Supporting Information

The substituent effect on the photophysical and charge transport property of the non-planar dibenzo[*a,m*]rubicenes

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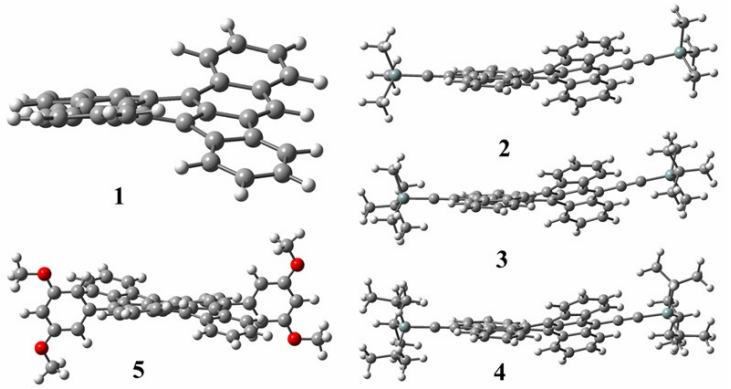

Figure S1. Side view of molecules 1 to 5, showing the changes of dihedral angles upon substitutions.

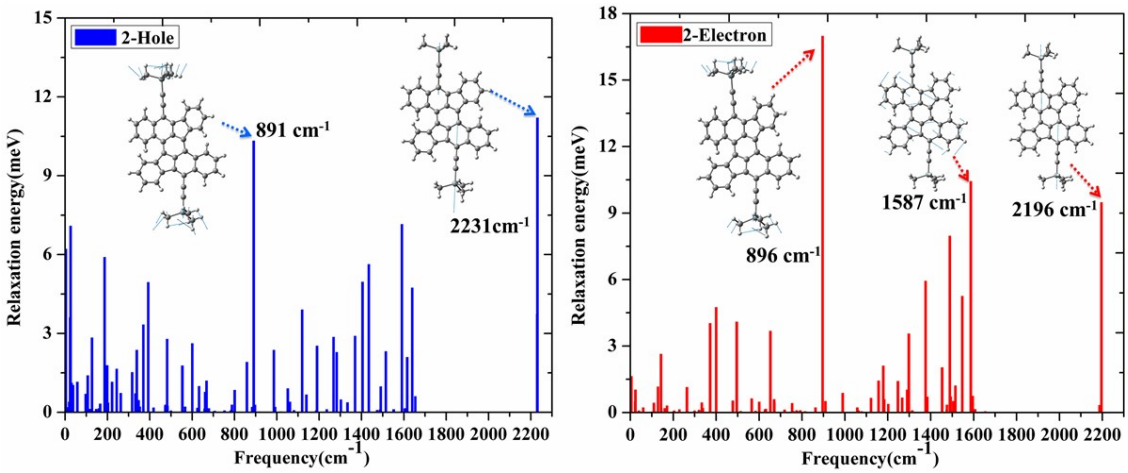

Figure S2. Contributions of the vibrational modes to the relaxation energies for molecule 2, embedded with the normal modes contribute the most for the reorganization energies of hole and electron.

