Quantum Chemical Study of the Reactivity of C₆₀HR and C₆₀(CHR) Derivatives

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Optimized geometries in Cartesian coordinates of the AM1 optimizations are provided for all structures under consideration:

1. C₆₀HR----- S10

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with R = -H, -OH, -OCH₃, -NH₂, -NHCH₃, -N(CH₃)₂, -CH₃, -CH=CH₂, -Ph, -CCH

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Table S1. Significant distances (Å) and angles (°) in a.u. for the acidic and basic forms of the series considered, fully optimized at the AM1 level, and $\Delta EC_{60\text{def}}$ in kcal/mol (see Figure 1 for atom numbering). *The experimental value for C_{60} is 1.401 Å (Ref: K. Hedberg, L. Hedberg, D. S. Bethune, C. A. Brown, H. C. Dorn, R. D. Johnson, M. De Vries Nature 1991, 254, 410).

	d(C ₁ -C ₂)*	d(C ₁ -H)	d(C ₂ -R)	d(C ₁ -C ₃)	d(C ₂ -C ₃)	d(C ₃ -H)	d(C ₃ -R)	$\alpha(C_1C_3C_2)$	$\Delta EC_{60\text{def}}$
C₆₀HR									
H	1.552	1.126	1.126						40.8
OH	1.565	1.131	1.414						45.6
OCH ₃	1.568	1.131	1.421						46.0
NH ₂	1.582	1.130	1.454						53.0
NHCH ₃	1.585	1.130	1.461						53.5
N(CH ₃) ₂	1.586	1.130	1.470						54.2
CH ₃	1.562	1.128	1.521						45.2
CH=CH ₂	1.568	1.128	1.498						46.5
Ph	1.569	1.128	1.504						47.3
C≡CH	1.571	1.128	1.442						47.7
C₆₀R⁻									
H	1.491		1.120						24.7
OH	1.493		1.411						27.3
OCH ₃	1.493		1.420						27.2
NH ₂	1.505		1.449						32.9
NHCH ₃	1.506		1.454						33.1
N(CH ₃) ₂	1.505		1.463						33.9
CH ₃	1.496		1.512						27.7
CH=CH ₂	1.498		1.490						28.4
Ph	1.498		1.498						28.7
C≡CH	1.498		1.440						28.6
C₆₀(CHR)									
H	1.580			1.494	1.494	1.108	1.108	63.59	29.2
OH	1.574			1.508	1.508	1.114	1.382	62.93	28.4
OCH ₃	1.575			1.507	1.507	1.111	1.397	62.91	28.5
NH ₂	1.568			1.525	1.509	1.119	1.412	62.29	27.2
NHCH ₃	1.569			1.524	1.510	1.119	1.417	62.27	27.3
N(CH ₃) ₂	1.569			1.525	1.508	1.124	1.421	62.24	27.9
CH ₃	1.574			1.502	1.502	1.114	1.490	63.06	28.5
CH=CH ₂	1.571			1.505	1.505	1.115	1.467	62.75	27.9
Ph	1.572			1.503	1.502	1.118	1.472	62.95	28.4
C≡CH	1.570			1.506	1.506	1.119	1.415	62.62	27.6
C₆₀(CR⁻)closed									
H	1.627			1.416	1.416		1.057	70.10	43.1
OH	1.577			1.524	1.524		1.380	62.34	30.4
OCH ₃	1.578			1.522	1.522		1.392	62.46	30.6

NH ₂	1.581	1.486	1.525	1.380	63.34	31.4
NHCH ₃	1.581	1.490	1.524	1.388	63.29	31.3
N(CH ₃) ₂	1.589	1.495	1.475	1.384	64.70	33.9
CH ₃	1.620	1.420	1.420	1.424	69.57	41.5
CH=CH ₂	1.617	1.430	1.430	1.380	68.84	39.6
Ph	1.616	1.433	1.433	1.378	68.66	38.9
C≡CH	1.615	1.429	1.429	1.342	68.84	39.2
C₆₀(CR⁻) open						
H	2.299	1.363	1.443	1.100	109.97	152.9
OH	2.362	1.388	1.435	1.343	113.61	158.0
OCH ₃	2.368	1.396	1.432	1.339	113.73	159.5
NH ₂	2.377	1.433	1.433	1.326	112.11	159.0
NHCH ₃	2.375	1.436	1.434	1.328	111.69	158.5
N(CH ₃) ₂	2.370	1.439	1.439	1.330	110.95	157.9
CH ₃	2.282	1.376	1.447	1.464	107.89	150.6
CH=CH ₂	2.236	1.398	1.441	1.418	103.93	142.7
Ph	2.212	1.421	1.421	1.416	102.24	138.6
C≡CH	2.210	1.420	1.420	1.375	102.28	138.6

Table S2. Electronic delocalization calculated from the Mulliken populations ($N_{C\text{ acid}}$, $N_{H\text{ acid}}$ and $N_{C\text{ base}}$)

for all the structures studied at B3LYP/6-31G*//AM1 level.

	$N_{C\text{ acid}}$	$N_{H\text{ acid}}$	$N_{C\text{ base}}$	Δ	$N_{C\text{ base}}$	Δ
$C_{60}HR/C_{60}R^{\cdot}$						
H	-0.239	0.178	0.013	-0.431		
OH	-0.289	0.210	-0.004	-0.495		
OCH ₃	-0.299	0.209	-0.020	-0.488		
NH ₂	-0.266	0.192	-0.034	-0.423		
NHCH ₃	-0.271	0.191	-0.052	-0.410		
N(CH ₃) ₂	-0.269	0.195	-0.054	-0.409		
CH ₃	-0.277	0.178	-0.013	-0.442		
CH=CH ₂	-0.281	0.186	-0.023	-0.444		
Ph	-0.270	0.193	0.010	-0.473		
C≡CH	-0.286	0.199	-0.024	-0.461		
$C_{60}(CHR)/C_{60}(CR^{\cdot})$			closed	closed	open	Open
H	-0.310	0.181	-0.654	0.163	-0.183	-0.308
OH	0.149	0.181	0.052	-0.084	0.244	-0.276
OCH ₃	0.169	0.155	0.099	-0.085	0.264	-0.250
NH ₂	0.028	0.171	0.030	-0.173	0.264	-0.407
NHCH ₃	0.052	0.168	0.046	-0.162	0.284	-0.400
N(CH ₃) ₂	0.029	0.164	0.033	-0.168	0.292	-0.427
CH ₃	-0.090	0.167	-0.212	-0.045	0.006	-0.263
CH=CH ₂	-0.144	0.166	0.033	-0.343	-0.032	-0.278
Ph	-0.210	0.184	-0.062	-0.332	-0.143	-0.251
C≡CH	-0.302	0.198	-0.238	-0.262	-0.277	-0.223

Table S3. Charges for the functional group R, the C₁, C₂ and C₃ carbon atoms, and the sum of the charges for the 58 non-functionalized carbon atoms of the cage for all systems (HF/3-21G//AM1).

	qR	qC ₁	qC ₂	qC ₃	q(58C)
C₆₀HR					
H	0.289	-0.311	-0.311		0.044
OH	-0.265	-0.303	0.180		0.056
OCH ₃	-0.281	-0.302	0.213		0.039
NH ₂	-0.104	-0.280	-0.008		0.083
NHCH ₃	-0.129	-0.276	0.037		0.057
N(CH ₃) ₂	-0.155	-0.274	0.083		0.033
CH ₃	0.170	-0.279	-0.317		0.135
CH=CH ₂	0.177	-0.270	-0.366		0.158
Ph	0.161	-0.267	-0.361		0.156
C≡CH	0.170	-0.274	-0.456		0.247
C₆₀R[•]					
H	0.201	-0.031	-0.316		-0.854
OH	-0.305	0.010	0.120		-0.825
OCH ₃	-0.337	-0.010	0.150		-0.824
NH ₂	-0.171	-0.008	-0.043		-0.778
NHCH ₃	-0.202	-0.011	-0.090		-0.778
N(CH ₃) ₂	-0.235	-0.023	0.028		-0.770
CH ₃	0.104	0.026	-0.365		-0.765
CH=CH ₂	0.116	0.035	-0.442		-0.709
Ph	0.093	0.051	-0.447		-0.697
C≡CH	0.131	0.032	-0.543		-0.618
C₆₀(CHR)					
H	0.263	-0.178	-0.177	-0.218	0.046
OH	-0.261	-0.215	-0.215	0.346	0.062
OCH ₃	-0.290	-0.200	-0.200	0.357	0.081
NH ₂	-0.149	-0.189	-0.174	0.216	0.025
NHCH ₃	-0.172	-0.186	-0.179	0.248	0.020
N(CH ₃) ₂	-0.200	-0.173	-0.189	0.273	0.024
CH ₃	0.101	-0.145	-0.145	-0.100	0.024
CH=CH ₂	0.122	-0.121	-0.121	-0.187	0.039
Ph	0.046	-0.148	-0.153	-0.083	0.054
C≡CH	0.044	-0.122	-0.122	-0.188	0.090
C₆₀(CR[•]) closed					
H	0.134	-0.129	-0.129	-0.290	-0.586
OH	-0.358	-0.240	-0.240	0.336	-0.498
OCH ₃	-0.417	-0.239	-0.239	0.378	-0.483
NH ₂	-0.307	-0.223	-0.230	0.310	-0.550
NHCH ₃	-0.352	-0.231	-0.227	0.347	-0.537
N(CH ₃) ₂	-0.397	-0.217	-0.213	0.360	-0.533
CH ₃	-0.198	-0.110	-0.110	-0.021	-0.561
CH=CH ₂	-0.340	-0.124	-0.098	0.020	-0.418
Ph	-0.517	-0.102	-0.102	0.093	-0.372

C≡CH	-0.665	0.018	0.019	-0.007	-0.365
C₆₀(CR⁺) open					
H	0.227	0.010	-0.112	-0.244	-0.881
OH	-0.250	-0.132	-0.244	0.512	-0.886
OCH ₃	-0.251	-0.166	-0.203	0.553	-0.933
NH ₂	-0.099	-0.192	-0.192	0.529	-1.046
NHCH ₃	-0.099	-0.203	-0.202	0.568	-1.064
N(CH ₃) ₂	-0.100	-0.211	-0.211	0.604	-1.082
CH ₃	0.028	0.003	-0.089	-0.050	-0.892
CH=CH ₂	-0.119	0.013	-0.056	-0.110	-0.728
Ph	-0.259	-0.020	-0.020	-0.064	-0.637
C≡CH	-0.270	0.048	0.045	-0.182	-0.641

Table S4. NICS (ppm-egs) for the rings labeled M to F' (**bold** = pentagonal rings) calculated at HF/3-21G//AMI using the GIAO method.

	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	A'	B'	C'	D'	E'	F'
C₆₀HR																				
H	4.1	-7.8	-7.8	4.1	-6.9	4.1	-7.7	-9.0	4.1	-6.9	-7.7	3.4	-7.7	5.1	-7.7	3.4	-7.7	5.1	-7.2	-7.2
OH	4.2	-7.7	-7.7	4.0	-6.9	4.0	-7.7	-7.8	4.2	-6.8	-7.7	3.5	-7.7	5.1	-7.7	3.5	-7.6	5.1	-7.2	-7.2
OCH ₃	4.2	-7.8	-7.8	3.9	-7.0	3.9	-7.8	-7.8	4.2	-6.9	-7.7	3.5	-7.7	5.1	-7.7	3.5	-7.7	5.1	-7.2	-7.2
NH ₂	4.2	-7.8	-7.8	4.0	-6.9	4.0	-7.7	-7.8	4.2	-6.9	-7.7	3.5	-7.7	5.1	-7.7	3.5	-7.7	5.1	-7.2	-7.2
NHCH ₃	4.2	-7.8	-7.8	4.0	-7.0	3.9	-7.8	-7.8	4.2	-6.9	-7.7	3.5	-7.7	5.1	-7.7	3.5	-7.7	5.1	-7.2	-7.2
N(CH ₃) ₂	4.2	-7.8	-7.8	3.9	-7.0	4.0	-7.8	-7.8	4.2	-6.9	-7.7	3.5	-7.8	5.1	-7.7	3.5	-7.7	5.1	-7.2	-7.2
CH ₃	4.1	-7.8	-7.8	4.1	-6.9	4.1	-7.8	-7.8	4.1	-6.9	-7.7	3.4	-7.7	5.1	-7.7	3.4	-7.7	5.1	-7.2	-7.2
CH=CH ₂	4.1	-7.8	-7.8	4.0	-7.0	4.1	-7.8	-9.1	4.1	-6.9	-7.7	3.4	-7.7	5.0	-7.7	3.4	-7.7	5.1	-7.2	-7.2
Ph	4.1	-7.7	-7.7	4.1	-6.9	4.1	-7.7	-7.7	4.1	-6.9	-7.7	3.5	-7.7	5.1	-7.7	3.5	-7.7	5.1	-7.2	-7.2
C≡CH	4.1	-7.8	-7.8	4.0	-7.0	4.0	-7.8	-7.8	4.1	-6.9	-7.7	3.4	-7.7	5.0	-7.7	3.4	-7.7	5.1	-7.3	-7.3
C₆₀R'																				
H	5.1	-7.5	-7.3	3.5	-6.9	3.5	-7.3	-7.5	5.1	-7.2	-6.5	2.5	-7.8	5.1	-7.8	2.5	-6.5	3.7	-7.1	-7.1
OH	5.7	-7.2	-6.8	4.1	-6.8	4.1	-6.8	-7.2	5.7	-6.9	-6.3	3.8	-7.4	5.6	-7.4	3.8	6.3	4.5	-6.8	-6.8
OCH ₃	5.7	-7.2	-6.8	4.1	-6.8	4.1	-6.8	-7.2	5.7	-6.9	-6.3	3.8	-7.4	5.6	-7.4	3.8	-6.3	4.5	-6.8	-6.8
NH ₂	5.3	-7.3	-7.0	4.0	-6.8	4.0	-7.0	-7.3	5.8	-7.0	-6.5	3.5	-7.6	5.5	-7.6	3.4	-6.4	4.3	-6.9	-7.0
NHCH ₃	5.3	-7.3	-7.0	3.9	-6.8	4.0	-7.0	-7.3	5.7	-7.0	-6.5	3.5	-7.6	5.4	-7.6	3.4	-6.4	4.4	-6.9	-7.0
N(CH ₃) ₂	5.4	-7.3	-7.0	4.0	-6.8	4.0	-6.9	-7.2	5.7	-7.0	-6.5	3.5	-7.6	5.4	-7.6	3.5	-6.4	4.4	-6.9	-6.9
CH ₃	5.3	-7.4	-7.2	3.6	-6.9	3.6	-7.2	-7.4	5.3	-7.1	-6.5	2.8	-7.8	5.2	-7.8	2.8	-6.5	3.9	-7.0	-7.0
CH=CH ₂	5.2	-7.4	-7.1	3.7	-6.9	3.6	-7.3	-8.5	5.3	-7.1	-6.5	2.9	-7.7	5.2	-7.7	2.8	-6.5	4.0	-7.0	-7.1
Ph	5.4	-7.3	-7.1	3.8	-6.9	3.8	-7.1	-7.3	5.4	-7.1	-6.4	3.1	-7.6	5.3	-7.6	3.1	-6.4	4.1	-7.0	-7.0
C≡CH	5.3	-7.4	-7.2	3.7	-6.9	3.7	-7.2	-7.4	5.3	-7.1	-6.5	3.0	-7.7	5.3	-7.7	3.0	-6.5	4.1	-7.0	-7.0
C₆₀(CHR)																				
H	4.5	-7.2	-7.2	4.5	-6.7	4.5	-7.2	-7.2	4.5	-6.7	-7.4	4.2	-7.4	5.3	-7.4	4.2	-7.4	5.3	-7.0	-7.0
OH	4.5	-7.3	-7.3	4.5	-6.8	4.5	-7.4	-7.4	4.5	-6.8	-7.4	4.1	-7.4	5.3	-7.4	4.0	-7.4	5.3	-7.0	-7.1
OCH ₃	4.5	-7.2	-7.2	4.5	-6.8	4.5	-7.4	-7.4	4.5	-6.8	-7.4	4.1	-7.4	5.3	-7.4	4.1	-7.4	5.3	-7.0	-7.0
NH ₂	4.5	-7.3	-7.3	4.5	-6.8	4.5	-7.4	-7.4	4.5	-6.8	-7.4	4.1	-7.4	5.3	-7.4	4.0	-7.4	5.3	-7.0	-7.1
NHCH ₃	4.5	-7.3	-7.4	4.5	-6.8	4.5	-7.4	-7.4	4.4	-6.8	-7.4	4.1	-7.4	5.3	-7.4	4.0	-7.4	5.3	-7.0	-7.1
N(CH ₃) ₂	4.4	-7.3	-7.3	4.5	-6.8	4.4	-7.4	-7.3	4.5	-6.8	-7.5	4.0	-7.5	5.3	-7.5	4.0	-7.4	5.3	-7.0	-7.1
CH ₃	4.5	-7.3	-7.3	4.5	-6.8	4.5	-7.3	-7.3	4.5	-6.8	-7.4	4.1	-7.4	5.3	-7.4	4.1	-7.4	5.3	-7.0	-7.0
CH=CH ₂	4.5	-7.3	-7.3	4.5	-6.8	4.5	-7.3	-7.3	4.5	-6.8	-7.4	4.2	-7.4	5.3	-7.4	4.1	-7.4	5.3	-7.0	-7.0
Ph	4.5	-7.3	-7.3	4.5	-6.7	4.5	-7.2	-7.2	4.6	-6.7	-7.4	4.1	-7.4	5.3	-7.4	4.2	-7.4	5.3	-7.0	-7.0
C≡CH	4.5	-7.3	-7.3	4.5	-6.8	4.5	-7.3	-7.3	4.5	-6.8	-7.4	4.1	-7.4	5.3	-7.4	4.1	-7.4	5.3	-7.0	-7.0
C₆₀(CR') closed																				
	4.5	-7.3	-7.3	4.5	-6.8	4.5	-7.3	-7.3	4.5	-6.8	-7.4	4.1	-7.4	5.3	-7.4	4.1	-7.4	5.3	-7.0	-7.0

H	4.6	-7.1	-7.1	4.6	-6.6	4.6	-7.1	-7.1	4.6	-6.6	-7.4	4.3	-7.4	5.5	-7.4	4.3	-7.4	5.5	-6.9	-8.1
OH	4.6	-7.2	-7.2	4.6	-6.7	4.5	-7.4	-7.4	4.5	-6.7	-7.4	3.8	-7.4	5.4	-7.4	3.8	-7.4	5.4	-7.0	-7.1
OCH ₃	4.6	-7.2	-7.2	4.6	-6.7	4.5	-7.4	-7.4	4.5	-6.7	-7.4	3.9	-7.4	5.4	-7.4	3.9	-7.4	5.4	-7.0	-7.1
NH ₂	4.4	-7.4	-7.4	4.4	-6.8	4.3	-7.4	-7.5	4.5	-6.8	-7.4	3.7	-7.5	5.3	-7.5	3.7	-7.4	5.2	-7.0	-7.2
NHCH ₃	4.4	-7.4	-7.4	4.4	-6.8	4.3	-7.4	-7.5	4.5	-6.8	-7.4	3.7	-7.5	5.3	-7.5	3.7	-7.4	5.2	-7.0	-7.2
N(CH ₃) ₂	4.4	-7.3	-7.3	4.4	-6.8	4.5	-7.5	-7.4	4.3	-6.7	-7.5	3.7	-7.5	5.2	-7.5	3.7	-7.5	5.3	-7.0	-7.2
CH ₃	4.7	-7.1	-7.1	4.7	-6.6	4.6	-7.1	-7.1	4.6	-6.6	-7.3	4.3	-7.3	5.5	-7.4	4.3	-7.3	5.5	-6.9	-6.9
CH=CH ₂	4.6	-7.2	-7.1	4.6	-6.6	4.6	-7.1	-7.2	4.6	-6.6	-7.4	4.2	-7.4	5.5	-7.4	4.2	-7.4	5.4	-7.0	-7.0
Ph	4.6	-7.1	-7.1	4.6	-6.6	4.6	-7.1	-7.1	4.6	-6.6	-7.4	4.2	-7.4	5.5	-7.4	4.2	-7.4	5.5	-6.9	-6.9
C≡CH	4.6	-7.2	-7.2	4.6	-6.7	4.6	-7.2	-7.2	4.6	-6.7	-7.4	4.2	-7.4	5.4	-7.4	4.2	-7.4	5.4	-7.0	-7.0
C₆₀(CR) open																				
H	2.6	-8.2	-7.9	4.9	-7.4	3.6	-8.7	-8.0	3.0	-7.3	-7.9	1.3	-6.4	-1.8	-6.7	1.6	-7.9	4.1	-7.5	-7.0
OH	2.1	-8.9	-8.8	3.2	-7.5	2.5	-9.4	-9.1	2.3	-7.4	-8.5	-1.3	-7.9	-2.4	-8.0	-1.4	-8.5	2.4	-7.9	-7.8
OCH ₃	3.0	-8.9	-9.0	1.9	-7.5	2.0	-9.2	-9.3	2.5	-7.5	-7.7	-1.8	-8.5	-1.9	-8.5	-1.8	-7.8	1.3	-8.0	-7.9
NH ₂	2.3	-9.0	-9.0	2.3	-7.5	2.2	-9.1	-9.1	2.2	-7.5	-8.3	-2.3	-8.3	-2.8	-8.3	-2.4	-8.3	1.3	-8.0	-8.0
NHCH ₃	2.3	-9.0	-9.0	2.3	-7.5	2.3	-8.9	-8.9	2.3	-7.6	-8.3	-2.3	-8.3	-2.7	-8.3	-2.3	-8.3	1.3	-8.0	-8.0
N(CH ₃) ₂	2.2	-8.9	-8.9	2.2	-7.5	2.2	-8.9	-8.9	2.2	-7.5	-8.3	-2.4	-8.3	-2.9	-8.3	-2.4	-8.3	1.2	-8.3	-8.0
CH ₃	2.8	-8.0	-7.7	4.9	-7.5	3.7	-8.6	-7.8	3.2	-7.2	-7.8	1.5	-6.5	-1.6	-6.8	1.7	-7.8	4.2	-7.4	-7.0
CH=CH ₂	4.4	-7.1	-6.7	5.5	-6.9	5.0	-7.4	-6.6	4.6	-7.0	-7.0	4.2	-6.2	0.3	-6.6	4.6	-6.9	5.2	-6.8	-6.5
Ph	5.4	-6.4	-6.9	5.1	-6.8	5.4	-6.4	-6.8	5.1	-6.8	-6.4	5.2	-6.7	1.0	-6.4	5.2	-6.7	5.3	-6.5	-6.5
C≡CH	5.4	-6.3	-6.7	5.3	-6.9	5.4	-6.3	-6.7	5.2	-6.9	-6.4	5.6	-6.6	1.1	-6.4	5.6	-6.6	5.5	-6.5	6.5

