0.000000
H	3.753098	4.624192	-0.000000
H	3.772040	-4.621389	-0.000000
H	5.894670	-0.964252	-0.000000
H	-2.115127	-5.582374	0.000000
H	2.128120	-5.562375	-0.000000
C	-7.324937	2.967574	0.000000
H	-8.072206	3.763965	0.000000
H	-7.443871	2.343811	-0.897277
H	-7.443871	2.343811	0.897277
C	1.092476	-7.827368	-0.000000
H	0.776415	-8.872717	-0.000000
H	1.692136	-7.618487	-0.897277
H	1.692136	-7.618487	0.897277
C	6.232463	4.859796	-0.000000
H	7.295791	5.108753	-0.000000
H	5.751735	5.274676	-0.897277
H	5.751735	5.274676	0.897277
O	-6.054352	3.627756	0.000000
O	6.168906	3.429344	-0.000000
O	-0.114553	-7.057100	0.000000
C	-6.224119	-3.565111	0.000000
O	-6.357536	-4.775091	0.000000
H	-7.116342	-2.891138	0.000000
C	0.024582	7.172801	-0.000000
O	-0.956582	7.893333	0.000000
H	1.054372	7.608502	-0.000000
C	6.199536	-3.607690	-0.000000
O	7.314118	-3.118241	-0.000000
H	6.061971	-4.717363	-0.000000

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CN_6

C	-1.2325620	3.5948690	0.0000000
C	-2.4966500	2.8648610	0.0000000
C	-2.4871910	1.4360590	0.0000000
C	-3.7292260	0.7298830	0.0000000
C	-3.7292260	-0.7298830	0.0000000
C	-2.4871910	-1.4360590	0.0000000
C	-2.4966500	-2.8648610	0.0000000
C	-1.2325620	-3.5948690	0.0000000
C	0.0000000	-2.8722640	0.0000000
C	1.2325620	-3.5948690	0.0000000
C	2.4966500	-2.8648610	0.0000000
C	2.4871910	-1.4360590	0.0000000
C	3.7292260	-0.7298830	0.0000000
C	3.7292260	0.7298830	0.0000000
C	2.4871910	1.4360590	0.0000000
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C	1.2325620	3.5948690	0.0000000
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C	-1.2089000	4.9949490	0.0000000
C	0.0000000	5.6931800	0.0000000
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C	-4.9298220	1.4504270	0.0000000
C	-4.9300800	2.8465140	0.0000000
C	-3.7209520	3.5443270	0.0000000
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C	-4.9300800	-2.8465150	0.0000000
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H	2.1204090	5.5764160	0.0000000
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H	-3.7685820	-4.6244030	0.0000000
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CN_3_NH2_3
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C       -1.235262     -0.713185     -0.005696
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H       -3.765757      4.622296     -0.047976
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NH2_6
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C	3.7277790	-0.7317930	-0.0053180
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C	-3.7277790	0.7317930	-0.0053180
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C	3.7252350	-3.5381370	-0.0035720
C	4.9411500	-2.8530630	-0.0031000
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C	-3.7252350	3.5381370	-0.0035720
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H	0.8334750	7.5364680	0.3180280
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H	-6.1102490	-4.4902550	0.3093960
H	-6.9439090	-3.0467510	0.3071850
N	6.1546650	-3.5539920	-0.0705180
H	6.9439090	-3.0467510	0.3071850
H	6.1102490	-4.4902550	0.3093960