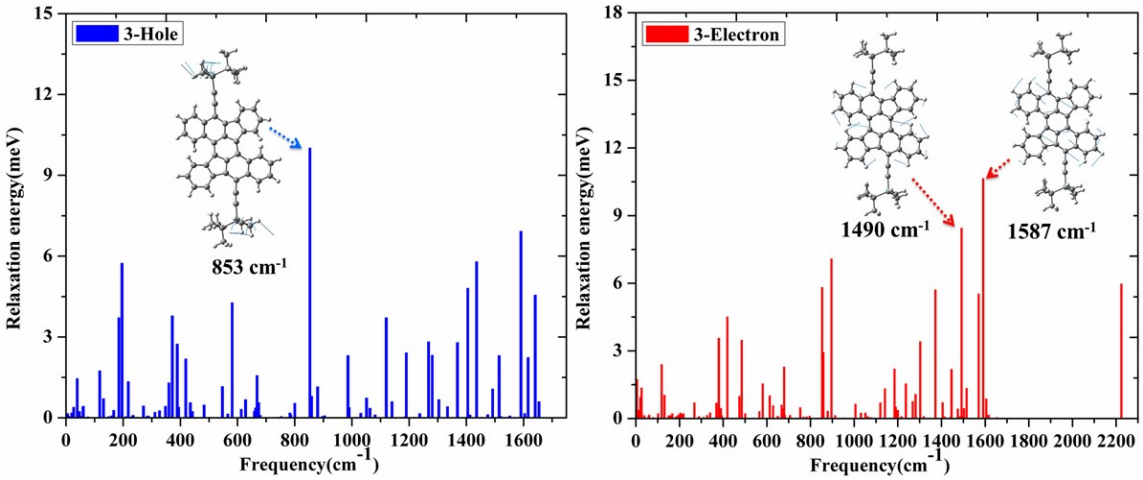

Figure S3. Contributions of the vibrational modes to the relaxation energies for molecule 3, embedded with the normal modes contribute the most for the reorganization energies of hole and electron.

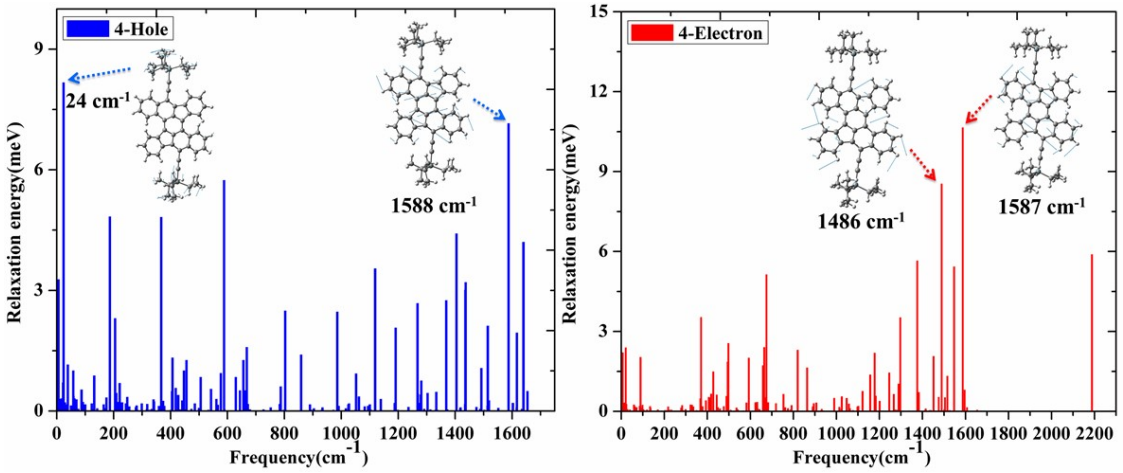

Figure S4. Contributions of the vibrational modes to the relaxation energies for molecule 4, embedded with the normal modes contribute the most for the reorganization energies of hole and electron.