Optimized geometries in Cartesian coordinates of the AM1 optimizations:

1. C₆₀HR

C₆₀H₂

C	-1.22828	3.29207	-0.7205
C	-1.2284	3.29192	0.74331
C	-0.02917	3.29193	1.43544
C	1.23879	3.29234	0.70373
C	1.23898	3.29125	-0.68132
C	-0.02898	3.29119	-1.4133
C	-2.33499	2.44818	-1.17264
C	-3.02111	1.92728	0.01135
C	-2.33551	2.44746	1.19548
C	-2.18208	1.6467	2.31517
C	0.13245	2.44713	2.61995
C	2.18419	2.44883	1.43642
C	3.07901	1.64983	0.74394
C	3.07938	1.64957	-0.72027
C	2.18365	2.44644	-1.41271
C	1.49845	1.92001	-2.59524
C	0.13182	2.44646	-2.5972
C	-0.91575	1.64963	-3.02676
C	-2.18346	1.64984	-2.29424
C	-3.51588	0.63342	0.01141
C	-3.35044	-0.21163	-1.17248
C	-2.70353	0.28165	-2.2916
C	-1.75199	-0.56272	-3.01695
C	-0.65573	0.28044	-3.47496
C	0.63615	-0.22247	-3.46541
C	1.74171	0.62388	-3.01692
C	2.68293	-0.22244	-2.2838
C	3.33722	0.28036	-1.16974
C	1.50027	1.92643	2.62093
C	2.29421	-2.37162	1.17904
C	2.16097	-1.57718	2.30889
C	0.9039	-1.57867	3.04528
C	-0.1393	-2.37847	2.60478
C	0.02974	-3.21919	1.42355
C	1.33824	-3.48757	-0.76592
C	2.31034	-2.38817	-1.17462
C	2.97501	-1.85185	-0.00021
C	3.48862	-0.5629	0.00857
C	3.33622	0.28125	1.1953
C	2.69085	-0.21177	2.31518
C	0.64163	-0.21281	3.50231
C	-0.65235	0.2798	3.49925
C	-1.7568	-0.56684	3.04286
C	-1.50611	-1.85737	2.60873
C	-2.18625	-2.37833	1.42314

C	-1.24787	-3.21896	0.68603
C	-1.2375	-3.22686	-0.68351
C	-0.00617	-3.48758	-1.54186
C	2.16594	-1.58756	-2.27653
C	0.88833	-1.58767	-3.01416
C	-0.13804	-2.3886	-2.58846
C	-1.48748	-1.85169	-2.57666
C	-2.16832	-2.37121	-1.39741
C	-3.08013	-1.5769	-0.71683
C	-3.08934	-1.57843	0.74002
C	-3.35409	-0.21254	1.19564
C	-2.70437	0.27989	2.31471
C	1.748	0.63301	3.05009
C	-0.91398	1.6466	3.04716
C	1.21059	-3.22764	0.72971
H	1.82197	-4.49121	-0.92925
H	-0.10707	-4.49146	-2.04184

C₆₀HOH

C	-1.23862	3.12122	-0.76841
C	-1.2294	3.12551	0.70726
C	-0.0393	3.13592	1.38316
C	1.3306	3.39907	0.73151
C	1.31407	3.37392	-0.83315
C	-0.0517	3.11762	-1.45166
C	-2.35458	2.28636	-1.20331
C	-3.03888	1.77408	-0.01628
C	-2.34144	2.29349	1.1593
C	-2.20075	1.49724	2.28481
C	0.11737	2.27687	2.54109
C	2.16411	2.27538	1.37433
C	3.02716	1.46316	0.68986
C	3.0202	1.458	-0.78589
C	2.14003	2.26155	-1.46063
C	1.44517	1.72571	-2.6185
C	0.08774	2.25602	-2.61316
C	-0.96585	1.46747	-3.05276
C	-2.22778	1.48122	-2.32474
C	-3.55048	0.48756	-0.0086
C	-3.40668	-0.36474	-1.19076
C	-2.76478	0.11921	-2.31801
C	-1.83037	-0.73649	-3.05201
C	-0.71881	0.09852	-3.51021
C	0.56995	-0.40473	-3.51626
C	1.68249	0.43327	-3.0639
C	2.62492	-0.41377	-2.34485
C	3.27177	0.08913	-1.22652
C	1.47549	1.74656	2.53644
C	2.26204	-2.56405	1.15534

C	2.12231	-1.76249	2.2757
C	0.85885	-1.75096	3.0153
C	-0.19657	-2.54347	2.59436
C	-0.04752	-3.39229	1.41126
C	1.13982	-3.40814	-0.75217
C	2.24907	-2.57319	-1.21412
C	2.94072	-2.04722	-0.03529
C	3.4363	-0.75453	-0.04289
C	3.28408	0.09652	1.1364
C	2.64957	-0.39664	2.2656
C	0.60951	-0.37875	3.46172
C	-0.67878	0.12344	3.46162
C	-1.79602	-0.71445	3.02425
C	-1.56038	-2.01155	2.59956
C	-2.25403	-2.53127	1.42019
C	-1.31919	-3.38555	0.68597
C	-1.32696	-3.39045	-0.69863
C	-0.0635	-3.40289	-1.43794
C	2.09687	-1.77926	-2.33817
C	0.82469	-1.77321	-3.06318
C	-0.22585	-2.56253	-2.62519
C	-1.58978	-2.03028	-2.61971
C	-2.26998	-2.54155	-1.42886
C	-3.15343	-1.73181	-0.73447
C	-3.14519	-1.72656	0.72965
C	-3.39315	-0.35603	1.1784
C	-2.73881	0.13561	2.29505
C	1.7157	0.45669	2.98882
C	-0.92999	1.48918	2.99744
C	1.14798	-3.40265	0.712
O	1.83344	4.68289	1.04585
H	1.86717	4.75428	2.00945
H	1.70509	4.37867	-1.17307

C₆₀HOCH₃

C	-1.99438	-1.47628	2.28837
C	-2.43565	-0.06814	2.28343
C	-3.06109	0.44983	1.18102
C	-3.5831	-0.38833	-0.00013
C	-3.08791	-1.87611	0.00287
C	-2.20311	-2.25324	1.18024
C	-0.73438	-1.54599	3.02261
C	-0.3885	-0.19882	3.4751
C	-1.43906	0.7089	3.01633
C	-1.10937	1.98855	2.59905
C	-2.68575	1.7755	0.72491
C	-3.06053	0.44517	-1.18436
C	-2.43451	-0.07719	-2.28437
C	-1.99321	-1.48532	-2.28359

C	-2.20245	-2.25793	-1.17253
C	-1.14358	-3.1452	-0.7229
C	-1.144	-3.14221	0.73459
C	0.05402	-3.23598	1.42796
C	0.26747	-2.41075	2.6095
C	0.93279	0.21489	3.48374
C	1.98846	-0.69675	3.03755
C	1.665	-1.97451	2.61377
C	2.31663	-2.54002	1.43066
C	1.32073	-3.3242	0.69852
C	1.32123	-3.32709	-0.68496
C	0.05481	-3.24169	-1.4153
C	0.2688	-2.42107	-2.59995
C	-0.73286	-1.55794	-3.01692
C	-2.68547	1.77261	-0.73329
C	1.28203	1.55223	-3.03832
C	0.28832	2.41797	-2.61412
C	0.50167	3.25425	-1.43146
C	1.69852	3.18095	-0.73795
C	2.74933	2.267	-1.18818
C	2.98432	0.07833	-2.30395
C	1.98996	-0.70875	-3.03393
C	0.93449	0.20112	-3.48421
C	-0.3868	-0.21255	-3.47456
C	-1.4376	0.69695	-3.01988
C	-1.10812	1.97823	-2.60749
C	-0.76299	3.32936	-0.6983
C	-0.7634	3.33233	0.68476
C	0.50097	3.25996	1.41878
C	1.69814	3.18381	0.72612
C	2.74874	2.27166	1.18044
C	3.39911	1.70558	-0.0026
C	3.81265	0.38415	0.00009
C	3.60051	-0.45205	-1.18263
C	1.66634	-1.98485	-2.60529
C	2.31746	-2.54574	-1.41969
C	3.25779	-1.80032	-0.72781
C	3.25729	-1.79733	0.73631
C	3.59988	-0.44735	1.18599
C	2.98318	0.08743	2.30494
C	2.54583	1.48472	2.30206
C	1.28055	1.56423	3.03268
C	0.28706	2.42831	2.60459
C	-1.75373	2.53309	-1.42515
C	-1.75443	2.53878	1.41424
C	2.54695	1.47562	-2.30676
O	-4.99658	-0.53312	-0.00025
H	-4.01586	-2.52249	0.00388
C	-5.73428	0.68087	-0.00061
H	-6.80068	0.33989	-0.00139

H	-5.50836	1.2776	0.91701
H	-5.50698	1.27799	-0.91759

C₆₀HNH₂

C	-1.26707	3.10877	-0.77198
C	-1.2695	3.10981	0.70278
C	-0.08537	3.12992	1.38757
C	1.29701	3.44638	0.76721
C	1.28585	3.39013	-0.81326
C	-0.07272	3.11575	-1.44054
C	-2.37003	2.26319	-1.21945
C	-3.05835	1.73998	-0.0397
C	-2.37522	2.26274	1.14276
C	-2.2372	1.46526	2.26756
C	0.07036	2.26826	2.54329
C	2.1241	2.29013	1.3927
C	3.00352	1.48927	0.71714
C	3.01138	1.48767	-0.75777
C	2.12612	2.28375	-1.43344
C	1.44787	1.74426	-2.59969
C	0.0852	2.26019	-2.60415
C	-0.9561	1.46339	-3.05768
C	-2.22486	1.46226	-2.34174
C	-3.55679	0.44823	-0.0399
C	-3.39409	-0.39908	-1.22318
C	-2.74751	0.09474	-2.34351
C	-1.79782	-0.74912	-3.07166
C	-0.69089	0.09864	-3.51766
C	0.60289	-0.39136	-3.51333
C	1.70277	0.45643	-3.04855
C	2.64822	-0.3834	-2.32521
C	3.28086	0.12281	-1.20028
C	1.43272	1.7512	2.54693
C	2.277	-2.54744	1.16535
C	2.11928	-1.75035	2.28641
C	0.84909	-1.75352	3.01448
C	-0.19444	-2.55581	2.58308
C	-0.0264	-3.39973	1.39912
C	1.17976	-3.39717	-0.75392
C	2.28451	-2.54977	-1.20395
C	2.96073	-2.02022	-0.01782
C	3.44326	-0.72246	-0.01767
C	3.27085	0.12414	1.16199
C	2.63201	-0.37903	2.28409
C	0.58136	-0.3851	3.46011
C	-0.71193	0.10489	3.45545
C	-1.81634	-0.74392	3.00526
C	-1.56359	-2.03724	2.57841
C	-2.24149	-2.56084	1.39163

C	-1.29177	-3.40355	0.66303
C	-1.28748	-3.40463	-0.72159
C	-0.01765	-3.40213	-1.44998
C	2.13393	-1.75411	-2.32702
C	0.86785	-1.75865	-3.06268
C	-0.17832	-2.56007	-2.63625
C	-1.54752	-2.04153	-2.64088
C	-2.23273	-2.56326	-1.45749
C	-3.13048	-1.76469	-0.76854
C	-3.13493	-1.76346	0.69563
C	-3.40096	-0.39697	1.14608
C	-2.76142	0.09832	2.26977
C	1.68241	0.46292	2.99931
C	-0.97243	1.46862	2.99032
C	1.17522	-3.39591	0.71022
N	1.75156	4.76549	1.17609
H	1.58216	4.91294	2.15123
H	2.72553	4.87859	0.97493
H	1.65512	4.38481	-1.20214

C₆₀HNHCH₃

C	-1.35918	2.94916	-0.90005
C	-1.37462	2.98016	0.57418
C	-0.19765	3.04533	1.27002
C	1.18321	3.38121	0.65779
C	1.18609	3.28738	-0.92412
C	-0.15923	2.96952	-1.55784
C	-2.43798	2.06943	-1.3406
C	-3.12491	1.55408	-0.1568
C	-2.46461	2.11594	1.02068
C	-2.32057	1.34438	2.1625
C	-0.03504	2.20522	2.44218
C	2.02884	2.25445	1.31206
C	2.93239	1.45992	0.66052
C	2.9547	1.42812	-0.81387
C	2.05765	2.18912	-1.51369
C	1.40348	1.61102	-2.6752
C	0.02946	2.09507	-2.70263
C	-0.98888	1.2657	-3.14965
C	-2.26395	1.24975	-2.44518
C	-3.59406	0.2515	-0.13551
C	-3.40082	-0.61533	-1.29991
C	-2.75505	-0.12925	-2.42406
C	-1.77938	-0.96541	-3.12637
C	-0.68797	-0.10147	-3.57944
C	0.61666	-0.56124	-3.55331
C	1.69231	0.32087	-3.09573
C	2.64975	-0.482	-2.34666
C	3.25957	0.06128	-1.22636

C	1.33865	1.72045	2.46948
C	2.29472	-2.58387	1.18336
C	2.10804	-1.76844	2.28661
C	0.83128	-1.78662	3.00296
C	-0.18945	-2.62123	2.57828
C	0.00932	-3.48446	1.41317
C	1.23579	-3.4969	-0.72832
C	2.32507	-2.63325	-1.18517
C	2.97739	-2.06445	-0.00383
C	3.42963	-0.75596	-0.02542
C	3.22619	0.11015	1.13501
C	2.58899	-0.38586	2.26121
C	0.52793	-0.41613	3.41826
C	-0.77614	0.0436	3.39161
C	-1.85651	-0.83924	2.94882
C	-1.57005	-2.13466	2.55057
C	-2.2243	-2.69735	1.36842
C	-1.2485	-3.53223	0.66573
C	-1.23084	-3.56085	-0.71849
C	0.04556	-3.54352	-1.43509
C	2.1671	-1.86398	-2.32547
C	0.90861	-1.91266	-3.07253
C	-0.12297	-2.72933	-2.63958
C	-1.50361	-2.24279	-2.66723
C	-2.18802	-2.75643	-1.47985
C	-3.11044	-1.9652	-0.81544
C	-3.12905	-1.93487	0.6483
C	-3.43067	-0.56616	1.06856
C	-2.81352	-0.03383	2.18782
C	1.61348	0.44773	2.9504
C	-1.06312	1.39116	2.89611
C	1.21713	-3.46654	0.73539
N	1.62863	4.72632	1.01221
H	2.60775	4.81185	0.80553
C	1.34294	5.15518	2.35522
H	0.23067	5.22602	2.48975
H	1.75177	4.46894	3.14693
H	1.78894	6.17548	2.49519
H	1.53539	4.28123	-1.33383

C₆₀HN(CH₃)₂

C	-0.77325	2.90822	-1.05438
C	-0.95558	3.11779	0.41318
C	0.33863	3.01759	1.294
C	1.60847	2.71568	0.56066
C	1.6825	2.67255	-0.81193
C	0.46384	2.77329	-1.63974
C	-1.89479	2.13741	-1.56981
C	-2.7016	1.70183	-0.43369

C	-2.07827	2.2077	0.78266
C	-2.05325	1.40791	1.90193
C	0.30196	2.01096	2.39847
C	2.40273	1.783	1.34577
C	3.27267	0.89478	0.7323
C	3.37201	0.87245	-0.72201
C	2.59006	1.73688	-1.47241
C	1.95019	1.25854	-2.6973
C	0.63908	1.89863	-2.79669
C	-0.43662	1.18787	-3.30665
C	-1.74328	1.30975	-2.67152
C	-3.31398	0.45827	-0.45962
C	-3.15166	-0.41908	-1.621
C	-2.38744	-0.00484	-2.69765
C	-1.47178	-0.94152	-3.35081
C	-0.26504	-0.20336	-3.72921
C	0.9761	-0.8083	-3.62869
C	2.11599	-0.05503	-3.10214
C	2.93178	-0.97028	-2.30155
C	3.5437	-0.51882	-1.14477
C	1.59532	1.34609	2.481
C	2.13005	-3.03977	1.17271
C	1.97385	-2.21144	2.27179
C	0.66257	-2.08246	2.91032
C	-0.42044	-2.78939	2.41643
C	-0.25483	-3.66732	1.25751
C	1.08665	-3.8132	-0.80804
C	2.29364	-3.07808	-1.18981
C	2.93903	-2.60085	0.0341
C	3.54843	-1.35721	0.05569
C	3.38235	-0.48243	1.21741
C	2.61748	-0.89699	2.29334
C	0.49805	-0.68727	3.32247
C	-0.73755	-0.06944	3.20966
C	-1.88137	-0.82059	2.69451
C	-1.72951	-2.14185	2.30986
C	-2.37638	-2.62753	1.0894
C	-1.46355	-3.56721	0.43739
C	-1.36725	-3.59332	-0.94397
C	-0.05644	-3.71849	-1.58365
C	2.29115	-2.28573	-2.32574
C	1.08247	-2.18561	-3.14588
C	-0.05852	-2.88327	-2.78587
C	-1.37094	-2.2439	-2.89039
C	-2.17995	-2.68265	-1.7517
C	-3.04625	-1.79552	-1.13441
C	-3.14648	-1.76676	0.3261
C	-3.31132	-0.37176	0.73886
C	-2.68922	0.09283	1.88721
C	1.70112	0.04298	2.94246

C	-0.83323	1.30578	2.72687
C	0.98497	-3.78815	0.65212
C	-0.40305	4.32453	1.16329
N	-1.03369	5.0444	2.21395
C	-1.14835	4.41399	3.50509
H	-1.47257	5.19241	4.24587
H	-1.89002	3.56862	3.52389
H	-0.14376	4.0205	3.81379
C	-2.23016	5.74118	1.79104
H	-2.51636	6.46764	2.5963
H	-2.0143	6.31039	0.84911
H	-3.0953	5.04846	1.60381
H	0.09534	5.0667	0.48215

C₆₀HCH₃

C	-1.33092	3.36829	-0.65175
C	-1.32687	3.3565	0.81179
C	-0.12558	3.35242	1.50113
C	1.13987	3.35949	0.76657
C	1.1368	3.37251	-0.61791
C	-0.13292	3.37597	-1.347
C	-2.43734	2.52496	-1.10785
C	-3.11666	1.99185	0.07385
C	-2.43086	2.50626	1.26044
C	-2.27486	1.69915	2.37463
C	0.03936	2.49901	2.67933
C	2.08662	2.50644	1.48816
C	2.97392	1.70863	0.78587
C	2.96929	1.71586	-0.67675
C	2.07815	2.53044	-1.35813
C	1.39342	2.01003	-2.5339
C	0.02682	2.53622	-2.53535
C	-1.0186	1.73939	-2.96601
C	-2.28666	1.734	-2.23487
C	-3.6081	0.69694	0.06511
C	-3.44794	-0.13882	-1.12519
C	-2.80696	0.36539	-2.24402
C	-1.85876	-0.47143	-2.98137
C	-0.75494	0.3721	-3.41946
C	0.53861	-0.12976	-3.40457
C	1.63981	0.70977	-2.95078
C	2.58938	-0.13728	-2.25097
C	3.22647	0.35734	-1.14459
C	1.40679	1.97849	2.67305
C	2.22055	-2.29219	1.19222
C	2.07459	-1.51669	2.33368
C	0.81254	-1.52883	3.07634
C	-0.23256	-2.32573	2.64511
C	-0.0725	-3.15399	1.44818