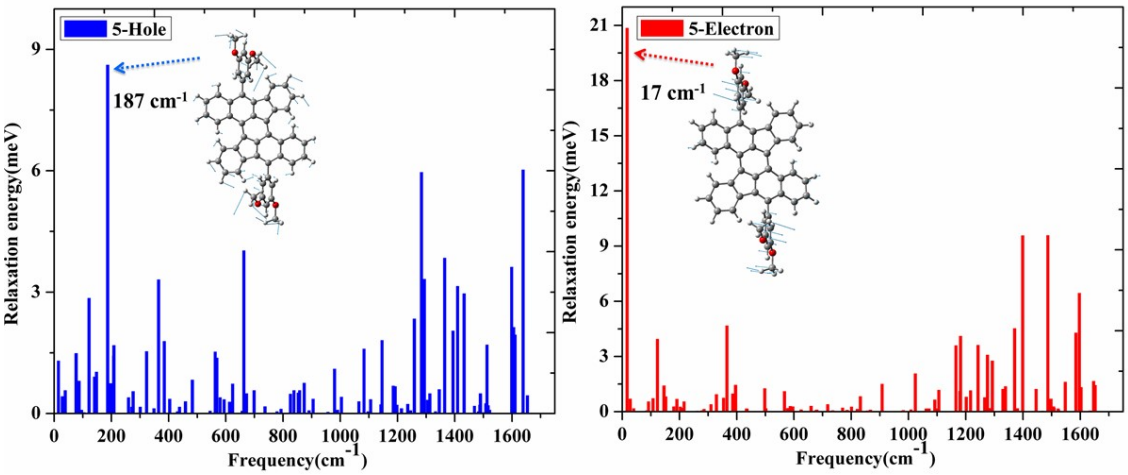

Figure S5. Contributions of the vibrational modes to the relaxation energies for molecule 5, embedded with the normal modes contribute the most for the reorganization energies of hole and electron.

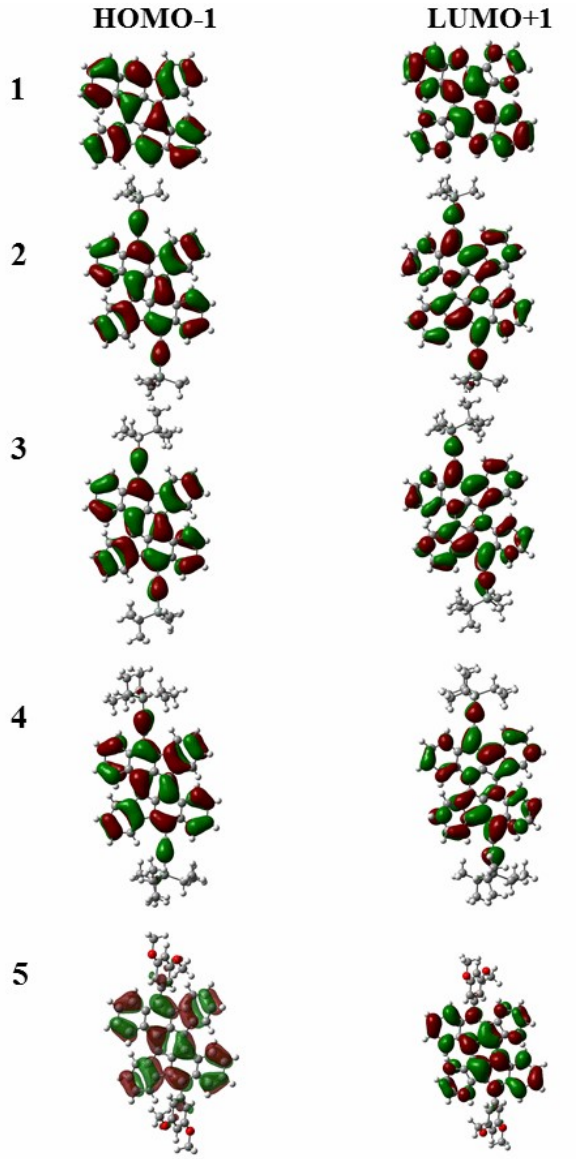

Figure S6. The HOMO-1, LUMO+1 distributions of molecules 1 to 5.