C	1.13275	-3.14304	-0.7138
C	2.43752	-2.5295	-1.2336
C	2.91208	-1.78621	0.01998
C	3.39187	-0.50369	0.04152
C	3.23417	0.33771	1.22426
C	2.59706	-0.15705	2.35148
C	0.55178	-0.16619	3.54321
C	-0.74295	0.32605	3.54821
C	-1.84916	-0.51748	3.09178
C	-1.60187	-1.80843	2.65484
C	-2.28731	-2.32385	1.46814
C	-1.33889	-3.15832	0.72836
C	-1.32937	-3.14216	-0.65759
C	-0.06222	-3.13757	-1.38284
C	2.24392	-1.60359	-2.47626
C	0.81201	-1.49257	-2.98391
C	-0.23002	-2.27834	-2.56993
C	-1.59668	-1.76578	-2.55951
C	-2.27967	-2.2974	-1.38047
C	-3.17914	-1.50889	-0.68322
C	-3.18106	-1.5199	0.78127
C	-3.44314	-0.15653	1.24326
C	-2.79562	0.33105	2.36637
C	1.65655	0.68351	3.09445
C	-1.00586	1.69576	3.10445
C	1.11949	-3.13178	0.73812
C	3.42469	-3.62992	-1.59225
H	4.40777	-3.18602	-1.8816
H	3.58101	-4.30426	-0.71548
H	3.03301	-4.23577	-2.44475
H	2.89292	-2.00572	-3.30634

C₆₀HCH=CH₂

C	-1.357867	3.479213	-0.697783
C	-1.348045	3.481479	0.766073
C	-0.144557	3.498009	1.450584
C	1.118509	3.513208	0.710703
C	1.109595	3.509485	-0.674346
C	-0.163009	3.492003	-1.398164
C	-2.457292	2.620959	-1.141399
C	-3.126777	2.092074	0.048395
C	-2.440964	2.623580	1.227078
C	-2.270554	1.827082	2.347312
C	0.035415	2.657520	2.635575
C	2.079246	2.683220	1.438863
C	2.979843	1.894480	0.742084
C	2.970583	1.891335	-0.722107
C	2.060200	2.675340	-1.410233
C	1.374065	2.137862	-2.587206

C	0.000930	2.647097	-2.581524
C	-1.039299	1.836316	-3.002883
C	-2.302400	1.822065	-2.262286
C	-3.605807	0.792415	0.054052
C	-3.437596	-0.052526	-1.129415
C	-2.804940	0.447215	-2.253678
C	-1.847145	-0.386334	-2.983380
C	-0.764678	0.469642	-3.450161
C	0.533473	-0.017103	-3.447821
C	1.630806	0.843826	-3.007539
C	2.586287	0.010651	-2.278145
C	3.242054	0.524350	-1.170327
C	1.409765	2.154282	2.628640
C	2.246986	-2.136887	1.187956
C	2.111587	-1.341378	2.316774
C	0.860238	-1.357060	3.062095
C	-0.174724	-2.170237	2.628094
C	-0.001856	-3.012200	1.447711
C	1.310859	-3.300690	-0.752046
C	2.252352	-2.160006	-1.165051
C	2.913381	-1.610171	0.004283
C	3.411107	-0.314834	0.008224
C	3.257041	0.530087	1.194168
C	2.624370	0.030249	2.318100
C	0.583912	0.005907	3.519410
C	-0.716202	0.482000	3.523900
C	-1.812575	-0.379557	3.075994
C	-1.548037	-1.667401	2.641703
C	-2.229470	-2.199764	1.462179
C	-1.285119	-3.030199	0.720875
C	-1.282149	-3.039087	-0.648168
C	-0.057349	-3.289407	-1.516961
C	2.087728	-1.361692	-2.265497
C	0.806282	-1.378068	-2.995706
C	-0.206587	-2.189654	-2.559661
C	-1.562945	-1.670576	-2.541571
C	-2.229403	-2.196966	-1.357448
C	-3.147353	-1.413399	-0.672897
C	-3.147301	-1.412528	0.783952
C	-3.426059	-0.049184	1.238763
C	-2.775545	0.453747	2.352726
C	1.676455	0.864716	3.058305
C	-0.997953	1.844561	3.071133
C	1.176117	-3.014313	0.748337
C	1.972235	-4.615729	-1.027750
H	2.288985	-4.738407	-2.077587
C	2.178723	-5.566662	-0.121106
H	1.880791	-5.470018	0.932345
H	2.668878	-6.515226	-0.381493
H	-0.170159	-4.290542	-2.023967

C₆₀HPh

C	-1.7321	2.43481	-0.86781
C	-1.71308	2.42668	0.60698
C	-0.5235	2.56389	1.27252
C	0.80219	3.00249	0.63367
C	0.77552	2.97597	-0.93495
C	-0.5554	2.57156	-1.5542
C	-2.74892	1.48361	-1.30597
C	-3.36255	0.88594	-0.12053
C	-2.72001	1.46979	1.05644
C	-2.48548	0.684	2.17375
C	-0.26882	1.71737	2.42421
C	1.75221	1.96189	1.244
C	2.70247	1.25864	0.55166
C	2.68848	1.26543	-0.92319
C	1.71755	1.97029	-1.58268
C	1.08197	1.37095	-2.74305
C	-0.32661	1.74357	-2.7254
C	-1.28663	0.8456	-3.16968
C	-2.53794	0.70901	-2.43628
C	-3.72514	-0.45032	-0.12347
C	-3.4928	-1.26931	-1.31514
C	-2.91683	-0.70508	-2.44074
C	-1.89568	-1.44202	-3.18793
C	-0.8887	-0.48192	-3.64296
C	0.44865	-0.83569	-3.65972
C	1.46182	0.11855	-3.20411
C	2.49876	-0.62336	-2.49938
C	3.0915	-0.06136	-1.37914
C	1.13938	1.34486	2.40657
C	2.40288	-2.83453	0.98047
C	2.17989	-2.06444	2.10929
C	0.92717	-2.20318	2.85448
C	-0.03401	-3.10642	2.4314
C	0.20328	-3.92155	1.23918
C	1.37188	-3.78168	-0.92994
C	2.37665	-2.82196	-1.38867
C	3.01133	-2.23233	-0.20786
C	3.35698	-0.89158	-0.20471
C	3.11486	-0.07371	0.98334
C	2.54874	-0.6477	2.11068
C	0.52616	-0.87246	3.31413
C	-0.81095	-0.51876	3.33089
C	-1.82804	-1.47434	2.88899
C	-1.44931	-2.73203	2.44913
C	-2.0864	-3.31586	1.26787
C	-1.06528	-4.05169	0.52029
C	-1.08067	-4.04428	-0.86424

C	0.1716	-3.90636	-1.60975
C	2.12877	-2.0398	-2.50396
C	0.85964	-2.17089	-3.22245
C	-0.09202	-3.07855	-2.78761
C	-1.50731	-2.70416	-2.76988
C	-2.11806	-3.30067	-1.58107
C	-3.08346	-2.60311	-0.87412
C	-3.06718	-2.61094	0.58993
C	-3.46634	-1.28194	1.054
C	-2.86542	-0.72981	2.1725
C	1.52812	0.08706	2.84541
C	-1.21817	0.81353	2.87982
C	1.38814	-3.78951	0.53411
C	1.17563	4.39355	1.06646
C	0.18234	5.35733	1.27743
C	0.53185	6.65077	1.66203
C	1.8726	6.99174	1.83885
C	2.86506	6.03431	1.63038
C	2.52033	4.73961	1.24571
H	-0.87848	5.09289	1.14492
H	-0.25494	7.40171	1.82796
H	2.14643	8.01254	2.14406
H	3.924	6.29758	1.77125
H	3.30841	3.98667	1.08814
H	1.045	4.01151	-1.29219

C₆₀HCCH

C	-1.2721	3.27458	-0.48389
C	-1.26005	3.27493	0.98007
C	-0.05434	3.27053	1.66066
C	1.20643	3.26909	0.91549
C	1.1923	3.26539	-0.46901
C	-0.07966	3.26423	-1.19105
C	-2.37095	2.42741	-0.92797
C	-3.05333	1.90673	0.25854
C	-2.36282	2.4281	1.43929
C	-2.20047	1.62406	2.55541
C	0.11689	2.42213	2.84049
C	2.15882	2.42501	1.64041
C	3.04948	1.62861	0.94084
C	3.03397	1.62859	-0.52312
C	2.1269	2.41957	-1.21059
C	1.44167	1.89613	-2.38914
C	0.06414	2.4235	-2.37588
C	-0.96585	1.62819	-2.80131
C	-2.20671	1.62288	-2.04638
C	-3.54711	0.61438	0.25855
C	-3.38552	-0.22858	-0.92804
C	-2.72673	0.26162	-2.04642

C	-1.80537	-0.56954	-2.80141
C	-0.80431	0.30731	-3.54069
C	0.66261	-0.253	-3.58603
C	1.67919	0.62252	-2.83132
C	2.6051	-0.21515	-2.09203
C	3.28061	0.26759	-0.97997
C	1.48459	1.89971	2.82803
C	2.29716	-2.40301	1.38741
C	2.15276	-1.60599	2.51107
C	0.89005	-1.60783	3.25115
C	-0.15998	-2.40581	2.82792
C	-0.00765	-3.24678	1.64026
C	1.17564	-3.23649	-0.52326
C	2.26681	-2.38645	-0.98004
C	2.96816	-1.87407	0.19883
C	3.46181	-0.58196	0.19886
C	3.3142	0.25958	1.38748
C	2.67513	-0.23825	2.51107
C	0.63221	-0.24159	3.70932
C	-0.66122	0.25246	3.72106
C	-1.77144	-0.59121	3.2754
C	-1.5277	-1.88339	2.84038
C	-2.2209	-2.40152	1.66051
C	-1.28023	-3.24094	0.91532
C	-1.28826	-3.22869	-0.46918
C	-0.02776	-3.2213	-1.21076
C	2.08518	-1.57629	-2.09211
C	0.83662	-1.58333	-2.83143
C	-0.18952	-2.37428	-2.38928
C	-1.56786	-1.84901	-2.37601
C	-2.23553	-2.37981	-1.19119
C	-3.13124	-1.5926	-0.48401
C	-3.12252	-1.60096	0.97995
C	-3.37998	-0.23463	1.43925
C	-2.72296	0.25637	2.55543
C	1.73522	0.60488	3.25119
C	-0.92624	1.62145	3.27543
C	1.18716	-3.24693	0.94071
C	1.05541	-0.40293	-4.96488
C	1.39055	-0.53105	-6.10541
H	1.68795	-0.64464	-7.11831
H	-1.15077	0.43967	-4.60564

2. C₆₀R⁻

C₆₀H⁻

C	3.25238	0.90073	-1.17753
C	3.57327	0.097	0.00229
C	3.34381	-1.26932	-0.00534
C	2.77526	-1.90771	-1.19293
C	2.46755	-1.1465	-2.30892
C	2.71113	0.29753	-2.30114
C	2.72934	2.18817	-0.71876
C	2.7286	2.18006	0.74547
C	3.25126	0.88768	1.19058
C	2.70886	0.27217	2.30694
C	2.77408	-1.92075	1.17458
C	1.85706	-2.95644	-0.74695
C	0.67977	-3.18635	-1.44075
C	0.3563	-2.38272	-2.62108
C	1.22508	-1.38951	-3.04138
C	0.70084	-0.09529	-3.48427
C	1.62326	0.94543	-3.03252
C	1.12255	2.16306	-2.59619
C	1.69737	2.80189	-1.40799
C	1.69592	2.78612	1.44042
C	0.60571	3.43609	0.71159
C	0.60643	3.44378	-0.67307
C	-0.63581	3.19651	-1.41069
C	-0.31339	2.41887	-2.59988
C	-1.19824	1.42422	-3.01747
C	-0.66443	0.13596	-3.47723
C	-1.5821	-0.90836	-3.02723
C	-1.08656	-2.13751	-2.61539
C	1.85637	-2.96455	0.7162
C	-2.67944	-2.155	0.71755
C	-1.65473	-2.79273	1.40656
C	-1.08919	-2.16624	2.5907
C	-1.58515	-0.94164	3.0154
C	-2.67402	-0.29646	2.28565
C	-3.82593	-0.12047	-0.00256
C	-3.22962	-0.88492	-1.19204
C	-2.67892	-2.14717	-0.74397
C	-1.65345	-2.77719	-1.43894
C	-0.564	-3.4334	-0.71049
C	-0.56466	-3.44107	0.67207
C	0.35371	-2.41146	2.59505
C	1.22209	-1.42292	3.0271
C	0.69736	-0.13365	3.48357
C	-0.66791	0.0977	3.47778
C	-1.20133	1.39093	3.03178
C	-2.4367	1.15448	2.32272
C	-2.73264	1.87781	1.16593

C	-3.31934	1.28138	0.00547
C	-2.67137	-0.2712	-2.29115
C	-2.43441	1.18	-2.31227
C	-2.73171	1.89064	-1.14807
C	-1.80729	2.95202	-0.71199
C	-1.80813	2.94421	0.74273
C	-0.63731	3.18089	1.44525
C	-0.31597	2.38998	2.62597
C	1.11993	2.13427	2.62092
C	1.62026	0.91195	3.04432
C	0.67841	-3.20212	1.40626
C	2.46526	-1.17186	2.29857
C	-3.23142	-0.89815	1.1794
H	-4.9443	-0.17309	-0.00381

C₆₀OH⁻

C	-1.25787	3.15505	-0.76463
C	-1.22741	3.13874	0.70359
C	-0.0379	3.16326	1.39671
C	1.33418	3.40843	0.71956
C	1.22504	3.14471	-0.74569
C	-0.03143	3.1192	-1.42953
C	-2.34864	2.3133	-1.2032
C	-3.03546	1.7887	-0.01646
C	-2.33884	2.30394	1.15991
C	-2.19559	1.50757	2.28582
C	0.12004	2.29027	2.54023
C	2.18171	2.29644	1.38754
C	3.03475	1.47423	0.686
C	3.05753	1.46969	-0.78243
C	2.12678	2.27648	-1.43839
C	1.4518	1.74544	-2.63643
C	0.09635	2.27499	-2.63112
C	-0.96275	1.49087	-3.05823
C	-2.2269	1.50493	-2.33216
C	-3.54539	0.50116	-0.0125
C	-3.40277	-0.34736	-1.19467
C	-2.75373	0.14449	-2.31711
C	-1.82079	-0.71469	-3.05281
C	-0.71074	0.12074	-3.51319
C	0.57916	-0.38303	-3.5186
C	1.69618	0.45238	-3.06921
C	2.64056	-0.39602	-2.35241
C	3.286	0.11275	-1.22659
C	1.48211	1.75826	2.53452
C	2.26612	-2.55146	1.15021
C	2.12527	-1.75144	2.27173
C	0.86081	-1.74096	3.00941
C	-0.19391	-2.53506	2.58835

C	-0.04374	-3.38132	1.40377
C	1.14654	-3.39033	-0.75912
C	2.25807	-2.55814	-1.21822
C	2.94649	-2.03417	-0.03948
C	3.44401	-0.7418	-0.04337
C	3.2894	0.10584	1.13655
C	2.65251	-0.38585	2.2657
C	0.61198	-0.3698	3.45556
C	-0.67571	0.13312	3.46093
C	-1.79112	-0.70525	3.02041
C	-1.55676	-2.00279	2.594
C	-2.24923	-2.51998	1.41294
C	-1.31478	-3.37381	0.67861
C	-1.32046	-3.37365	-0.70673
C	-0.05709	-3.38591	-1.44493
C	2.10611	-1.75348	-2.33738
C	0.83251	-1.7509	-3.06383
C	-0.21762	-2.54179	-2.6295
C	-1.5815	-2.00914	-2.62383
C	-2.26305	-2.52438	-1.43575
C	-3.14611	-1.71385	-0.74125
C	-3.13945	-1.71315	0.72307
C	-3.38717	-0.34365	1.17373
C	-2.73333	0.14607	2.29192
C	1.72027	0.46689	2.98797
C	-0.92697	1.50076	2.99894
C	1.15266	-3.38944	0.70523
O	1.84117	4.7039	0.9574
H	1.88633	4.81241	1.91567

C ₆₀ OCH ₃ ⁻			
C	2.00506	-1.4991	-2.31517
C	2.4442	-0.09801	-2.2872
C	3.09056	0.43107	-1.19191
C	3.57994	-0.42769	0.00036
C	2.86225	-1.73735	0.00163
C	2.19884	-2.25237	-1.15659
C	0.74629	-1.56539	-3.02285
C	0.39875	-0.2136	-3.47693
C	1.45268	0.6892	-3.02045
C	1.134	1.97249	-2.60392
C	2.71082	1.75086	-0.73277
C	3.09056	0.43335	1.19099
C	2.44423	-0.09355	2.28733
C	2.00508	-1.49457	2.31801
C	2.19887	-2.25006	1.16087
C	1.13256	-3.17223	0.73071
C	1.13253	-3.17365	-0.72459
C	-0.06049	-3.24847	-1.4245

C	-0.26902	-2.42678	-2.6101
C	-0.92064	0.20681	-3.4845
C	-1.98047	-0.6961	-3.03784
C	-1.65573	-1.97341	-2.60679
C	-2.31529	-2.53066	-1.42173
C	-1.32592	-3.32218	-0.68912
C	-1.32588	-3.32076	0.69556
C	-0.06045	-3.24567	1.43079
C	-0.26897	-2.42172	2.61481
C	0.74634	-1.55952	3.02586
C	2.71086	1.75228	0.72932
C	-1.25883	1.56554	3.03297
C	-0.25989	2.42417	2.60566
C	-0.46873	3.25771	1.42041
C	-1.66755	3.19106	0.72849
C	-2.72321	2.28434	1.18167
C	-2.96795	0.09915	2.30417
C	-1.98041	-0.69021	3.03923
C	-0.92057	0.21357	3.48411
C	0.39882	-0.20685	3.47733
C	1.45274	0.69508	3.01907
C	1.13406	1.97755	2.60006
C	0.79632	3.32258	0.68799
C	0.79627	3.32116	-0.69443
C	-0.46877	3.25492	-1.42671
C	-1.66757	3.18964	-0.73464
C	-2.72324	2.28205	-1.18604
C	-3.37715	1.7244	-0.00164
C	-3.79601	0.40387	-0.00035
C	-3.58942	-0.42946	1.18457
C	-1.65567	-1.96835	2.61065
C	-2.31525	-2.52788	1.42666
C	-3.25226	-1.78028	0.73386
C	-3.25227	-1.78168	-0.73035
C	-3.58943	-0.43174	-1.18366
C	-2.96799	0.09469	-2.3043
C	-2.52429	1.49021	-2.30532
C	-1.25889	1.55966	-3.03598
C	-0.25994	2.4191	-2.61035
C	1.78399	2.52402	1.41826
C	1.78394	2.52124	-1.42318
C	-2.52424	1.49467	2.30247
O	4.97898	-0.66938	0.00057
C	5.78176	0.49715	-0.0004
H	6.83085	0.10896	-0.00079
H	5.58837	1.10978	-0.91577
H	5.58934	1.11056	0.91466

$C_{60}NH_2^-$

C	-2.26063	1.75308	-1.97993
C	-2.54242	0.3449	-2.29757
C	-3.12969	-0.49149	-1.37655
C	-3.75896	0.00296	-0.04135
C	-3.1637	1.34257	0.29724
C	-2.54788	2.1849	-0.68717
C	-1.01158	2.11849	-2.60918
C	-0.51074	0.95611	-3.35195
C	-1.46132	-0.13608	-3.15543
C	-1.00445	-1.44044	-3.03904
C	-2.61438	-1.83432	-1.22411
C	-3.15042	-1.054	0.93761
C	-2.58088	-0.73576	2.14954
C	-2.30556	0.65617	2.52438
C	-2.56994	1.63355	1.56108
C	-1.61047	2.74138	1.39782
C	-1.59755	3.08673	-0.0152
C	-0.41357	3.45392	-0.63569
C	-0.10326	2.96201	-1.97079
C	0.84724	0.69241	-3.41067
C	1.79513	1.57297	-2.72866
C	1.32604	2.6711	-2.02435
C	1.90741	3.00067	-0.71935
C	0.82813	3.48671	0.14175
C	0.81504	3.15871	1.48689
C	-0.44089	2.77635	2.13856
C	-0.15181	1.72581	3.10656
C	-1.06854	0.68752	3.26937
C	-2.62613	-2.17831	0.19584
C	1.27558	-2.11843	2.61884
C	0.38346	-2.95422	1.96815
C	0.69528	-3.45786	0.6294
C	1.88533	-3.10231	0.01487
C	2.82831	-2.22027	0.70389
C	2.81574	-0.34737	2.31262
C	1.73945	0.13629	3.17617
C	0.78378	-0.95468	3.36051
C	-0.57439	-0.68832	3.40587
C	-1.51537	-1.56442	2.71286
C	-1.05171	-2.67054	2.01722
C	-0.54796	-3.48283	-0.14212
C	-0.5352	-3.15606	-1.48528
C	0.72118	-2.78466	-2.13679
C	1.89876	-2.75646	-1.40677
C	2.85004	-1.66069	-1.59663
C	3.42623	-1.33089	-0.29258
C	3.69428	-0.01083	0.03127
C	3.3845	0.49315	1.36958
C	1.2763	1.43709	3.0454
C	1.88013	2.32671	2.04819