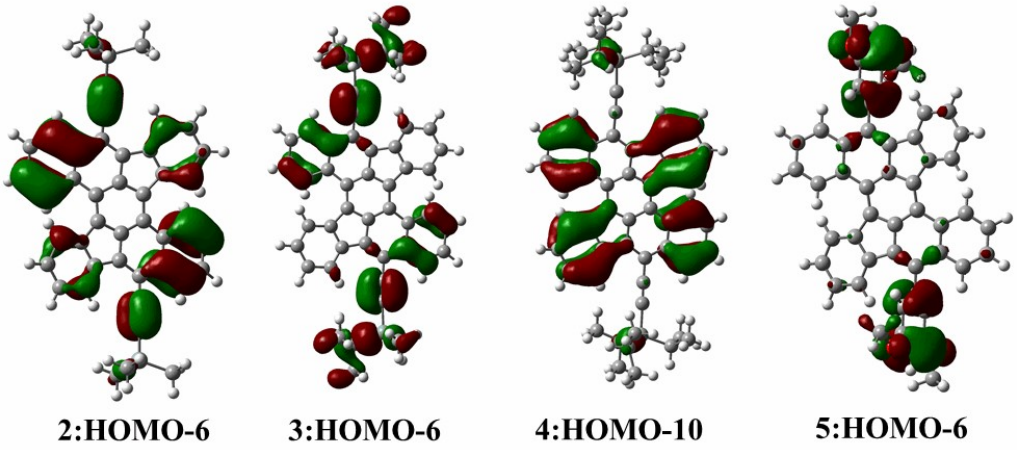

Figure S7. The HOMO-6 distributions of molecules 2, 3 and 5, the HOMO-10 distributions of molecule 4.

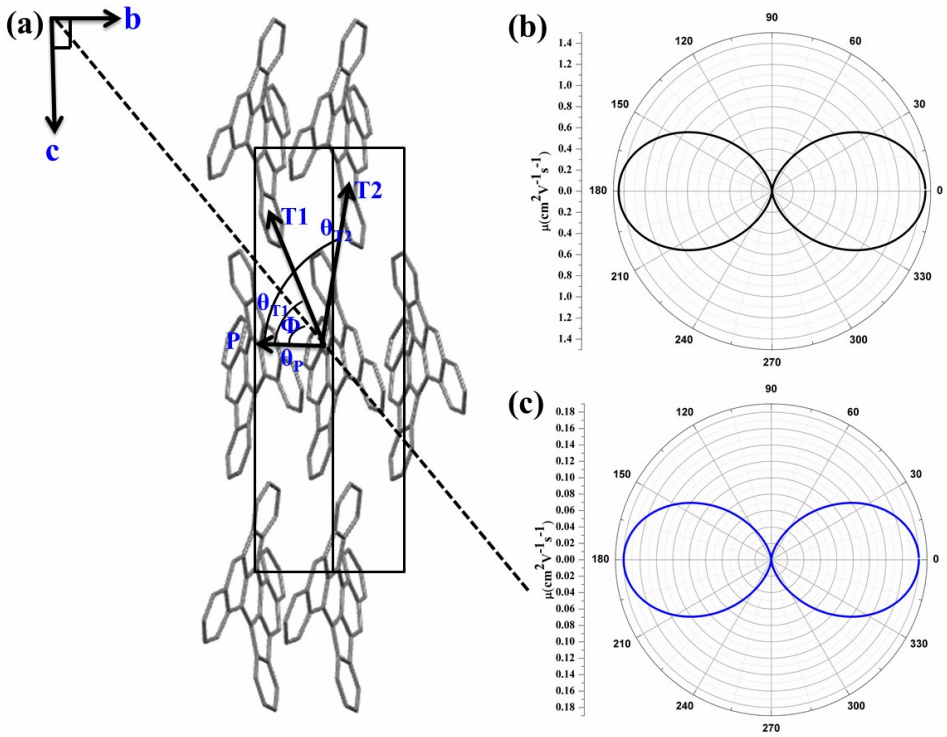

Figure S8. The projecting angle-dependent hopping paths to a transistor channel in the *bc* plane (a) and the calculated angle-resolved anisotropic hole (b) and electron (c) mobilities of molecule 1.

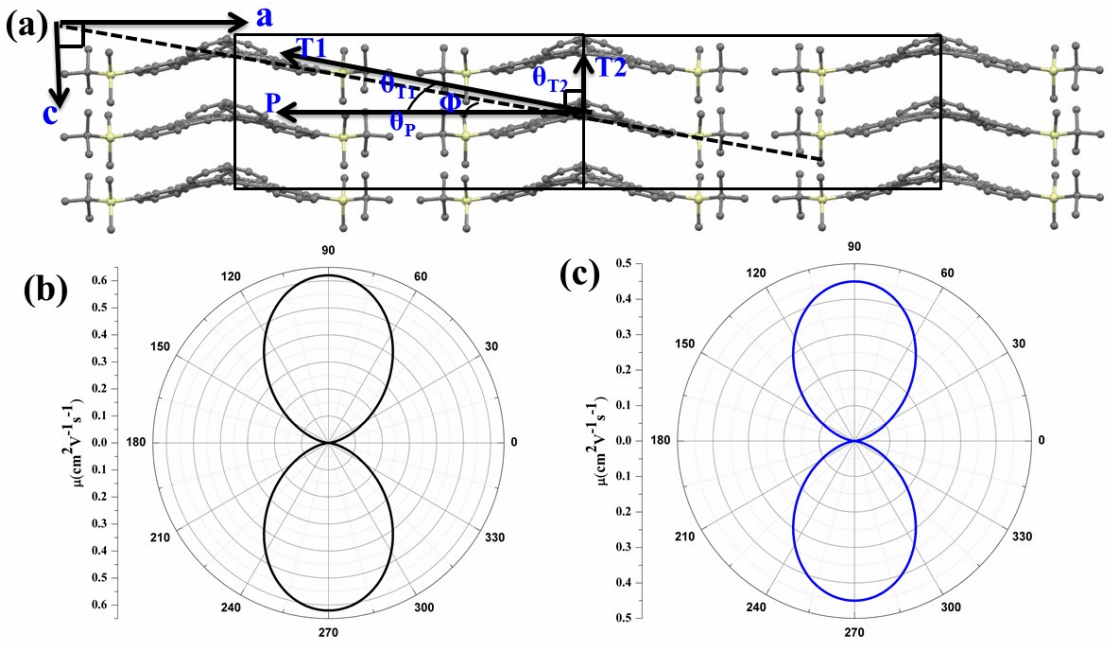

Figure S9. The projecting angle-dependent hopping paths to a transistor channel in the *ac* plane (a) and the calculated angle-resolved anisotropic hole (b) and electron (c) mobilities of molecule 3.