C	2.90187	1.86796	1.23424
C	2.91565	2.21423	-0.18843
C	3.40623	1.05285	-0.93143
C	2.85821	0.74167	-2.16514
C	2.57366	-0.65349	-2.507
C	1.33104	-0.68382	-3.27804
C	0.43069	-1.72092	-3.0999
C	-1.62542	-2.98888	0.71876
C	-1.59937	-2.31662	-2.04188
C	2.5316	-1.74259	1.97006
N	-5.20675	0.00744	-0.09543
H	-5.5674	-0.91706	0.02906
H	-5.57801	0.61665	0.60565

C₆₀NHCH₃⁻

C	1.918	-2.00446	-1.98808
C	2.35755	-0.63617	-2.2998
C	3.037	0.12487	-1.37631
C	3.60745	-0.44246	-0.04335
C	2.85989	-1.70607	0.29003
C	2.1539	-2.47013	-0.6964
C	0.63545	-2.22374	-2.61748
C	0.26929	-1.00938	-3.35566
C	1.33744	-0.03265	-3.15531
C	1.03097	1.31448	-3.03426
C	2.67495	1.51655	-1.21854
C	3.12362	0.67271	0.9401
C	2.51966	0.41695	2.15062
C	2.08698	-0.93639	2.52037
C	2.238	-1.93366	1.55418
C	1.15996	-2.92527	1.38711
C	1.10784	-3.2615	-0.02723
C	-0.10999	-3.49003	-0.64849
C	-0.36262	-2.96135	-1.98175
C	-1.05017	-0.5935	-3.41277
C	-2.09159	-1.36355	-2.73352
C	-1.74968	-2.51027	-2.03338
C	-2.36465	-2.77677	-0.72933
C	-1.34741	-3.38511	0.12946
C	-1.29722	-3.06581	1.47586
C	-0.00612	-2.83061	2.12844
C	-0.17394	-1.75753	3.10001
C	0.85446	-0.83028	3.26618
C	2.72573	1.85158	0.20258
C	-1.15693	2.22542	2.62719
C	-0.17595	2.95721	1.97913
C	-0.42902	3.49787	0.64239
C	-1.65171	3.28166	0.02715
C	-2.68839	2.50952	0.71343

C	-2.88773	0.64132	2.31523
C	-1.87293	0.03568	3.17633
C	-0.79975	1.01076	3.36409
C	0.51951	0.59204	3.40738
C	1.55371	1.35808	2.71662
C	1.21774	2.51257	2.02633
C	0.80885	3.38455	-0.12974
C	0.75911	3.06641	-1.47408
C	-0.53127	2.8422	-2.12639
C	-1.70432	2.94479	-1.39576
C	-2.77354	1.96447	-1.58913
C	-3.38321	1.69723	-0.28598
C	-3.79897	0.41482	0.03314
C	-3.54811	-0.12592	1.36944
C	-1.56037	-1.30868	3.04072
C	-2.26117	-2.12056	2.04067
C	-3.22438	-1.54605	1.22883
C	-3.27736	-1.88324	-0.19505
C	-3.63331	-0.67107	-0.93358
C	-3.05368	-0.41941	-2.16642
C	-2.61306	0.93583	-2.50331
C	-1.37511	0.82813	-3.27491
C	-0.36313	1.75598	-3.0935
C	1.82335	2.76817	0.72864
C	1.72123	2.11385	-2.03407
C	-2.44745	1.99662	1.97766
N	5.04627	-0.64713	-0.09889
H	5.31437	-1.33282	0.5823
C	5.85061	0.53764	0.0047
H	5.55668	1.25449	-0.80709
H	5.75167	1.07091	0.99117
H	6.92511	0.2475	-0.13691

$C_{60}N(CH_3)_2^-$

C	1.88254	-0.59779	-2.69312
C	2.19397	0.78464	-2.30327
C	2.84155	1.06634	-1.12223
C	3.51374	-0.01558	-0.22241
C	2.88109	-1.34281	-0.54438
C	2.20505	-1.60141	-1.78106
C	0.59998	-0.60362	-3.35896
C	0.10638	0.77709	-3.42404
C	1.09606	1.62998	-2.77003
C	0.68355	2.71915	-2.01751
C	2.37041	2.17156	-0.31633
C	2.97138	0.44098	1.17299
C	2.43506	-0.41693	2.10676
C	2.12862	-1.81425	1.77521
C	2.32599	-2.20612	0.44977

C	1.32915	-3.08871	-0.18197
C	1.25308	-2.708	-1.58351
C	0.0364	-2.72036	-2.24718
C	-0.30925	-1.64281	-3.16393
C	-1.24432	1.04757	-3.28337
C	-2.19208	-0.04487	-3.06638
C	-1.72976	-1.35041	-3.00205
C	-2.27142	-2.26463	-1.99175
C	-1.17575	-3.11504	-1.52418
C	-1.1025	-3.47839	-0.19011
C	0.18784	-3.46895	0.50478
C	-0.0324	-3.01459	1.87149
C	0.92067	-2.19189	2.47137
C	2.44784	1.78708	1.09088
C	-1.35985	0.59844	3.36721
C	-0.46774	1.63697	3.15878
C	-0.81442	2.72723	2.24534
C	-2.03701	2.72304	1.59297
C	-2.97975	1.62587	1.8151
C	-2.96341	-0.79112	2.31828
C	-1.87044	-1.64083	2.78903
C	-0.87572	-0.78267	3.43106
C	0.47447	-1.04899	3.27727
C	1.41536	0.04471	3.04822
C	0.9589	1.35279	2.99657
C	0.39901	3.11093	1.5231
C	0.32559	3.4742	0.1914
C	-0.96509	3.47498	-0.49787
C	-2.11452	3.10735	0.18327
C	-3.10505	2.24773	-0.46609
C	-3.64141	1.33373	0.54299
C	-3.93696	0.02385	0.20221
C	-3.59243	-1.06659	1.11504
C	-1.45276	-2.72048	2.02544
C	-2.12021	-3.01248	0.75281
C	-3.15729	-2.20888	0.31056
C	-3.23488	-1.82441	-1.10018
C	-3.71776	-0.4446	-1.16659
C	-3.20738	0.41931	-2.1218
C	-2.89388	1.80357	-1.76135
C	-1.6809	2.19232	-2.48045
C	-0.74355	3.00675	-1.86725
C	1.49247	2.25296	1.98613
C	1.34165	2.99855	-0.75069
C	-2.65014	0.59342	2.67813
N	4.96929	0.00118	-0.36516
C	5.59072	1.21827	0.10138
H	5.06564	2.09886	-0.35395
H	5.56544	1.32896	1.22086
H	6.66159	1.22104	-0.23256

C	5.63795	-1.18585	0.11243
H	6.70801	-1.14328	-0.22369
H	5.62199	-1.28448	1.23265
H	5.15354	-2.09309	-0.33484

C₆₀CH₃⁻

C	2.91296	-2.09296	0.76115
C	3.39773	-0.78214	1.19497
C	2.83823	-0.17358	2.30668
C	1.76948	-0.83895	3.05039
C	1.30504	-2.07886	2.6378
C	1.89889	-2.72316	1.46204
C	2.91292	-2.11326	-0.70293
C	3.39769	-0.81496	-1.17291
C	3.69554	0.00772	-0.00016
C	3.42585	1.36654	-0.01898
C	2.55216	1.2625	2.28649
C	0.81631	0.18256	3.48175
C	-0.54151	-0.08889	3.47879
C	-1.0369	-1.40075	3.04438
C	-0.12278	-2.37643	2.64602
C	-0.42155	-3.18605	1.47245
C	0.82771	-3.41077	0.73962
C	0.82768	-3.42999	-0.64485
C	1.89884	-2.76267	-1.38606
C	2.83815	-0.23747	-2.30106
C	1.76939	-0.92319	-3.02602
C	1.30492	-2.15118	-2.5792
C	-0.12283	-2.4489	-2.5792
C	-0.42162	-3.22566	-1.38361
C	-1.59907	-3.0094	-0.68563
C	-1.59903	-2.98926	0.76878
C	-2.55442	-1.94714	1.18387
C	-2.27918	-1.20652	2.33474
C	1.30258	1.48283	3.01406
C	-2.6203	2.07909	0.70187
C	-1.61445	2.75278	1.38412
C	-0.54453	3.42713	0.64382
C	-0.54455	3.40798	-0.73854
C	-1.61445	2.71336	-1.45983
C	-3.13706	0.77899	-1.19724
C	-3.72778	0.00643	-0.00007
C	-3.13692	0.81186	1.17519
C	-2.55934	0.23579	2.28468
C	-1.48903	0.91868	3.00797
C	-1.02978	2.15355	2.57317
C	0.70548	3.23148	1.3789
C	1.8895	3.02308	0.68973
C	1.88949	3.00281	-0.77328

C	0.70546	3.19204	-1.46794
C	0.4051	2.36937	-2.64123
C	-1.0298	2.08138	-2.63175
C	-1.48907	0.83494	-3.03215
C	-2.55949	0.17236	-2.29033
C	-3.15934	-1.37739	0.01912
C	-2.5546	-1.97921	-1.12936
C	-2.27932	-1.27082	-2.30044
C	-1.03702	-1.4846	-3.00433
C	-0.54158	-0.18527	-3.47494
C	0.81622	0.08597	-3.48544
C	1.30252	1.39873	-3.05403
C	2.55211	1.19864	-2.32067
C	2.83791	1.9779	-1.21134
C	0.40514	2.44164	2.57455
C	2.83793	2.01072	1.15599
C	-2.62026	2.05877	-0.75917
C	-5.24001	0.02757	-0.00026
H	-5.6257	-0.4834	0.91421
H	-5.61682	1.07817	-0.01521
H	-5.62582	-0.5093	-0.89971

$C_{60}CH=CH_2^-$

C	-1.363453	3.458073	-0.718822
C	-1.358996	3.465154	0.744347
C	-0.158005	3.491145	1.434582
C	1.106863	3.506466	0.699003
C	1.103221	3.495881	-0.686439
C	-0.166301	3.469456	-1.415987
C	-2.456671	2.592714	-1.163287
C	-3.128953	2.066312	0.026264
C	-2.450691	2.606703	1.205022
C	-2.282037	1.812763	2.327760
C	0.019871	2.655280	2.622411
C	2.067785	2.683244	1.434391
C	2.972576	1.892633	0.744036
C	2.969233	1.883432	-0.720063
C	2.058514	2.661614	-1.415015
C	1.378143	2.118662	-2.593298
C	0.006058	2.624190	-2.596635
C	-1.026840	1.799468	-3.016383
C	-2.294322	1.789221	-2.279009
C	-3.602121	0.765223	0.035026
C	-3.431538	-0.083548	-1.145137
C	-2.795853	0.414230	-2.269932
C	-1.834547	-0.416919	-3.000318
C	-0.753589	0.439959	-3.468615
C	0.552110	-0.051107	-3.455128
C	1.642530	0.824375	-3.008352

C	2.596971	-0.000648	-2.271418
C	3.248171	0.515886	-1.160685
C	1.396011	2.157166	2.623037
C	2.250131	-2.142168	1.201893
C	2.110709	-1.340811	2.328502
C	0.858331	-1.355361	3.067627
C	-0.176130	-2.172033	2.635178
C	-0.001630	-3.019293	1.457215
C	1.309142	-3.305357	-0.742420
C	2.282886	-2.178074	-1.156482
C	2.920988	-1.616642	0.015241
C	3.416467	-0.318287	0.018593
C	3.252770	0.531150	1.201318
C	2.617884	0.033986	2.324278
C	0.574333	0.008097	3.517577
C	-0.727732	0.479844	3.515156
C	-1.820970	-0.386420	3.067489
C	-1.550335	-1.675784	2.641306
C	-2.225523	-2.225980	1.459622
C	-1.288383	-3.063093	0.748204
C	-1.245536	-3.042004	-0.646655
C	-0.021150	-3.058989	-1.386525
C	2.099013	-1.374509	-2.259386
C	0.839980	-1.396764	-3.017944
C	-0.182792	-2.209569	-2.526066
C	-1.565322	-1.700612	-2.553313
C	-2.233260	-2.223697	-1.371833
C	-3.146154	-1.443847	-0.679877
C	-3.152916	-1.438768	0.776787
C	-3.422428	-0.076251	1.222424
C	-2.784009	0.439435	2.340310
C	1.665345	0.868943	3.056927
C	-1.012224	1.839414	3.056786
C	1.193249	-3.034547	0.771973
C	1.860751	-4.646385	-1.086957
H	1.965346	-4.809682	-2.172978
C	2.186347	-5.588250	-0.206189
H	2.081292	-5.451819	0.878216
H	2.577548	-6.564908	-0.517933

C₆₀Ph⁻

C	1.71855	-2.31463	1.23757
C	1.99354	-2.2879	-0.20575
C	2.57157	-1.18959	-0.80332
C	3.17061	-0.00046	-0.01908
C	2.59804	0.00361	1.36547
C	1.99645	-1.15159	1.95743
C	0.47655	-3.02108	1.44794
C	-0.02317	-3.47705	0.14524

C	0.92071	-3.02233	-0.87303
C	0.4579	-2.60852	-2.11333
C	2.04945	-0.73669	-2.07557
C	2.57179	1.18424	-0.81019
C	1.99401	2.28612	-0.21901
C	1.71903	2.32127	1.22415
C	1.99667	1.16235	1.95073
C	1.04444	0.73576	2.99126
C	1.04427	-0.71876	2.99544
C	-0.13235	-1.41881	3.20821
C	-0.43404	-2.60604	2.41939
C	-1.38186	-3.48452	-0.12182
C	-2.33157	-3.03589	0.8954
C	-1.863	-2.60268	2.12666
C	-2.4544	-1.41606	2.75309
C	-1.38082	-0.68231	3.42485
C	-1.38067	0.70228	3.42083
C	-0.13204	1.43727	3.19995
C	-0.4335	2.61997	2.40424
C	0.47718	3.02918	1.4304
C	2.0496	0.72408	-2.0798
C	-1.87158	3.03034	-1.44581
C	-0.97738	2.60119	-2.4123
C	-1.28024	1.4143	-3.21419
C	-2.46368	0.72304	-3.00951
C	-3.40879	1.17832	-1.98902
C	-3.40202	2.30507	0.20774
C	-2.33094	3.04136	0.87778
C	-1.38114	3.48389	-0.14202
C	-0.02245	3.4777	0.12508
C	0.92134	3.0169	-0.89054
C	0.45845	2.596	-2.12842
C	-0.03088	0.68125	-3.42169
C	-0.03102	-0.70121	-3.41768
C	-1.28053	-1.43279	-3.20594
C	-2.46384	-0.74011	-3.00527
C	-3.40903	-1.18927	-1.98216
C	-3.99476	-0.00359	-1.35581
C	-4.26005	0.00038	0.00398
C	-3.95946	1.18674	0.80594
C	-1.86245	2.61519	2.11152
C	-2.4541	1.43235	2.74483
C	-3.47036	0.73852	2.11034
C	-3.47051	-0.72571	2.11458
C	-3.95971	-1.18139	0.8128
C	-3.4025	-2.30328	0.22111
C	-3.12107	-2.30713	-1.21603
C	-1.8722	-3.03843	-1.42822
C	-0.97792	-2.61507	-2.39718
C	1.04135	1.41353	-2.74244

C	1.04106	-1.42976	-2.7342
C	-3.12059	2.30053	-1.22938
C	4.66882	-0.00036	-0.02679
C	5.37784	-1.20791	-0.01591
C	6.77153	-1.20566	0.00146
C	7.47132	0.0003	0.00927
C	6.77097	1.20596	0.0014
C	5.37729	1.20755	-0.01587
H	4.82666	-2.16127	-0.01839
H	7.31819	-2.15929	0.01058
H	8.56996	0.00056	0.02304
H	7.31719	2.15984	0.01064
H	4.82558	2.1606	-0.0185

C₆₀CCH⁻

C	0.03876	-2.44847	-2.58005
C	-1.38831	-2.14628	-2.58012
C	-1.84869	-0.91669	-3.02642
C	-0.89213	0.08942	-3.48573
C	0.46472	-0.18643	-3.4753
C	0.95593	-1.48754	-3.00532
C	0.33491	-3.22666	-1.38473
C	-0.91505	-3.42724	-0.64604
C	-1.98405	-2.75621	-1.38709
C	-2.99601	-2.10372	-0.70377
C	-2.91524	-0.22763	-2.30131
C	-1.37394	1.40362	-3.05356
C	-0.47334	2.37106	-2.64033
C	0.96063	2.07788	-2.6306
C	1.41545	0.8305	-3.03187
C	2.48467	0.16376	-2.29081
C	2.19916	-1.27783	-2.30094
C	2.47221	-1.98787	-1.13089
C	1.51293	-3.01436	-0.68667
C	-0.91505	-3.40853	0.73837
C	0.3349	-3.18804	1.47137
C	1.51291	-2.99471	0.7678
C	2.4722	-1.95662	1.18421
C	3.07712	-1.38896	0.01878
C	3.65587	-0.00706	0.0001
C	3.06487	0.77142	-1.20025
C	2.5519	2.05056	-0.75828
C	1.54751	2.70797	-1.4584
C	-2.62431	1.20748	-2.32035
C	-0.77092	3.23282	1.38001
C	-1.95559	3.02864	0.69073
C	-2.90742	2.01929	1.15663
C	-2.6243	1.26973	2.28688
C	-1.37394	1.48561	3.01452

C	0.96064	2.14821	2.57352
C	1.54751	2.74639	1.38472
C	0.47979	3.42453	0.64505
C	0.47979	3.40585	-0.73732
C	-0.77092	3.19436	-1.46685
C	-1.95559	3.00888	-0.7723
C	-3.49742	1.37746	-0.01861
C	-3.77169	0.01959	-0.00026
C	-3.47653	-0.77168	1.19461
C	-2.91524	-0.16537	2.30662
C	-1.8487	-0.83459	3.05009
C	-0.89214	0.18357	3.48204
C	0.46472	-0.09246	3.47909
C	1.41545	0.91211	3.00835
C	2.55191	2.07031	0.70261
C	3.06488	0.80358	1.17898
C	2.48467	0.22561	2.28557
C	2.19917	-1.21518	2.3346
C	0.95591	-1.40577	3.0444
C	0.03877	-2.37785	2.64522
C	-1.38833	-2.07579	2.63717
C	-1.98406	-2.71774	1.46105
C	-2.99602	-2.08394	0.76035
C	-2.90741	1.9873	-1.21076
C	-3.47653	-0.80368	-1.17332
C	-0.47334	2.44152	2.5753
C	5.09581	0.01435	-0.0002
C	6.2916	0.01835	-0.00023
H	7.34952	0.01894	-0.00029

3. C₆₀(CHR)

C₆₀CH₂

C	-1.22519	3.16621	-0.65374
C	-1.24233	3.11999	0.82173
C	-0.07039	3.1177	1.54207
C	1.26761	3.30816	0.90884
C	1.28588	3.35767	-0.67045
C	-0.03684	3.20817	-1.34539
C	-2.32884	2.33812	-1.13632
C	-3.02915	1.78163	0.02051
C	-2.35631	2.26419	1.2258
C	-2.23606	1.43032	2.3266
C	0.06735	2.21442	2.67611
C	2.1363	2.2725	1.54144
C	3.00939	1.49143	0.82029
C	3.02648	1.53764	-0.65518
C	2.1698	2.36292	-1.34612
C	1.49149	1.85506	-2.53052
C	0.12786	2.37745	-2.53019
C	-0.91311	1.59296	-3.00133
C	-2.1825	1.57463	-2.28406
C	-3.53646	0.49413	-0.02566
C	-3.36943	-0.31558	-1.23409
C	-2.71195	0.21044	-2.3329
C	-1.7626	-0.61517	-3.08203
C	-0.65011	0.24053	-3.49719
C	0.64216	-0.25444	-3.49744
C	1.7417	0.57606	-3.00214
C	2.67449	-0.2858	-2.28572
C	3.29418	0.18427	-1.13827
C	1.43103	1.69209	2.67577
C	2.26808	-2.55964	1.13131
C	2.10351	-1.79896	2.27613
C	0.82799	-1.82478	2.99485
C	-0.21427	-2.60829	2.52772
C	-0.0389	-3.41336	1.31806
C	1.18541	-3.34491	-0.82332
C	2.29558	-2.48554	-1.23613
C	2.96154	-1.99489	-0.02799
C	3.44424	-0.69797	0.01823
C	3.26678	0.1103	1.22388
C	2.62094	-0.43014	2.32498
C	0.56099	-0.47314	3.48886
C	-0.7312	0.02193	3.48901
C	-1.83321	-0.80536	2.99565
C	-1.58145	-2.0846	2.52813
C	-2.25059	-2.56624	1.31884
C	-1.29785	-3.38879	0.57154
C	-1.28175	-3.34545	-0.81224

C	-0.00581	-3.32427	-1.52944
C	2.15707	-1.65463	-2.33463
C	0.89859	-1.63454	-3.08296
C	-0.15365	-2.44501	-2.69013
C	-1.52078	-1.92124	-2.68954
C	-2.21749	-2.47708	-1.52861
C	-3.11726	-1.69682	-0.82176
C	-3.13423	-1.74261	0.64143
C	-3.39699	-0.38966	1.13335
C	-2.7656	0.06614	2.27784
C	1.67119	0.38586	3.07212
C	-0.98373	1.40287	3.07294
C	1.16841	-3.39072	0.63988
C	1.72988	4.51646	0.16107
H	1.09095	5.42125	0.18192
H	2.80982	4.76296	0.18117

C₆₀CHOH

C	-1.29457	3.0669	-0.63065
C	-1.33374	2.99804	0.84418
C	-0.17251	2.9888	1.58105
C	1.17364	3.19364	0.96859
C	1.21536	3.26696	-0.60344
C	-0.09596	3.12342	-1.30268
C	-2.38726	2.24236	-1.14211
C	-3.10255	1.66551	-0.00455
C	-2.44991	2.13213	1.21806
C	-2.34259	1.28186	2.30783
C	-0.0478	2.06959	2.70319
C	2.03625	2.15067	1.59895
C	2.92544	1.38445	0.88179
C	2.96452	1.4533	-0.59296
C	2.11258	2.28511	-1.28168
C	1.45554	1.79494	-2.48478
C	0.09021	2.31246	-2.49739
C	-0.94043	1.53134	-2.99646
C	-2.22032	1.49703	-2.29911
C	-3.60358	0.37689	-0.07802
C	-3.41513	-0.41357	-1.2961
C	-2.74341	0.13171	-2.37674
C	-1.77944	-0.67867	-3.12385
C	-0.66418	0.18759	-3.50871
C	0.62985	-0.3025	-3.49728
C	1.71856	0.52433	-2.97243
C	2.64399	-0.34508	-2.25593
C	3.24525	0.10915	-1.09226
C	1.3176	1.55212	2.71468
C	2.19545	-2.6725	1.1196
C	2.01063	-1.93011	2.27332

C	0.72449	-1.97148	2.97213
C	-0.30747	-2.75175	2.47748
C	-0.11072	-3.53761	1.25846
C	1.14537	-3.43176	-0.86297
C	2.2582	-2.56201	-1.2459
C	2.90419	-2.08761	-0.02044
C	3.38163	-0.79002	0.05283
C	3.18265	-0.00108	1.26788
C	2.52179	-0.56025	2.35073
C	0.44466	-0.62848	3.48231
C	-0.84939	-0.13839	3.47085
C	-1.94059	-0.9623	2.94851
C	-1.67666	-2.23326	2.46535
C	-2.32565	-2.69889	1.23886
C	-1.35847	-3.50633	0.49349
C	-1.32178	-3.44175	-0.88912
C	-0.03522	-3.40472	-1.58658
C	2.13286	-1.71493	-2.3336
C	0.88562	-1.68785	-3.1003
C	-0.16913	-2.50824	-2.73579
C	-1.53831	-1.98975	-2.74789
C	-2.25015	-2.566	-1.60619
C	-3.16352	-1.79999	-0.90111
C	-3.20231	-1.86827	0.56085
C	-3.47792	-0.52405	1.0694
C	-2.8657	-0.08346	2.23017
C	1.55758	0.24096	3.09511
C	-1.10148	1.24793	3.0721
C	1.10658	-3.50004	0.59897
C	1.63015	4.4386	0.25061
H	0.98355	5.34535	0.27579
O	2.94474	4.85588	0.30482
H	3.52192	4.0769	0.28389

C₆₀CHOCH₃

C	-1.296790	2.993263	-0.545886
C	-1.380306	2.851236	0.921793
C	-0.241244	2.784375	1.689793
C	1.126116	2.997840	1.127930
C	1.215172	3.148959	-0.436524
C	-0.078625	3.063206	-1.180366
C	-2.387214	2.214671	-1.129292
C	-3.144692	1.594148	-0.043314
C	-2.520737	1.987410	1.219389
C	-2.458846	1.081851	2.267299
C	-0.164013	1.808341	2.767185
C	1.954103	1.911534	1.729380
C	2.849377	1.165344	0.998811
C	2.933218	1.307325	-0.468368

C	2.117899	2.188802	-1.138902
C	1.487056	1.769553	-2.382838
C	0.130488	2.309592	-2.408131
C	-0.897602	1.572653	-2.975186
C	-2.197863	1.525596	-2.317222
C	-3.663795	0.319741	-0.196181
C	-3.452166	-0.411742	-1.446870
C	-2.740340	0.175260	-2.478919
C	-1.767825	-0.613120	-3.238372
C	-0.628165	0.251863	-3.546935
C	0.657141	-0.260227	-3.522970
C	1.743152	0.520352	-2.926556
C	2.633000	-0.400193	-2.228974
C	3.206400	-0.015176	-1.027065
C	1.192526	1.268530	2.791604
C	2.048433	-2.885912	1.010347
C	1.841707	-2.199063	2.194380
C	0.535125	-2.253088	2.853104
C	-0.494189	-2.989649	2.290512
C	-0.274322	-3.716769	1.039449
C	1.045047	-3.526357	-1.037286
C	2.182382	-2.658062	-1.343796
C	2.799434	-2.256977	-0.077962
C	3.294540	-0.973019	0.074457
C	3.072631	-0.242407	1.321736
C	2.372130	-0.843972	2.355681
C	0.262001	-0.932528	3.422287
C	-1.023397	-0.420574	3.399190
C	-2.111723	-1.198121	2.804904
C	-1.854042	-2.447637	2.265668
C	-2.474068	-2.839801	0.999180
C	-1.498382	-3.625522	0.241750
C	-1.420084	-3.492320	-1.134225
C	-0.113231	-3.442701	-1.791989
C	2.102522	-1.755265	-2.390239
C	0.878869	-1.668141	-3.189703
C	-0.199040	-2.487476	-2.897603
C	-1.558863	-1.945439	-2.922540
C	-2.312972	-2.565701	-1.832212
C	-3.234435	-1.820373	-1.115556
C	-3.317207	-1.961204	0.339344
C	-3.586150	-0.639626	0.907270
C	-3.001248	-0.268502	2.105834
C	1.399573	-0.064216	3.111872
C	-1.241281	0.987979	3.063851
C	0.962255	-3.667191	0.417673
C	1.599263	4.277084	0.478125
H	0.931412	5.164083	0.539746
O	2.958762	4.594803	0.504849
C	3.292742	5.539618	1.519673

H	2.737897	6.496378	1.361206
H	3.070630	5.122293	2.531256
H	4.393292	5.690480	1.384052

C₆₀CHNH₂

C	-1.26746	3.07994	-0.61473
C	-1.31502	3.00082	0.85935
C	-0.15638	2.97476	1.60028
C	1.19287	3.17012	0.99479
C	1.24412	3.25636	-0.57046
C	-0.06485	3.13156	-1.27999
C	-2.3643	2.26818	-1.13764
C	-3.0902	1.68914	-0.00793
C	-2.43995	2.1416	1.2214
C	-2.34515	1.2824	2.30545
C	-0.04543	2.04731	2.71733
C	2.04431	2.11881	1.62328
C	2.93202	1.35018	0.90653
C	2.97946	1.42939	-0.5673
C	2.13757	2.27311	-1.25351
C	1.4822	1.7977	-2.46338
C	0.12125	2.32711	-2.47908
C	-0.91338	1.55838	-2.98931
C	-2.19724	1.52978	-2.29908
C	-3.60149	0.4053	-0.09327
C	-3.41335	-0.37788	-1.31611
C	-2.73144	0.16953	-2.38929
C	-1.77043	-0.64353	-3.13732
C	-0.64591	0.21606	-3.51001
C	0.64382	-0.28514	-3.49566
C	1.73687	0.52853	-2.95936
C	2.65132	-0.35411	-2.24487
C	3.25077	0.08637	-1.07495
C	1.31551	1.5183	2.73186
C	2.1656	-2.702	1.11133
C	1.98122	-1.96628	2.26939
C	0.69118	-2.00166	2.96129
C	-0.34485	-2.76955	2.45588
C	-0.14858	-3.54832	1.23226
C	1.11922	-3.43785	-0.88198
C	2.24138	-2.57495	-1.25293
C	2.88514	-2.11503	-0.02081
C	3.37344	-0.82221	0.06429
C	3.17514	-0.04021	1.28408
C	2.50378	-0.60156	2.35942
C	0.42018	-0.65999	3.47965
C	-0.86963	-0.1589	3.46529
C	-1.96511	-0.96971	2.9316
C	-1.70952	-2.23937	2.44062

C	-2.3562	-2.69065	1.20759
C	-1.3921	-3.5009	0.46127
C	-1.34779	-3.42664	-0.92064
C	-0.05742	-3.39552	-1.61131
C	2.12879	-1.71885	-2.33498
C	0.8857	-1.67553	-3.10769
C	-0.17783	-2.4896	-2.75458
C	-1.54246	-1.95938	-2.76982
C	-2.26501	-2.53781	-1.63598
C	-3.17549	-1.7692	-0.92997
C	-3.22233	-1.84771	0.53124
C	-3.48923	-0.50493	1.04816
C	-2.87915	-0.07785	2.21511
C	1.54251	0.20256	3.1044
C	-1.10805	1.2323	3.07529
C	1.07236	-3.51635	0.57922
C	1.67286	4.42797	0.2787
H	0.9617	5.29119	0.31524
N	3.01142	4.8764	0.27893
H	3.21537	5.43088	1.08581
H	3.67603	4.13664	0.17191

C₆₀CHNHCH₃

C	-1.31839	2.96982	-0.62101
C	-1.39526	2.86624	0.85036
C	-0.25163	2.82466	1.61354
C	1.11021	3.02698	1.03843
C	1.19231	3.13838	-0.52414
C	-0.10268	3.02901	-1.26137
C	-2.40663	2.17	-1.17897
C	-3.15617	1.57421	-0.07368
C	-2.52923	2.00424	1.17562
C	-2.45811	1.12679	2.24681
C	-0.16512	1.87825	2.71671
C	1.946	1.96218	1.66536
C	2.84597	1.20319	0.95365
C	2.9227	1.30673	-0.51743
C	2.09655	2.16416	-1.20577
C	1.46414	1.71082	-2.43617
C	0.10507	2.24423	-2.46989
C	-0.9212	1.4871	-3.0133
C	-2.2185	1.45063	-2.34913
C	-3.66892	0.29343	-0.19062
C	-3.4586	-0.46973	-1.42246
C	-2.75421	0.09359	-2.47263
C	-1.78063	-0.70958	-3.21508
C	-0.64682	0.15293	-3.55104
C	0.64113	-0.35207	-3.51961
C	1.72541	0.44941	-2.94828

C	2.62331	-0.4476	-2.2308
C	3.20052	-0.02836	-1.04202
C	1.19397	1.34524	2.74917
C	2.06542	-2.84981	1.07537
C	1.86001	-2.13297	2.24171
C	0.55643	-2.17629	2.90731
C	-0.4713	-2.93273	2.36877
C	-0.25281	-3.69152	1.1364
C	1.05685	-3.54931	-0.95025
C	2.18829	-2.68353	-1.28447
C	2.80865	-2.24604	-0.03234
C	3.29834	-0.95618	0.08403
C	3.07788	-0.19403	1.31254
C	2.38407	-0.77144	2.3649
C	0.27859	-0.8427	3.44262
C	-1.00944	-0.33782	3.41123
C	-2.09616	-1.13652	2.84252
C	-1.83408	-2.39853	2.33547
C	-2.45735	-2.82732	1.08252
C	-1.48071	-3.62772	0.3419
C	-1.40888	-3.53052	-1.03744
C	-0.10502	-3.49152	-1.70187
C	2.09927	-1.80916	-2.35403
C	0.87181	-1.74944	-3.15029
C	-0.20053	-2.5663	-2.83195
C	-1.56327	-2.03204	-2.86525
C	-2.30955	-2.62728	-1.75575
C	-3.23189	-1.86797	-1.05506
C	-3.30783	-1.97075	0.40343
C	-3.58156	-0.63606	0.93739
C	-2.99362	-0.23025	2.12315
C	1.41026	0.02283	3.10409
C	-1.23664	1.06036	3.03996
C	0.9809	-3.65208	0.50823
C	1.60422	4.29575	0.35381
H	0.89356	5.15861	0.39184
N	2.95014	4.73778	0.37622
H	3.60277	3.97873	0.31527
C	3.28262	5.66162	1.42884
H	3.2068	5.21619	2.45826
H	4.33765	6.00638	1.26284
H	2.59939	6.54996	1.37577

C₆₀CHCH₃

C	-1.19966	3.03077	-0.90119
C	-1.32313	3.22767	0.57445
C	0.0261	3.25309	1.38394
C	1.27514	3.07739	0.5836
C	1.27851	3.03423	-0.79115

C	0.01262	3.01038	-1.55064
C	-2.26501	2.14745	-1.35332
C	-2.96225	1.64009	-0.17498
C	-2.32801	2.21054	1.00532
C	-2.16222	1.42708	2.12397
C	0.14674	2.25713	2.49004
C	2.19941	2.23156	1.32518
C	3.11735	1.4292	0.66566
C	3.13894	1.40812	-0.79205
C	2.23644	2.18744	-1.4991
C	1.58103	1.64125	-2.68674
C	0.21008	2.14927	-2.71483
C	-0.81642	1.33361	-3.16512
C	-2.09269	1.33105	-2.46018
C	-3.45021	0.3427	-0.16602
C	-3.26584	-0.52162	-1.33359
C	-2.6051	-0.04059	-2.45023
C	-1.63871	-0.88712	-3.15149
C	-0.53246	-0.03671	-3.59555
C	0.76557	-0.51666	-3.56233
C	1.85284	0.34779	-3.09917
C	2.79663	-0.47841	-2.34377
C	3.42304	0.0378	-1.22239
C	1.50194	1.72419	2.50338
C	2.39107	-2.59533	1.17062
C	2.21414	-1.77969	2.27602
C	0.93293	-1.77521	2.98494
C	-0.10053	-2.58784	2.55135
C	0.08739	-3.45252	1.3858
C	1.32281	-3.47915	-0.74974
C	2.42943	-2.63178	-1.19731
C	3.09026	-2.0863	-0.01074
C	3.5751	-0.78891	-0.02339
C	3.38753	0.07229	1.14512
C	2.72656	-0.40874	2.26164
C	0.65497	-0.40042	3.40486
C	-0.63952	0.09344	3.36009
C	-1.72986	-0.76943	2.90743
C	-1.47037	-2.07187	2.51581
C	-2.1316	-2.6261	1.33278
C	-1.16789	-3.47616	0.63268
C	-1.14447	-3.50131	-0.75187
C	0.13565	-3.50151	-1.46199
C	2.28776	-1.85041	-2.33201
C	1.03249	-1.87405	-3.08513
C	-0.01341	-2.6778	-2.66293
C	-1.38594	-2.17061	-2.6963
C	-2.08512	-2.67964	-1.51493
C	-2.99958	-1.8779	-0.85203
C	-3.02256	-1.84972	0.61179

C	-3.30032	-0.47493	1.03181
C	-2.66576	0.05528	2.14439
C	1.75941	0.44083	2.95955
C	-0.89628	1.4509	2.88346
C	1.29838	-3.45529	0.71376
C	-0.88162	4.44791	1.32978
C	-1.6191	4.89251	2.54503
H	-1.9672	4.02028	3.1522
H	-0.95281	5.5261	3.18124
H	-2.51091	5.49711	2.24628
H	-0.5249	5.30114	0.70837

C₆₀CHCH=CH₂

C	-1.24195	3.03889	-0.47853
C	-1.33441	2.87297	0.98573
C	-0.19972	2.7768	1.75717
C	1.17294	2.97999	1.20378
C	1.27131	3.15651	-0.35412
C	-0.019	3.10112	-1.10495
C	-2.34019	2.28572	-1.08041
C	-3.11153	1.65732	-0.00868
C	-2.48819	2.02013	1.26344
C	-2.44376	1.09599	2.29584
C	-0.14134	1.78161	2.81816
C	1.98261	1.87163	1.79218
C	2.8718	1.12588	1.05336
C	2.96426	1.29181	-0.41094
C	2.1633	2.1959	-1.06953
C	1.53321	1.807	-2.3235
C	0.18469	2.36672	-2.34538
C	-0.8508	1.65432	-2.92998
C	-2.1549	1.6144	-2.2791
C	-3.64755	0.39307	-0.18578
C	-3.44019	-0.31981	-1.44785
C	-2.71527	0.27475	-2.46637
C	-1.75024	-0.51421	-3.23475
C	-0.59706	0.33981	-3.5231
C	0.68076	-0.19086	-3.50239
C	1.77463	0.56393	-2.88749
C	2.64828	-0.38079	-2.2019
C	3.2214	-0.02459	-0.99097
C	1.2072	1.22193	2.83973
C	2.01357	-2.9131	0.99141
C	1.81082	-2.24373	2.1861
C	0.50046	-2.29053	2.83792
C	-0.53635	-3.00277	2.25807
C	-0.32072	-3.71141	0.99571
C	1.01106	-3.50422	-1.07143
C	2.1619	-2.64689	-1.35783

C	2.77852	-2.2763	-0.08252
C	3.29104	-1.00229	0.09421
C	3.07341	-0.29016	1.35273
C	2.35941	-0.8992	2.37302
C	0.24314	-0.97622	3.42844
C	-1.0347	-0.4456	3.40805
C	-2.13101	-1.19755	2.79569
C	-1.88831	-2.44122	2.23635
C	-2.50777	-2.80294	0.96055
C	-1.53959	-3.58927	0.19417
C	-1.45289	-3.43368	-1.17895
C	-0.14232	-3.39124	-1.82981
C	2.0997	-1.72531	-2.38897
C	0.88122	-1.60721	-3.19238
C	-0.20945	-2.4161	-2.91923
C	-1.56142	-1.85455	-2.94098
C	-2.32936	-2.48277	-1.86495
C	-3.24366	-1.73684	-1.1398
C	-3.33534	-1.90137	0.3121
C	-3.58852	-0.58602	0.90138
C	-3.00414	-0.24367	2.10873
C	1.39418	-0.11885	3.13798
C	-1.23129	0.97148	3.09603
C	0.91938	-3.66875	0.38048
C	1.67993	4.25584	0.58834
H	0.98811	5.12843	0.64352
C	3.09595	4.61728	0.71868
H	3.80694	3.77413	0.66735
C	3.51029	5.87189	0.88771
H	4.57582	6.12137	0.98319
H	2.82434	6.72815	0.9421

C₆₀CHPh

C	-1.40878	2.77786	-0.59107
C	-1.58878	2.60338	0.86395
C	-0.50363	2.45043	1.69499
C	0.9059	2.60034	1.22054
C	1.09787	2.7867	-0.3289
C	-0.15186	2.79173	-1.14929
C	-2.50433	2.07945	-1.26024
C	-3.36016	1.47647	-0.23928
C	-2.79236	1.80016	1.06885
C	-2.84517	0.86604	2.09178
C	-0.54713	1.44457	2.74628
C	1.63241	1.45135	1.83922
C	2.52575	0.6726	1.14093
C	2.70521	0.84684	-0.31391
C	1.98455	1.79289	-1.00542
C	1.40688	1.44158	-2.29561

C	0.08719	2.05992	-2.38466
C	-0.94473	1.39919	-3.03283
C	-2.28311	1.41123	-2.45451
C	-3.94037	0.23878	-0.45942
C	-3.69532	-0.47149	-1.71621
C	-2.89035	0.09938	-2.68706
C	-1.91992	-0.72464	-3.41052
C	-0.7165	0.08013	-3.62605
C	0.53394	-0.50643	-3.54147
C	1.62417	0.19401	-2.8595
C	2.41676	-0.79447	-2.13806
C	2.93701	-0.47439	-0.89379
C	0.77266	0.82632	2.8351
C	1.498	-3.32416	0.98753
C	1.25932	-2.65696	2.17679
C	-0.08564	-2.65155	2.75563
C	-1.11912	-3.31227	2.11228
C	-0.86559	-4.01867	0.85572
C	0.58546	-3.85236	-1.13337
C	1.78657	-3.04419	-1.34708
C	2.34775	-2.71234	-0.03597
C	2.90451	-1.46367	0.18262
C	2.64929	-0.75357	1.43526
C	1.85486	-1.33961	2.4083
C	-0.31742	-1.33232	3.34583
C	-1.56798	-0.74588	3.26194
C	-2.66073	-1.44331	2.58239
C	-2.44211	-2.6915	2.02321
C	-3.00572	-3.01431	0.71158
C	-2.0321	-3.83585	-0.00965
C	-1.86343	-3.67222	-1.37418
C	-0.51849	-3.68196	-1.95218
C	1.82132	-2.11182	-2.36979
C	0.65513	-1.93298	-3.23696
C	-0.48314	-2.69532	-3.0327
C	-1.80611	-2.07452	-3.12182
C	-2.65863	-2.6776	-2.09628
C	-3.578	-1.89845	-1.41373
C	-3.75636	-2.07147	0.02909
C	-3.98392	-0.75145	0.61835
C	-3.45239	-0.44586	1.85953
C	0.88406	-0.52398	3.12812
C	-1.68504	0.68108	2.95539
C	0.40711	-4.02538	0.30949
C	1.48549	3.86205	0.64554
H	0.80851	4.75123	0.66905
C	2.88549	4.25597	0.87092
C	3.34027	4.49348	2.17431
C	4.64731	4.92647	2.3892
C	5.50571	5.12847	1.30823

C	5.0549	4.89562	0.00912
C	3.74906	4.46076	-0.2116
H	2.66441	4.33436	3.02794
H	5.00072	5.10845	3.41499
H	6.53701	5.47026	1.4805
H	5.72952	5.05351	-0.8454
H	3.39494	4.27222	-1.23663

C₆₀CHCCH

C	-1.26068	3.04829	-0.60175
C	-1.32375	2.95517	0.87063
C	-0.17416	2.90281	1.62387
C	1.18662	3.08308	1.03307
C	1.25369	3.18221	-0.5323
C	-0.05081	3.08486	-1.25486
C	-2.36643	2.26132	-1.14363
C	-3.11334	1.68379	-0.02694
C	-2.46741	2.11229	1.21305
C	-2.3977	1.24102	2.28908
C	-0.08927	1.96212	2.73157
C	2.01431	2.01037	1.66096
C	2.8921	1.2325	0.94229
C	2.95519	1.32561	-0.52995
C	2.13765	2.19242	-1.21723
C	1.48509	1.73875	-2.43753
C	0.13323	2.29046	-2.46075
C	-0.90963	1.54515	-2.98849
C	-2.20059	1.53191	-2.3108
C	-3.64577	0.4099	-0.13032
C	-3.45904	-0.3641	-1.35919
C	-2.75728	0.18211	-2.42013
C	-1.80309	-0.63983	-3.16714
C	-0.66039	0.20385	-3.52033
C	0.62049	-0.31933	-3.49823
C	1.72207	0.47008	-2.94349
C	2.61388	-0.43548	-2.22893
C	3.20853	-0.01688	-1.04878
C	1.26258	1.4104	2.75444
C	2.05502	-2.80818	1.0984
C	1.87189	-2.08099	2.26206
C	0.57473	-2.10102	2.94102
C	-0.46927	-2.84591	2.41787
C	-0.27438	-3.61566	1.18834
C	1.01584	-3.50588	-0.91236
C	2.15624	-2.65881	-1.26368
C	2.79553	-2.2224	-0.02075
C	3.30447	-0.93892	0.08223
C	3.10755	-0.16593	1.30789
C	2.41675	-0.72638	2.37104

C	0.32186	-0.76003	3.47036
C	-0.95904	-0.23688	3.44883
C	-2.06292	-1.02328	2.89628
C	-1.82443	-2.29219	2.39484
C	-2.46657	-2.71981	1.15104
C	-1.50922	-3.53907	0.40584
C	-1.45005	-3.45176	-0.97476
C	-0.15263	-3.436	-1.6526
C	2.06903	-1.79009	-2.33799
C	0.83457	-1.71759	-3.12213
C	-0.2462	-2.51671	-2.78767
C	-1.60135	-1.96299	-2.81076
C	-2.34483	-2.54016	-1.68988
C	-3.24893	-1.76312	-0.98489
C	-3.31148	-1.85543	0.47491
C	-3.56025	-0.51347	1.00287
C	-2.9544	-0.10879	2.17998
C	1.46242	0.08692	3.11518
C	-1.16927	1.16197	3.07059
C	0.95328	-3.5982	0.54747
C	1.66615	4.33463	0.34568
H	0.9615	5.20313	0.37044
C	3.01978	4.73926	0.4291
C	4.15379	5.11328	0.50149
H	5.16004	5.44528	0.56522

4. C₆₀(CR⁻) open

C₆₀CH⁻ open

C	0.	0.	0.
C	1.4804	0.	0.
C	2.253	1.1759	0.
C	1.7846	2.4925	0.2159
C	-0.5137	2.5154	0.2306
C	-0.8382	1.0989	-0.0038
C	-0.4408	-1.1964	-0.7299
C	0.7352	-1.8885	-1.2334
C	1.9093	-1.1294	-0.7981
C	3.0166	-1.0791	-1.6506
C	3.3364	1.2621	-1.0109
C	2.0851	3.2539	-0.9962
C	1.1892	3.9589	-1.8151
C	-0.3081	3.9424	-1.7669
C	-1.1335	3.2599	-0.8769
C	-2.2112	2.4307	-1.4039
C	-2.0537	1.0944	-0.8177
C	-2.4449	-0.0257	-1.5291
C	-1.617	-1.2159	-1.4691
C	0.7037	-2.5194	-2.467
C	-0.5189	-2.4889	-3.2712
C	-1.65	-1.8595	-2.7824
C	-2.4694	-1.0298	-3.6699
C	-2.9636	0.107	-2.8928
C	-3.0491	1.36	-3.4736
C	-2.6453	2.5444	-2.7119
C	-1.926	3.437	-3.6067
C	-0.7886	4.0925	-3.1453
C	3.2337	2.5778	-1.6218
C	1.5161	3.0777	-5.8725
C	2.6733	3.0187	-5.1152
C	3.4734	1.7889	-5.102
C	3.0505	0.6791	-5.8138
C	1.8227	0.7423	-6.6074
C	-0.3811	1.8544	-6.5844
C	-0.8464	2.9845	-5.7801
C	0.3287	3.7229	-5.3174
C	0.3552	4.2373	-4.0309
C	1.5607	4.152	-3.2106
C	2.7097	3.5984	-3.7751
C	4.0194	1.6272	-3.7545
C	4.0958	0.3687	-3.1816
C	3.6285	-0.8013	-3.9241
C	3.1294	-0.6526	-5.2072
C	1.9494	-1.4089	-5.6271
C	1.145	-0.5498	-6.4961
C	-0.2384	-0.6046	-6.4415

C	-1.0226	0.6296	-6.4927
C	-1.9403	2.8431	-4.9444
C	-2.6283	1.5517	-4.8603
C	-2.1741	0.4737	-5.6034
C	-2.0945	-0.8543	-4.9921
C	-0.8961	-1.5184	-5.5072
C	-0.1346	-2.3204	-4.6724
C	1.3277	-2.2656	-4.7326
C	1.844	-2.4105	-3.3728
C	2.9618	-1.6957	-2.9698
C	3.5596	2.7596	-2.9509
C	3.7284	0.182	-1.776
C	1.0807	1.9121	-6.6411
C	0.5959	3.022	0.8389
H	0.6318	3.9998	1.3342

C₆₀COH⁻ open

C	0.	0.	0.
C	1.4907	0.	0.
C	2.2834	1.1515	0.
C	1.8623	2.4968	0.2223
C	-0.5001	2.5114	0.221
C	-0.8293	1.1098	-0.0062
C	-0.4332	-1.1831	-0.7397
C	0.7437	-1.8894	-1.2279
C	1.9192	-1.1449	-0.7804
C	3.0437	-1.1135	-1.6108
C	3.3906	1.221	-0.9754
C	2.1846	3.2429	-0.9918
C	1.3071	3.9457	-1.8266
C	-0.195	3.9421	-1.799
C	-1.0303	3.2555	-0.9173
C	-2.1244	2.4513	-1.463
C	-2.0203	1.1199	-0.8641
C	-2.4065	0.0027	-1.5833
C	-1.5989	-1.1976	-1.5028
C	0.7251	-2.5276	-2.4574
C	-0.4817	-2.4879	-3.2835
C	-1.6122	-1.8414	-2.8152
C	-2.4032	-1.004	-3.7222
C	-2.8949	0.1421	-2.9577
C	-2.9481	1.3949	-3.5428
C	-2.5341	2.5742	-2.7789
C	-1.7916	3.4543	-3.6617
C	-0.6496	4.0929	-3.1784
C	3.3268	2.5393	-1.5916
C	1.6813	3.0374	-5.8707
C	2.8267	2.9657	-5.0971
C	3.607	1.7238	-5.0657

C	3.1789	0.6171	-5.7798
C	1.9651	0.6953	-6.5931
C	-0.2222	1.8403	-6.6088
C	-0.6836	2.9801	-5.8171
C	0.494	3.7018	-5.3362
C	0.5085	4.2203	-4.0515
C	1.7016	4.1272	-3.2163
C	2.8524	3.5519	-3.759
C	4.1283	1.5601	-3.7089
C	4.1759	0.3038	-3.1296
C	3.7032	-0.8627	-3.8742
C	3.2276	-0.7128	-5.1664
C	2.0431	-1.4529	-5.6017
C	1.2666	-0.5862	-6.4885
C	-0.1181	-0.6202	-6.4557
C	-0.8832	0.6251	-6.525
C	-1.7917	2.8576	-4.997
C	-2.5014	1.5766	-4.9231
C	-2.0514	0.4895	-5.6548
C	-2.0023	-0.838	-5.0378
C	-0.8053	-1.5209	-5.5299
C	-0.0704	-2.3299	-4.6778
C	1.3932	-2.2959	-4.714
C	1.8837	-2.4389	-3.3444
C	3.0056	-1.7411	-2.9282
C	3.6751	2.7061	-2.9189
C	3.7806	0.1291	-1.7295
C	1.2412	1.8761	-6.6424
C	0.6551	2.9762	0.8333
O	0.639	4.0884	1.5854
H	1.5589	4.3779	1.7291

C₆₀COCH₃⁻ open

C	0.	0.	0.
C	1.4913	0.	0.
C	2.319	1.1122	0.
C	1.9908	2.5095	0.2419
C	-0.3773	2.4971	0.2204
C	-0.7953	1.1502	0.0035
C	-0.4283	-1.1432	-0.7819
C	0.7475	-1.8831	-1.2359
C	1.9244	-1.1767	-0.7476
C	3.0879	-1.1851	-1.5158
C	3.5027	1.1306	-0.8676
C	2.4899	3.2548	-0.9125
C	1.6527	3.9479	-1.787
C	0.1508	3.9592	-1.8117
C	-0.7227	3.2525	-0.9736
C	-1.8606	2.5401	-1.5746

C	-1.9095	1.2187	-0.9649
C	-2.2984	0.1269	-1.7199
C	-1.5565	-1.1128	-1.6083
C	0.7635	-2.5165	-2.4681
C	-0.3986	-2.4286	-3.3504
C	-1.5213	-1.7361	-2.9274
C	-2.2263	-0.8576	-3.868
C	-2.701	0.3045	-3.1175
C	-2.6614	1.5629	-3.6928
C	-2.2119	2.7091	-2.9007
C	-1.3965	3.562	-3.7408
C	-0.246	4.141	-3.1985
C	3.5902	2.4634	-1.4638
C	2.1374	3.009	-5.81
C	3.2484	2.8872	-4.9939
C	3.9641	1.6091	-4.9281
C	3.5162	0.5233	-5.663
C	2.3444	0.6579	-6.5287
C	0.2145	1.9012	-6.6339
C	-0.2278	3.058	-5.857
C	0.9583	3.7244	-5.3228
C	0.9453	4.2381	-4.0361
C	2.1053	4.1088	-3.166
C	3.2489	3.477	-3.6555
C	4.416	1.4229	-3.5501
C	4.3711	0.1672	-2.9706
C	3.8813	-0.9775	-3.7382
C	3.4747	-0.8071	-5.0516
C	2.2786	-1.4925	-5.5423
C	1.5847	-0.5908	-6.4619
C	0.1996	-0.5619	-6.4897
C	-0.5042	0.7171	-6.5871
C	-1.3707	2.9793	-5.0797
C	-2.1453	1.7335	-5.0506
C	-1.715	0.6312	-5.77
C	-1.7561	-0.7012	-5.1613
C	-0.5702	-1.4349	-5.6034
C	0.0861	-2.2788	-4.7212
C	1.55	-2.3076	-4.6904
C	1.967	-2.47	-3.2986
C	3.0972	-1.8219	-2.8314
C	3.9973	2.5965	-2.7799
C	3.8899	0.0183	-1.5945
C	1.6782	1.8708	-6.6051
C	0.8204	2.9713	0.8463
O	0.7399	4.0345	1.6556
C	1.9679	4.7227	1.9434
H	2.7927	3.992	2.13
H	2.2201	5.3825	1.0784
H	1.725	5.3201	2.8561

C₆₀CNH₂⁻ open

C	0.	0.	0.
C	1.4926	0.	0.
C	2.3071	1.1315	0.
C	1.9347	2.5029	0.2174
C	-0.4421	2.5029	0.2174
C	-0.8145	1.1315	0.
C	-0.4305	-1.159	-0.7643
C	0.7463	-1.8823	-1.2355
C	1.923	-1.159	-0.7643
C	3.0703	-1.151	-1.563
C	3.454	1.1737	-0.9239
C	2.3367	3.2451	-0.9596
C	1.4959	3.9596	-1.818
C	-0.0033	3.9596	-1.818
C	-0.8442	3.2451	-0.9596
C	-1.9727	2.4985	-1.5326
C	-1.9614	1.1737	-0.9239
C	-2.3496	0.0696	-1.6623
C	-1.5777	-1.151	-1.563
C	0.7463	-2.5183	-2.4663
C	-0.4368	-2.4537	-3.3235
C	-1.5638	-1.7827	-2.8797
C	-2.3084	-0.923	-3.8065
C	-2.7906	0.2322	-3.0503
C	-2.7923	1.4887	-3.6305
C	-2.3556	2.6508	-2.8532
C	-1.578	3.5177	-3.7136
C	-0.43	4.127	-3.1988
C	3.4653	2.4985	-1.5326
C	1.9293	3.0257	-5.8476
C	3.0564	2.9274	-5.0499
C	3.8015	1.6645	-4.9994
C	3.3626	0.5687	-5.724
C	2.171	0.6771	-6.5659
C	0.0141	1.876	-6.6299
C	-0.4367	3.0257	-5.8476
C	0.7463	3.7182	-5.3385
C	0.7463	4.2373	-4.0539
C	1.9226	4.127	-3.1988
C	3.0705	3.5177	-3.7136
C	4.2849	1.4887	-3.6306
C	4.2832	0.2322	-3.0503
C	3.801	-0.923	-3.8065
C	3.3625	-0.762	-5.1105
C	2.1711	-1.4726	-5.5753
C	1.4391	-0.5868	-6.4807
C	0.0534	-0.5868	-6.4807

C	-0.6785	0.6771	-6.5659
C	-1.5639	2.9274	-5.0499
C	-2.309	1.6645	-4.9994
C	-1.8701	0.5687	-5.7239
C	-1.87	-0.762	-5.1105
C	-0.6785	-1.4726	-5.5752
C	0.014	-2.3002	-4.7054
C	1.4785	-2.3002	-4.7054
C	1.9294	-2.4537	-3.3235
C	3.0563	-1.7827	-2.8797
C	3.8481	2.6508	-2.8532
C	3.8422	0.0696	-1.6623
C	1.4785	1.876	-6.6299
C	0.7463	2.9453	0.8837
N	0.7463	3.8392	1.8632
H	1.6032	4.2166	2.2033
H	-0.1106	4.2166	2.2033

C₆₀CNHCH₃⁻ open

C	0.	0.	0.
C	1.4973	0.	0.
C	2.3329	1.1201	0.
C	1.9358	2.4979	0.1889
C	-0.4393	2.4982	0.1856
C	-0.8352	1.1205	-0.0014
C	-0.4277	-1.1666	-0.7561
C	0.7486	-1.8936	-1.2204
C	1.925	-1.1664	-0.7567
C	3.0726	-1.1693	-1.5551
C	3.4636	1.1587	-0.939
C	2.308	3.2119	-1.0035
C	1.4915	3.9369	-1.8713
C	-0.0011	3.9381	-1.8713
C	-0.8174	3.2136	-1.0026
C	-1.9618	2.4745	-1.5635
C	-1.9681	1.1577	-0.9383
C	-2.3524	0.0464	-1.6669
C	-1.5758	-1.1704	-1.5538
C	0.7484	-2.5452	-2.4431
C	-0.4348	-2.4917	-3.3005
C	-1.5619	-1.8166	-2.8638
C	-2.3075	-0.968	-3.8001
C	-2.7906	0.195	-3.0568
C	-2.7902	1.4459	-3.649
C	-2.3502	2.6157	-2.8841
C	-1.5787	3.4752	-3.7569
C	-0.4316	4.0937	-3.2509
C	3.4536	2.4752	-1.5647
C	1.9283	2.9607	-5.886

C	3.0554	2.8712	-5.0868
C	3.8006	1.609	-5.0219
C	3.3624	0.5051	-5.7346
C	2.1708	0.6039	-6.5777
C	0.0133	1.8013	-6.6542
C	-0.4379	2.9599	-5.8856
C	0.7451	3.6592	-5.3855
C	0.7451	4.1957	-4.1081
C	1.9218	4.0935	-3.251
C	3.0693	3.4762	-3.7575
C	4.283	1.4483	-3.6507
C	4.2851	0.1973	-3.0587
C	3.8024	-0.966	-3.8019
C	3.3632	-0.819	-5.1073
C	2.1718	-1.535	-5.5638
C	1.4394	-0.6592	-6.4787
C	0.0537	-0.6597	-6.4782
C	-0.6788	0.6028	-6.577
C	-1.5646	2.8697	-5.0858
C	-2.3086	1.6068	-5.0204
C	-1.8699	0.5032	-5.7333
C	-1.8692	-0.8209	-5.1057
C	-0.6776	-1.536	-5.563
C	0.0155	-2.3539	-4.6845
C	1.4799	-2.3534	-4.6849
C	1.9312	-2.4909	-3.3013
C	3.0582	-1.8154	-2.8653
C	3.8418	2.6173	-2.8853
C	3.8482	0.0479	-1.6685
C	1.4778	1.8018	-6.6546
C	0.7482	2.7621	0.9485
N	0.7187	3.06	2.2418
H	-0.1713	3.137	2.6947
C	1.891	3.2042	3.062
H	1.8514	4.1938	3.5901
H	1.9243	2.3791	3.823
H	2.8156	3.1544	2.4223

$C_{60}CN(CH_3)_2^-$ open

C	0.	0.	0.
C	1.4939	0.	0.
C	2.3174	1.1276	0.
C	1.9322	2.5013	0.2026
C	-0.4382	2.5013	0.2026
C	-0.8235	1.1276	0.
C	-0.4296	-1.1611	-0.7624
C	0.7469	-1.8856	-1.2313
C	1.9235	-1.1611	-0.7623
C	3.071	-1.1573	-1.5611

C	3.4565	1.1689	-0.9317
C	2.3171	3.2296	-0.9795
C	1.494	3.9553	-1.8428
C	0.0002	3.9553	-1.8429
C	-0.823	3.2296	-0.9796
C	-1.9624	2.4899	-1.5473
C	-1.9626	1.169	-0.9318
C	-2.35	0.0623	-1.6662
C	-1.5771	-1.1572	-1.5612
C	0.747	-2.5272	-2.4592
C	-0.4361	-2.4667	-3.3167
C	-1.5629	-1.7939	-2.8756
C	-2.3075	-0.9381	-3.8062
C	-2.7895	0.2203	-3.0549
C	-2.7894	1.4749	-3.6394
C	-2.3498	2.6397	-2.867
C	-1.5769	3.5046	-3.7331
C	-0.4295	4.1187	-3.2222
C	3.4564	2.4899	-1.5472
C	1.9301	3.0029	-5.8649
C	3.057	2.9078	-5.0661
C	3.8015	1.6448	-5.0094
C	3.3631	0.5458	-5.7295
C	2.1718	0.6506	-6.5722
C	0.0149	1.8493	-6.6414
C	-0.4359	3.0029	-5.865
C	0.7471	3.6983	-5.3597
C	0.7471	4.2258	-4.0786
C	1.9237	4.1186	-3.2222
C	3.0711	3.5045	-3.733
C	4.2835	1.4747	-3.6392
C	4.2835	0.2202	-3.0548
C	3.8015	-0.9382	-3.806
C	3.3631	-0.7824	-5.1107
C	2.1717	-1.495	-5.5726
C	1.4399	-0.6129	-6.4817
C	0.0542	-0.6129	-6.4818
C	-0.6776	0.6507	-6.5723
C	-1.5628	2.9079	-5.0662
C	-2.3074	1.6449	-5.0095
C	-1.869	0.5459	-5.7296
C	-1.869	-0.7823	-5.1108
C	-0.6777	-1.495	-5.5726
C	0.0148	-2.3191	-4.6994
C	1.4792	-2.3191	-4.6993
C	1.93	-2.4667	-3.3166
C	3.0569	-1.794	-2.8755
C	3.844	2.6396	-2.8669
C	3.844	0.0622	-1.6661
C	1.4793	1.8493	-6.6414

C	0.747	2.8441	0.9423
N	0.747	3.4011	2.1498
C	1.9746	3.7218	2.8462
H	2.8619	3.4328	2.2171
H	2.0045	4.8244	3.0527
H	2.0052	3.1609	3.8177
C	-0.4807	3.7216	2.8463
H	-0.5101	4.824	3.054
H	-1.3679	3.4336	2.2166
H	-0.5118	3.1596	3.8171

C₆₀CHCH₃⁻ open

C	0.	0.	0.
C	1.479	0.	0.
C	2.2486	1.1757	0.
C	1.7604	2.4892	0.2081
C	-0.5211	2.521	0.2291
C	-0.834	1.1033	-0.0093
C	-0.4405	-1.1967	-0.7289
C	0.7356	-1.8889	-1.2341
C	1.9096	-1.1297	-0.8007
C	3.0141	-1.0738	-1.6545
C	3.3264	1.2679	-1.0144
C	2.0527	3.2473	-1.0044
C	1.1668	3.9625	-1.8228
C	-0.3259	3.9489	-1.7727
C	-1.1384	3.259	-0.8766
C	-2.2167	2.4276	-1.4047
C	-2.0532	1.0928	-0.8203
C	-2.4457	-0.029	-1.5271
C	-1.6171	-1.219	-1.4669
C	0.7031	-2.5192	-2.4679
C	-0.5205	-2.491	-3.2705
C	-1.6516	-1.863	-2.7798
C	-2.4742	-1.0352	-3.6663
C	-2.9689	0.1012	-2.889
C	-3.0586	1.3539	-3.4704
C	-2.6563	2.5401	-2.7109
C	-1.9445	3.4356	-3.6091
C	-0.8092	4.0958	-3.15
C	3.2101	2.5818	-1.6273
C	1.4964	3.0808	-5.8774
C	2.6542	3.0246	-5.1207
C	3.4571	1.7967	-5.1068
C	3.0369	0.6857	-5.8183
C	1.8082	0.7455	-6.6109
C	-0.3984	1.8522	-6.5862
C	-0.8659	2.9823	-5.7832
C	0.3077	3.7245	-5.3227

C	0.3338	4.2421	-4.0375
C	1.5401	4.1582	-3.218
C	2.6892	3.6048	-3.7808
C	4.0036	1.6366	-3.7593
C	4.0855	0.3782	-3.1869
C	3.6213	-0.7932	-3.9292
C	3.1202	-0.6457	-5.2118
C	1.9416	-1.4051	-5.63
C	1.134	-0.5483	-6.4985
C	-0.2491	-0.6064	-6.4417
C	-1.0366	0.6259	-6.4926
C	-1.9582	2.8391	-4.9456
C	-2.6417	1.5454	-4.8584
C	-2.1861	0.4678	-5.6013
C	-2.1022	-0.8597	-4.9893
C	-0.9033	-1.5214	-5.5061
C	-0.1387	-2.3216	-4.6723
C	1.3233	-2.2635	-4.7349
C	1.8421	-2.407	-3.3756
C	2.9591	-1.6903	-2.9748
C	3.5388	2.7667	-2.9551
C	3.7221	0.1898	-1.7807
C	1.0632	1.9135	-6.6446
C	0.5887	2.9973	0.8874
C	0.6286	4.1613	1.7744
H	1.5505	4.7714	1.6072
H	-0.2734	4.8086	1.6355
H	0.6394	3.7974	2.8359

$C_{60}CCH=CH_2^-$ open

C	0.	0.	0.
C	1.474	0.	0.
C	2.2506	1.1652	0.
C	1.7242	2.4793	0.1833
C	-0.5113	2.5275	0.2027
C	-0.8283	1.1117	-0.0204
C	-0.4408	-1.199	-0.7281
C	0.7352	-1.8982	-1.2279
C	1.9091	-1.1411	-0.7985
C	3.0115	-1.0837	-1.6471
C	3.3222	1.2587	-1.0149
C	2.019	3.2243	-1.033
C	1.1588	3.9575	-1.8556
C	-0.3224	3.9556	-1.8082
C	-1.1157	3.253	-0.9054
C	-2.201	2.4238	-1.4349
C	-2.0443	1.0941	-0.8429
C	-2.4388	-0.0299	-1.5405
C	-1.6128	-1.2242	-1.4701

C	0.7045	-2.5339	-2.4594
C	-0.5162	-2.5078	-3.2654
C	-1.6464	-1.8742	-2.7799
C	-2.4662	-1.0498	-3.6725
C	-2.9604	0.092	-2.9029
C	-3.0473	1.342	-3.4916
C	-2.6442	2.5314	-2.7389
C	-1.9359	3.4253	-3.6448
C	-0.8054	4.0922	-3.1887
C	3.1916	2.568	-1.6399
C	1.5093	3.0514	-5.8998
C	2.6642	2.9981	-5.1386
C	3.4659	1.7701	-5.1122
C	3.0486	0.6552	-5.8197
C	1.8227	0.7112	-6.617
C	-0.3835	1.819	-6.6064
C	-0.8531	2.9558	-5.8135
C	0.3189	3.7017	-5.3559
C	0.3407	4.2325	-4.0757
C	1.5443	4.1495	-3.2526
C	2.6914	3.5861	-3.8017
C	4.0058	1.617	-3.7612
C	4.0881	0.3612	-3.1827
C	3.6272	-0.8139	-3.9212
C	3.1299	-0.6727	-5.2062
C	1.9522	-1.4341	-5.6236
C	1.1476	-0.5817	-6.4997
C	-0.2354	-0.6386	-6.4455
C	-1.0224	0.5938	-6.5062
C	-1.9467	2.818	-4.9764
C	-2.6294	1.5244	-4.8807
C	-2.1735	0.4419	-5.6158
C	-2.0918	-0.8822	-4.9958
C	-0.8928	-1.5483	-5.5066
C	-0.131	-2.3453	-4.6674
C	1.3307	-2.2884	-4.7273
C	1.8462	-2.4244	-3.3648
C	2.963	-1.7081	-2.9666
C	3.5336	2.7487	-2.9636
C	3.7238	0.1802	-1.7767
C	1.0782	1.879	-6.661
C	0.5953	2.9476	0.9465
C	0.6535	3.8682	2.0235
C	-0.4239	4.3977	2.6282
H	-0.3308	5.1021	3.4623
H	-1.4485	4.159	2.3189
H	1.6707	4.1248	2.371

C₆₀CPh⁻ open

C	0.	0.	0.
C	1.4747	0.	0.
C	2.2983	1.1214	0.
C	1.9693	2.525	0.2415
C	-0.242	2.4628	0.2345
C	-0.7951	1.1451	0.034
C	-0.4383	-1.1344	-0.8198
C	0.7359	-1.8738	-1.269
C	1.9121	-1.1767	-0.7605
C	3.0781	-1.1856	-1.5132
C	3.5037	1.1235	-0.8452
C	2.5426	3.2704	-0.8531
C	1.7619	4.007	-1.7433
C	0.2878	3.99	-1.7819
C	-0.5485	3.2255	-0.9743
C	-1.7312	2.5853	-1.573
C	-1.8657	1.2627	-0.9689
C	-2.27	0.2008	-1.7529
C	-1.5456	-1.0603	-1.6556
C	0.7609	-2.4846	-2.5132
C	-0.3888	-2.3605	-3.4079
C	-1.5071	-1.66	-2.9892
C	-2.1823	-0.749	-3.9186
C	-2.6428	0.4086	-3.1528
C	-2.5683	1.6763	-3.7054
C	-2.0919	2.7921	-2.8878
C	-1.2617	3.651	-3.7185
C	-0.116	4.215	-3.175
C	3.6376	2.4622	-1.413
C	2.2668	3.0813	-5.7714
C	3.3656	2.9321	-4.9426
C	4.0543	1.6395	-4.8768
C	3.599	0.5693	-5.6295
C	2.4413	0.7328	-6.5093
C	0.334	2.0101	-6.624
C	-0.0967	3.1652	-5.836
C	1.0956	3.813	-5.2911
C	1.0811	4.3219	-4.0018
C	2.2345	4.1698	-3.1222
C	3.3623	3.5148	-3.6009
C	4.4812	1.4316	-3.4937
C	4.4066	0.1686	-2.9302
C	3.9128	-0.9602	-3.7189
C	3.5283	-0.7677	-5.0356
C	2.3293	-1.4297	-5.5516
C	1.6604	-0.5043	-6.4668
C	0.2769	-0.4535	-6.5108
C	-0.405	0.8384	-6.5966
C	-1.2459	3.0906	-5.0686
C	-2.0411	1.859	-5.0578

C	-1.6245	0.7603	-5.7913
C	-1.6952	-0.5797	-5.2044
C	-0.5169	-1.3269	-5.6453
C	0.1157	-2.1964	-4.7719
C	1.5779	-2.2474	-4.7231
C	1.9745	-2.4375	-3.3277
C	3.104	-1.8066	-2.8364
C	4.0745	2.6021	-2.7151
C	3.8962	0.0163	-1.5676
C	1.7962	1.9566	-6.581
C	0.8509	2.8544	1.0536
C	0.8307	3.4266	2.3482
C	2.0328	3.7489	3.0149
C	2.0063	4.315	4.2835
C	0.7905	4.5641	4.9219
C	-0.4053	4.2458	4.2764
C	-0.3921	3.6886	3.0036
H	2.9901	3.5434	2.5134
H	2.9501	4.5648	4.7892
H	0.7748	5.0079	5.926
H	-1.3648	4.4407	4.7767
H	-1.3336	3.4452	2.4893

C₆₀CCCH⁻ open

C	0.	0.	0.
C	1.4745	0.	0.
C	2.299	1.1211	0.
C	1.9722	2.5255	0.2416
C	-0.2372	2.4604	0.235
C	-0.796	1.1442	0.0356
C	-0.4384	-1.1342	-0.8211
C	0.7357	-1.8738	-1.2697
C	1.9118	-1.177	-0.7604
C	3.0783	-1.1869	-1.5121
C	3.5057	1.1218	-0.8437
C	2.5496	3.2711	-0.8503
C	1.7696	4.0074	-1.7415
C	0.2959	3.9892	-1.7808
C	-0.5408	3.224	-0.9748
C	-1.725	2.5865	-1.5735
C	-1.864	1.264	-0.9692
C	-2.2685	0.2033	-1.7546
C	-1.5448	-1.0585	-1.6575
C	0.7613	-2.4843	-2.5141
C	-0.3877	-2.3588	-3.4096
C	-1.5058	-1.6576	-2.9915
C	-2.1793	-0.7455	-3.9209
C	-2.6392	0.4121	-3.1548
C	-2.5627	1.6801	-3.7069

C	-2.0851	2.7946	-2.8882
C	-1.2533	3.653	-3.7182
C	-0.1075	4.2156	-3.1742
C	3.6431	2.4607	-1.4105
C	2.2752	3.0813	-5.7698
C	3.3734	2.9309	-4.9403
C	4.0606	1.6375	-4.8742
C	3.6047	0.5679	-5.6274
C	2.4478	0.7327	-6.508
C	0.3418	2.0122	-6.6238
C	-0.0882	3.1674	-5.8355
C	1.1045	3.8141	-5.29
C	1.0898	4.3226	-4.0005
C	2.2428	4.1696	-3.1204
C	3.37	3.5136	-3.5986
C	4.4863	1.4291	-3.4908
C	4.4098	0.166	-2.9276
C	3.9154	-0.9622	-3.7169
C	3.5321	-0.7691	-5.0338
C	2.3329	-1.4299	-5.5509
C	1.6655	-0.5036	-6.4663
C	0.2821	-0.4514	-6.5113
C	-0.3984	0.8412	-6.5971
C	-1.2377	3.0934	-5.0687
C	-2.0344	1.8627	-5.0588
C	-1.6186	0.764	-5.7926
C	-1.691	-0.5761	-5.2063
C	-0.5131	-1.3243	-5.6466
C	0.118	-2.1948	-4.7731
C	1.5801	-2.2471	-4.7232
C	1.9754	-2.4379	-3.3275
C	3.1049	-1.8079	-2.8352
C	4.0808	2.6	-2.7122
C	3.8977	0.0144	-1.5656
C	1.8039	1.9572	-6.5799
C	0.8535	2.85	1.0539
C	0.8342	3.3927	2.3173
C	0.8174	3.8682	3.4214
H	0.8027	4.2859	4.3911

5. C₆₀(CR⁻) closed

C₆₀CH⁻ closed

C	-1.25229	3.18134	-0.7476
C	-1.37531	3.3934	0.73367
C	0.03207	3.39769	1.54906
C	1.25715	3.18892	0.70663
C	1.23285	3.1665	-0.67183
C	-0.04406	3.16265	-1.41181
C	-2.31689	2.29985	-1.2088
C	-2.99796	1.76928	-0.03101
C	-2.34833	2.32762	1.14767
C	-2.15885	1.5151	2.24549
C	0.1612	2.33512	2.60193
C	2.19045	2.31337	1.40334
C	3.09658	1.52122	0.71463
C	3.09333	1.53191	-0.74184
C	2.17381	2.32783	-1.41016
C	1.50121	1.80778	-2.59955
C	0.13251	2.32172	-2.59315
C	-0.90095	1.51997	-3.05666
C	-2.16624	1.50548	-2.33536
C	-3.49106	0.47331	-0.04419
C	-3.32698	-0.36739	-1.23112
C	-2.68152	0.13551	-2.34743
C	-1.72753	-0.69875	-3.07916
C	-0.62562	0.15977	-3.51984
C	0.67137	-0.32564	-3.51809
C	1.76634	0.52536	-3.05045
C	2.72024	-0.31952	-2.33068
C	3.36439	0.17169	-1.20747
C	1.50937	1.78277	2.58112
C	2.36288	-2.51148	1.14227
C	2.20549	-1.7178	2.26688
C	0.9345	-1.72145	2.9949
C	-0.10794	-2.52301	2.56057
C	0.05938	-3.36337	1.37487
C	1.26209	-3.35001	-0.77942
C	2.36458	-2.49698	-1.22565
C	3.04552	-1.97962	-0.03833
C	3.53367	-0.68304	-0.03007
C	3.36932	0.15358	1.15928
C	2.72378	-0.3493	2.27554
C	0.67064	-0.35562	3.44804
C	-0.62141	0.15008	3.42398
C	-1.71995	-0.70186	2.97129
C	-1.47472	-1.9998	2.55486
C	-2.15681	-2.52914	1.37317
C	-1.20743	-3.36716	0.6407
C	-1.20519	-3.36473	-0.74465

C	0.06383	-3.3536	-1.47386
C	2.20761	-1.68964	-2.34044
C	0.94081	-1.69342	-3.0746
C	-0.10088	-2.50434	-2.65449
C	-1.47191	-1.99312	-2.65639
C	-2.15457	-2.52498	-1.47581
C	-3.05568	-1.73354	-0.7822
C	-3.0555	-1.73339	0.68254
C	-3.32363	-0.36757	1.13322
C	-2.6627	0.14397	2.24101
C	1.77172	0.48905	3.00578
C	-0.88193	1.51892	2.98545
C	1.26028	-3.35736	0.6842
C	-0.88534	4.47562	1.50448
H	-1.07858	5.46122	1.83306

C₆₀COH⁻ closed

C	-1.21873	3.04719	-0.85115
C	-1.3376	3.24902	0.62067
C	0.02162	3.27284	1.42079
C	1.2558	3.09055	0.60552
C	1.25755	3.05814	-0.77381
C	-0.013	3.03588	-1.52174
C	-2.28207	2.15931	-1.30794
C	-2.96726	1.64122	-0.12753
C	-2.31485	2.2094	1.04621
C	-2.15287	1.41586	2.16282
C	0.15061	2.25259	2.49754
C	2.19388	2.23772	1.32689
C	3.11271	1.44424	0.65672
C	3.12459	1.43315	-0.79942
C	2.20854	2.21521	-1.48992
C	1.54595	1.67267	-2.67597
C	0.17371	2.17955	-2.68774
C	-0.85379	1.36345	-3.14134
C	-2.1212	1.35255	-2.42429
C	-3.45781	0.34402	-0.12378
C	-3.2802	-0.51115	-1.29931
C	-2.63015	-0.02052	-2.41832
C	-1.66777	-0.86008	-3.13288
C	-0.56796	-0.00224	-3.58039
C	0.73179	-0.48029	-3.56325
C	1.81952	0.38377	-3.10235
C	2.77241	-0.44454	-2.36201
C	3.40529	0.06737	-1.24149
C	1.50781	1.71962	2.50678
C	2.40258	-2.58693	1.14109
C	2.23195	-1.77808	2.25282
C	0.95668	-1.78132	2.97338

C	-0.07756	-2.59604	2.54347
C	0.1034	-3.45106	1.37035
C	1.32094	-3.46062	-0.77572
C	2.42117	-2.60729	-1.22671
C	3.09012	-2.06799	-0.04228
C	3.56979	-0.76832	-0.04972
C	3.39004	0.08495	1.12554
C	2.73987	-0.40567	2.24448
C	0.68067	-0.4121	3.40787
C	-0.61643	0.08139	3.37378
C	-1.70759	-0.78376	2.92412
C	-1.44839	-2.08353	2.5225
C	-2.1182	-2.63179	1.34223
C	-1.15824	-3.47316	0.62767
C	-1.1463	-3.48991	-0.75748
C	0.12752	-3.48153	-1.47824
C	2.2674	-1.81744	-2.35438
C	1.00575	-1.83954	-3.09707
C	-0.03402	-2.65031	-2.67199
C	-1.40783	-2.14679	-2.69006
C	-2.09534	-2.66574	-1.50667
C	-3.00545	-1.86984	-0.83024
C	-3.01677	-1.85093	0.63436
C	-3.29835	-0.48182	1.06557
C	-2.65234	0.04572	2.17531
C	1.77618	0.43573	2.95728
C	-0.88338	1.4381	2.91012
C	1.30887	-3.4469	0.68779
C	-0.85014	4.51768	1.30968
O	-1.53011	4.89176	2.45344
H	-1.51769	5.85608	2.40343

$C_{60}COCH_3^-$ closed

C	-1.25491	2.83505	-1.04628
C	-1.40787	3.09294	0.41392
C	-0.06455	3.19145	1.23687
C	1.19006	3.01442	0.45158
C	1.21831	2.92574	-0.92488
C	-0.03665	2.83367	-1.6937
C	-2.28184	1.89658	-1.48458
C	-2.97318	1.40583	-0.29608
C	-2.36092	2.04129	0.86471
C	-2.19573	1.29915	2.01555
C	0.07466	2.21995	2.3568
C	2.13937	2.22092	1.22399
C	3.09423	1.42965	0.6034
C	3.13389	1.35979	-0.85062
C	2.20782	2.0843	-1.58881
C	1.5846	1.47374	-2.76306

C	0.19812	1.93686	-2.82002
C	-0.79536	1.07153	-3.25779
C	-2.07532	1.0504	-2.56362
C	-3.42405	0.09522	-0.24759
C	-3.19838	-0.80112	-1.38353
C	-2.5424	-0.33643	-2.51012
C	-1.54161	-1.17403	-3.1723
C	-0.45999	-0.30135	-3.63517
C	0.85308	-0.73769	-3.57529
C	1.90517	0.17775	-3.13114
C	2.86851	-0.58984	-2.34057
C	3.46424	-0.01345	-1.23106
C	1.44693	1.7301	2.41181
C	2.49739	-2.59862	1.24066
C	2.28127	-1.75096	2.31494
C	0.99324	-1.76451	3.01228
C	-0.00751	-2.62771	2.59804
C	0.22149	-3.52368	1.46454
C	1.47926	-3.5826	-0.65741
C	2.56149	-2.71455	-1.12359
C	3.19122	-2.10708	0.04928
C	3.63138	-0.79453	-0.00318
C	3.40362	0.09978	1.13259
C	2.74749	-0.36492	2.25908
C	0.66766	-0.38795	3.38494
C	-0.64285	0.06322	3.30757
C	-1.69858	-0.8529	2.87471
C	-1.3926	-2.15927	2.53168
C	-2.02297	-2.77556	1.36331
C	-1.02458	-3.6151	0.70116
C	-0.98586	-3.68771	-0.6817
C	0.30057	-3.66907	-1.3795
C	2.40529	-1.97632	-2.28538
C	1.15921	-2.06774	-3.04877
C	0.1366	-2.89245	-2.60916
C	-1.25125	-2.43299	-2.67231
C	-1.94505	-2.92452	-1.48091
C	-2.89153	-2.13044	-0.85408
C	-2.93119	-2.05241	0.60806
C	-3.26215	-0.67625	0.97742
C	-2.65361	-0.0843	2.07572
C	1.74541	0.47446	2.91937
C	-0.94186	1.39113	2.78372
C	1.43901	-3.50981	0.80385
C	-0.96995	4.40168	1.05601
O	-1.68934	4.78701	2.18371
C	-1.82109	6.20169	2.23173
H	-2.40732	6.39582	3.16458
H	-0.8179	6.689	2.2881
H	-2.37131	6.57666	1.33525

C₆₀CNH₂⁻ closed

C	-1.2326	3.05015	-0.82867
C	-1.36136	3.24192	0.64953
C	0.00215	3.25139	1.45046
C	1.24018	3.09128	0.64348
C	1.24692	3.07134	-0.73715
C	-0.02194	3.04811	-1.48889
C	-2.28671	2.15886	-1.29676
C	-2.97554	1.6241	-0.12521
C	-2.33478	2.1828	1.05711
C	-2.17009	1.38002	2.16558
C	0.12888	2.22208	2.51447
C	2.17967	2.2332	1.35914
C	3.10423	1.45025	0.68483
C	3.1221	1.4543	-0.77121
C	2.20382	2.23911	-1.45652
C	1.54922	1.70448	-2.65088
C	0.17482	2.20395	-2.66334
C	-0.84631	1.38777	-3.13027
C	-2.11711	1.36328	-2.4201
C	-3.45915	0.32433	-0.13733
C	-3.27172	-0.5182	-1.32037
C	-2.61889	-0.01245	-2.43088
C	-1.64899	-0.83972	-3.14955
C	-0.55156	0.02825	-3.58292
C	0.75052	-0.44311	-3.56459
C	1.83173	0.42171	-3.08982
C	2.78573	-0.40935	-2.35436
C	3.41088	0.09457	-1.22582
C	1.48973	1.69778	2.5287
C	2.41085	-2.58926	1.12503
C	2.23109	-1.79269	2.2441
C	0.95233	-1.80916	2.95852
C	-0.07563	-2.62511	2.51587
C	0.11513	-3.46734	1.33502
C	1.34239	-3.44881	-0.80546
C	2.44031	-2.5855	-1.24274
C	3.10113	-2.05482	-0.04988
C	3.5744	-0.75286	-0.04208
C	3.38536	0.08743	1.14108
C	2.73272	-0.41806	2.25204
C	0.66736	-0.44606	3.40548
C	-0.63215	0.04174	3.37056
C	-1.71671	-0.82493	2.90747
C	-1.44868	-2.11933	2.49377
C	-2.11034	-2.65903	1.30495
C	-1.14293	-3.48848	0.58638
C	-1.12465	-3.49098	-0.79878

C	0.15232	-3.4688	-1.51365
C	2.28758	-1.78475	-2.36284
C	1.02941	-1.80578	-3.11144
C	-0.0081	-2.62618	-2.6995
C	-1.38444	-2.12966	-2.7188
C	-2.07459	-2.66427	-1.54406
C	-2.99195	-1.87996	-0.8638
C	-3.0099	-1.87605	0.60082
C	-3.30013	-0.51259	1.04455
C	-2.66238	0.00623	2.1628
C	1.76137	0.41131	2.9684
C	-0.90435	1.4014	2.91956
C	1.32359	-3.45011	0.65803
C	-0.91085	4.46957	1.35572
N	-1.58668	5.07916	2.39363
H	-1.83301	4.48684	3.16801
H	-1.06038	5.86302	2.72174

$C_{60}CNHCH_3^-$ closed

C	-1.36126	2.80366	-1.02557
C	-1.51738	3.04847	0.44157
C	-0.16714	3.16941	1.25533
C	1.08783	3.04427	0.46733
C	1.11192	2.96694	-0.9109
C	-0.14453	2.84171	-1.67352
C	-2.35885	1.83612	-1.46553
C	-3.03067	1.31321	-0.27891
C	-2.43561	1.95571	0.88476
C	-2.24051	1.21054	2.02802
C	0.0039	2.19363	2.36347
C	2.06449	2.27075	1.2279
C	3.03905	1.51312	0.59638
C	3.07403	1.45719	-0.85829
C	2.12209	2.16011	-1.5852
C	1.51244	1.54034	-2.76201
C	0.11272	1.96141	-2.80899
C	-0.85597	1.07061	-3.25067
C	-2.13189	1.00493	-2.55237
C	-3.44143	-0.01087	-0.24038
C	-3.19356	-0.89038	-1.38477
C	-2.55651	-0.39591	-2.50945
C	-1.53377	-1.19709	-3.18301
C	-0.48099	-0.2881	-3.64228
C	0.84488	-0.68486	-3.5914
C	1.87076	0.2581	-3.14335
C	2.86045	-0.4869	-2.36409
C	3.4432	0.09788	-1.25201
C	1.39135	1.74711	2.41256
C	2.56528	-2.53684	1.20091

C	2.32831	-1.70543	2.28339
C	1.04399	-1.7634	2.98553
C	0.06814	-2.65323	2.56804
C	0.31935	-3.53218	1.42589
C	1.56923	-3.53474	-0.70156
C	2.62281	-2.63051	-1.16451
C	3.23891	-2.01432	0.01106
C	3.63922	-0.68878	-0.03184
C	3.38977	0.18842	1.11271
C	2.75287	-0.30579	2.2378
C	0.67863	-0.40081	3.37147
C	-0.64537	0.01172	3.30345
C	-1.67465	-0.93268	2.8671
C	-1.33046	-2.22626	2.51129
C	-1.94696	-2.85132	1.34013
C	-0.92658	-3.65482	0.66675
C	-0.89162	-3.71425	-0.71683
C	0.39064	-3.65075	-1.41968
C	2.43939	-1.88713	-2.31902
C	1.19336	-2.00967	-3.07813
C	0.19802	-2.86876	-2.64174
C	-1.20338	-2.45108	-2.69533
C	-1.8769	-2.97375	-1.50562
C	-2.84434	-2.21412	-0.86812
C	-2.87999	-2.14992	0.59478
C	-3.25051	-0.7874	0.97742
C	-2.65589	-0.18743	2.07874
C	1.72861	0.49729	2.90894
C	-0.98695	1.33414	2.79265
C	1.53302	-3.47584	0.76043
C	-1.14058	4.33108	1.09863
N	-1.87888	4.92395	2.11358
H	-2.10523	4.32788	2.8919
C	-1.36935	6.19013	2.56211
H	-2.17037	6.70268	3.15985
H	-0.45342	6.10458	3.21108
H	-1.10906	6.82136	1.67354

$C_{60}CN(CH_3)_2^-$ closed

C	-2.46098	-1.77392	0.9568
C	-3.21782	-0.55645	0.54202
C	-3.16348	-0.19777	-1.00546
C	-2.34843	-1.1268	-1.85156
C	-1.81161	-2.30532	-1.37786
C	-1.86919	-2.63826	0.05851
C	-1.7947	-1.52462	2.22996
C	-1.95606	-0.10893	2.54726
C	-2.71169	0.5031	1.46075
C	-2.36996	1.77604	1.05262

C	-2.60311	1.1503	-1.33196
C	-1.59342	-0.35783	-2.83245
C	-0.38778	-0.81734	-3.34135
C	0.15874	-2.07822	-2.86041
C	-0.5362	-2.79248	-1.89403
C	0.19726	-3.4256	-0.79872
C	-0.62823	-3.3225	0.40445
C	-0.01996	-3.11468	1.63524
C	-0.62299	-2.18088	2.5757
C	-0.94043	0.57662	3.19661
C	0.29964	-0.11466	3.55567
C	0.454	-1.45633	3.25314
C	1.72778	-1.94576	2.72424
C	1.43325	-2.97304	1.72235
C	2.21083	-3.0664	0.58004
C	1.57439	-3.30478	-0.71611
C	2.3024	-2.53508	-1.72595
C	1.612	-1.93863	-2.76787
C	-1.75548	1.05781	-2.51307
C	2.81958	1.52314	-2.23561
C	1.64623	2.17834	-2.5724
C	1.03225	3.1145	-1.62797
C	1.62725	3.34586	-0.39891
C	2.86721	2.65534	-0.04425
C	3.99928	0.5017	-0.45442
C	3.71075	-0.527	-1.45469
C	2.98254	0.10427	-2.55578
C	1.96331	-0.5824	-3.19538
C	0.7248	0.11099	-3.55174
C	0.57075	1.45258	-3.24911
C	-0.41974	2.96368	-1.72366
C	-1.20373	3.03425	-0.58062
C	-0.57294	3.28435	0.71512
C	0.80055	3.43786	0.80542
C	1.53526	2.81489	1.9072
C	2.81027	2.327	1.38149
C	3.33645	1.12959	1.83798
C	3.94545	0.19115	0.89424
C	3.37993	-1.81063	-1.05213
C	3.32313	-2.13898	0.37365
C	3.60031	-1.16593	1.31997
C	2.78003	-1.06636	2.52761
C	2.61686	0.35257	2.84779
C	1.4102	0.81516	3.34704
C	0.85277	2.08011	2.86253
C	-0.59918	1.92795	2.77276
C	-1.29614	2.50341	1.7191
C	-0.7048	1.93949	-2.71958
C	-2.31302	2.10724	-0.3828
C	3.44705	1.7685	-0.93663

C	-4.41594	-0.61968	-0.3504
N	-5.64204	0.02073	-0.3124
C	-5.73917	1.34525	0.25739
H	-6.70342	1.81589	-0.07054
H	-5.71643	1.34789	1.38271
H	-4.88389	1.9691	-0.11276
C	-6.72108	-0.84712	0.10204
H	-7.69003	-0.39958	-0.24729
H	-6.58448	-1.85499	-0.36669
H	-6.77894	-0.97535	1.2185

C₆₀CCH₃⁻ closed

C	-1.30759	3.03119	-0.7504
C	-1.45583	3.20484	0.73339
C	-0.06733	3.23553	1.56688
C	1.17775	3.08612	0.74153
C	1.17513	3.09126	-0.63713
C	-0.09023	3.06329	-1.39672
C	-2.33782	2.12688	-1.24426
C	-3.01931	1.55163	-0.08784
C	-2.40389	2.10381	1.11167
C	-2.20739	1.27564	2.19599
C	0.07997	2.1587	2.60271
C	2.12669	2.22554	1.43575
C	3.06718	1.47578	0.74547
C	3.08552	1.51594	-0.71032
C	2.1522	2.29684	-1.37723
C	1.5135	1.78057	-2.58681
C	0.1296	2.25214	-2.59138
C	-0.87177	1.42849	-3.08585
C	-2.1462	1.36058	-2.38409
C	-3.47207	0.24162	-0.13428
C	-3.26457	-0.56916	-1.33523
C	-2.61869	-0.02402	-2.43123
C	-1.62883	-0.8136	-3.16494
C	-0.54772	0.08703	-3.57169
C	0.76353	-0.35828	-3.55973
C	1.82472	0.51624	-3.05872
C	2.79356	-0.31342	-2.34112
C	3.40551	0.17439	-1.19859
C	1.44521	1.65029	2.59218
C	2.45317	-2.58549	1.08172
C	2.25465	-1.82012	2.21937
C	0.97391	-1.87794	2.92771
C	-0.03664	-2.70211	2.46151
C	0.1741	-3.51248	1.26194
C	1.40737	-3.41818	-0.87295
C	2.4893	-2.52275	-1.28514
C	3.13626	-2.00896	-0.07744

C	3.58369	-0.69841	-0.0359
C	3.37565	0.10844	1.16714
C	2.72978	-0.43669	2.26315
C	0.66104	-0.53043	3.40405
C	-0.64584	-0.06493	3.37107
C	-1.71072	-0.9407	2.88443
C	-1.4189	-2.22141	2.44544
C	-2.06667	-2.74697	1.24289
C	-1.08103	-3.54022	0.50849
C	-1.05849	-3.50938	-0.87633
C	0.22015	-3.44441	-1.58563
C	2.32382	-1.69813	-2.38595
C	1.06868	-1.72586	-3.13941
C	0.04656	-2.57673	-2.7515
C	-1.33948	-2.10786	-2.76419
C	-2.02257	-2.6844	-1.60504
C	-2.95786	-1.93531	-0.90967
C	-2.97937	-1.9653	0.55457
C	-3.29644	-0.61788	1.0284
C	-2.66865	-0.10963	2.15679
C	1.74138	0.35683	2.99532
C	-0.94206	1.3036	2.95556
C	1.38425	-3.4554	0.59004
C	-1.01249	4.29406	1.52859
C	-1.3589	5.56945	2.05876
H	-1.93485	5.50443	3.0246
H	-0.43802	6.17547	2.26672
H	-1.99793	6.13931	1.33395

$C_{60}CCH=CH_2^-$ closed

C	-1.35337	2.9174	-0.7349
C	-1.52444	3.03864	0.74862
C	-0.15128	3.07722	1.60116
C	1.10613	2.98532	0.79147
C	1.12421	3.0308	-0.58563
C	-0.1297	2.99594	-1.36364
C	-2.35877	2.00704	-1.26748
C	-3.04308	1.3851	-0.13713
C	-2.45624	1.91519	1.08675
C	-2.25742	1.06253	2.15083
C	0.00325	1.98319	2.61327
C	2.06498	2.12905	1.4779
C	3.0311	1.41989	0.78041
C	3.06898	1.50069	-0.67356
C	2.12931	2.27965	-1.33339
C	1.51837	1.78326	-2.5656
C	0.12432	2.22422	-2.57764
C	-0.85205	1.39252	-3.10684
C	-2.13413	1.27739	-2.42512

C	-3.46577	0.0674	-0.22561
C	-3.22377	-0.70473	-1.44547
C	-2.57516	-0.11546	-2.51678
C	-1.55825	-0.86256	-3.25796
C	-0.49194	0.07215	-3.62463
C	0.82855	-0.34435	-3.60583
C	1.8634	0.539	-3.06637
C	2.8402	-0.28888	-2.35751
C	3.42545	0.18027	-1.19345
C	1.3807	1.50724	2.6084
C	2.50322	-2.66163	0.99671
C	2.27209	-1.93278	2.15199
C	0.98347	-2.03866	2.84013
C	-0.00195	-2.87145	2.33705
C	0.24328	-3.64334	1.11875
C	1.50332	-3.46264	-0.99488
C	2.57061	-2.53264	-1.3668
C	3.18929	-2.03844	-0.13627
C	3.60673	-0.72008	-0.0525
C	3.3639	0.0484	1.16901
C	2.71543	-0.54093	2.24036
C	0.63377	-0.71211	3.34888
C	-0.68273	-0.27556	3.31146
C	-1.72113	-1.16036	2.7853
C	-1.39437	-2.42122	2.31469
C	-2.01354	-2.92684	1.08863
C	-1.00041	-3.67762	0.34689
C	-0.95954	-3.60765	-1.03605
C	0.32692	-3.49514	-1.72497
C	2.402	-1.68179	-2.44695
C	1.15827	-1.71611	-3.21876
C	0.15005	-2.59941	-2.86896
C	-1.24582	-2.16079	-2.88864
C	-1.93159	-2.78388	-1.75552
C	-2.89288	-2.07524	-1.0533
C	-2.93396	-2.14679	0.409
C	-3.28723	-0.82021	0.91547
C	-2.68766	-0.33092	2.06706
C	1.69954	0.20991	2.97999
C	-1.00373	1.09721	2.92925
C	1.4609	-3.5409	0.46608
C	-1.12338	4.12506	1.58887
C	-1.48176	5.3713	2.05992
H	-2.45405	5.73945	1.67444
C	-0.78331	6.14877	2.91189
H	0.18013	5.84956	3.33002
H	-1.15425	7.12708	3.22725

C₆₀CPh⁻ closed

C	2.19946	-1.44822	1.17636
C	2.86752	-0.80802	-0.0011
C	2.86753	0.80801	-0.00052
C	2.19951	1.44739	1.17741
C	1.75393	0.73725	2.27054
C	1.75391	-0.73888	2.27002
C	1.43376	-2.60447	0.72882
C	1.43348	-2.604	-0.7317
C	2.19902	-1.44743	-1.17876
C	1.75292	-0.73727	-2.27167
C	2.19898	1.44825	-1.17772
C	1.4338	2.60393	0.73065
C	0.31352	3.03975	1.4217
C	-0.13227	2.30685	2.59919
C	0.56865	1.17924	3.00141
C	-0.16396	-0.00124	3.4572
C	0.56863	-1.1814	3.00056
C	-0.13229	-2.30873	2.59755
C	0.31351	-3.04083	1.41956
C	0.31285	-3.0398	-1.4222
C	-0.87197	-3.49553	-0.69321
C	-0.87161	-3.49606	0.69075
C	-2.05387	-3.04078	1.42337
C	-1.5956	-2.30687	2.60511
C	-2.28593	-1.18517	3.03253
C	-1.54873	-0.00125	3.47652
C	-2.28593	1.183	3.03338
C	-1.59559	2.305	2.60677
C	1.43348	2.60452	-0.72986
C	-3.17481	2.61081	-0.73048
C	-2.05449	3.04077	-1.42281
C	-1.59677	2.30688	-2.60474
C	-2.28728	1.18517	-3.03184
C	-3.47216	0.7329	-2.30254
C	-4.35505	0.69246	0.00101
C	-3.90287	1.4243	1.18519
C	-3.1744	2.61021	0.73333
C	-2.05384	3.0397	1.42552
C	-0.87161	3.49542	0.69322
C	-0.87191	3.4962	-0.69082
C	-0.13346	2.30872	-2.59784
C	0.56729	1.18139	-3.00114
C	-0.16551	0.00123	-3.45741
C	-1.55028	0.00124	-3.47614
C	-2.28729	-1.18299	-3.03269
C	-3.47215	-0.73122	-2.30305
C	-3.90346	-1.42431	-1.18385
C	-4.35506	-0.69244	0.00053
C	-3.47111	0.73124	2.30424
C	-3.47111	-0.73288	2.30373

C	-3.90291	-1.42515	1.1842
C	-3.1745	-2.61078	0.73153
C	-3.1748	-2.61022	-0.7323
C	-2.0545	-3.03967	-1.42494
C	-1.59678	-2.305	-2.60638
C	-0.13347	-2.30686	-2.59945
C	0.56729	-1.17926	-3.00197
C	0.31288	3.04088	-1.4201
C	1.75289	0.73887	-2.27114
C	-3.90345	1.42519	-1.18284
C	4.05067	-0.00003	-0.00102
C	5.4278	-0.00003	-0.00053
C	6.16486	-1.21441	-0.00041
C	7.54996	-1.20329	0.00014
C	8.25838	0.00001	0.00056
C	7.54994	1.20329	0.00046
C	6.16483	1.21438	-0.00007
H	5.61718	-2.16543	-0.00075
H	8.10038	-2.15564	0.00022
H	9.35426	0.00001	0.00105
H	8.10034	2.15566	0.00083
H	5.61713	2.1654	-0.00014

C₆₀CCCH⁻ closed

C	-1.33244	2.93725	-0.7567
C	-1.48696	3.08704	0.72626
C	-0.10586	3.13284	1.56285
C	1.14334	3.0195	0.74298
C	1.14716	3.03849	-0.63477
C	-0.11506	2.99659	-1.39933
C	-2.34886	2.02311	-1.26097
C	-3.02561	1.42739	-0.11191
C	-2.4229	1.97667	1.09568
C	-2.21809	1.14342	2.17381
C	0.05318	2.05868	2.59538
C	2.10388	2.17093	1.43613
C	3.05854	1.4426	0.74244
C	3.08187	1.49532	-0.71304
C	2.14011	2.26721	-1.37824
C	1.51346	1.7511	-2.59438
C	0.12198	2.2003	-2.6007
C	-0.86477	1.36447	-3.10364
C	-2.14034	1.27016	-2.40663
C	-3.45648	0.11058	-0.17073
C	-3.23142	-0.68623	-1.37798
C	-2.59045	-0.12146	-2.46691
C	-1.58561	-0.88875	-3.20387
C	-0.51772	0.03228	-3.59948
C	0.80043	-0.39186	-3.58627

C	1.84594	0.49537	-3.07454
C	2.82515	-0.32473	-2.35985
C	3.42525	0.163	-1.21113
C	1.4276	1.5749	2.5854
C	2.50894	-2.63079	1.0425
C	2.29402	-1.87862	2.18589
C	1.01204	-1.96357	2.88906
C	0.01657	-2.79971	2.41211
C	0.24463	-3.59625	1.20642
C	1.48382	-3.4637	-0.923
C	2.55263	-2.54746	-1.32359
C	3.18691	-2.03358	-0.10919
C	3.61303	-0.71642	-0.05503
C	3.38731	0.07674	1.15391
C	2.7463	-0.48804	2.24289
C	0.67536	-0.62537	3.3758
C	-0.63896	-0.18183	3.34363
C	-1.68798	-1.07014	2.84514
C	-1.37341	-2.34164	2.3954
C	-2.00815	-2.86683	1.18568
C	-1.00719	-3.63777	0.44816
C	-0.98024	-3.59452	-0.93621
C	0.29974	-3.50296	-1.64022
C	2.37788	-1.71641	-2.41808
C	1.12607	-1.75792	-3.17633
C	0.11637	-2.62822	-2.79928
C	-1.27695	-2.1815	-2.81294
C	-1.95493	-2.77888	-1.66142
C	-2.90464	-2.05102	-0.96309
C	-2.93094	-2.09427	0.50069
C	-3.27131	-0.7562	0.98521
C	-2.6571	-0.24872	2.12119
C	1.74257	0.2829	2.97844
C	-0.95582	1.18523	2.93834
C	1.45605	-3.51371	0.53953
C	-1.0716	4.18564	1.54015
C	-1.38428	5.41106	1.98875
C	-1.66366	6.51269	2.39242
H	-1.91041	7.47364	2.74304