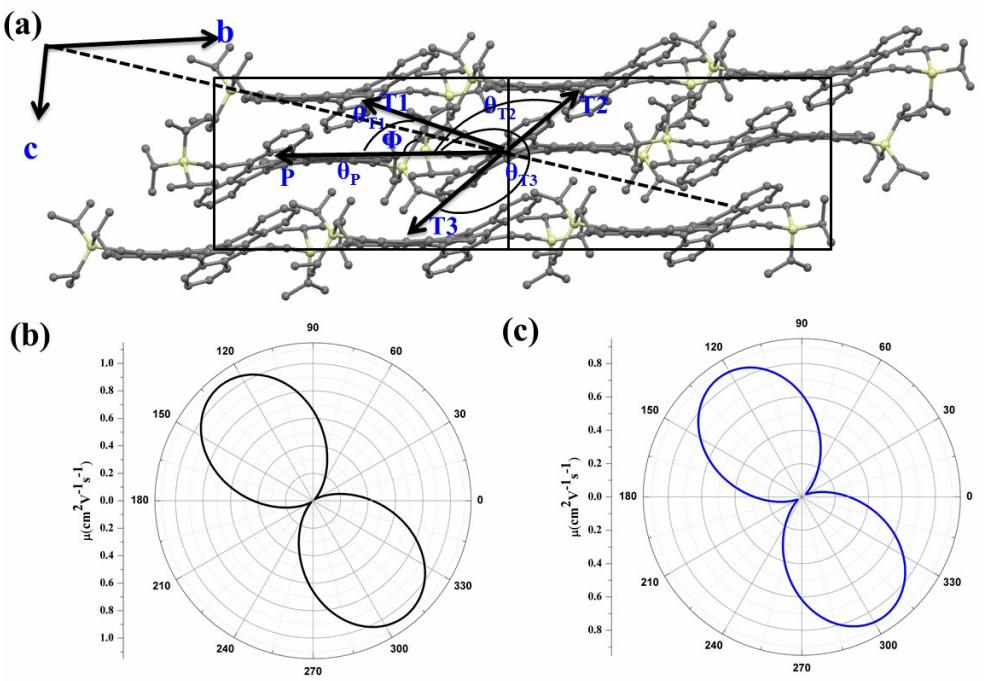

Figure S10. The projecting angle-dependent hopping paths to a transistor channel in the *bc* plane (a) and the calculated angle-resolved anisotropic hole (b) and electron (c) mobilities of molecule 4.

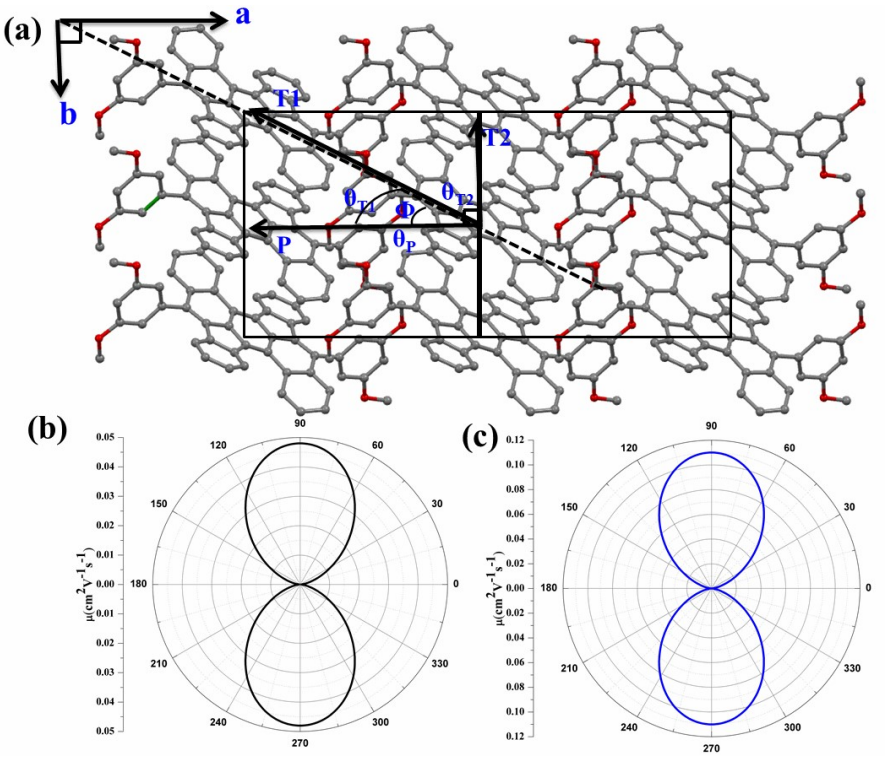

Figure S11. The projecting angle-dependent hopping paths to a transistor channel in the *ab* plane (a) and the calculated angle-resolved anisotropic hole (b) and electron (c) mobilities of molecule 5.

Table S1. the reorganization energies of hole (λ^+) and electron (λ^-) for molecules 1 to 5 using B3LYP functional and different basis sets.

Molecules	λ^+ (eV)			λ^- (eV)		
	6-31G (d, p)	6-31+G (d, p)	6-311++G (d, p)	6-31G (d, p)	6-31+G (d, p)	6-311++G (d, p)
1	0.200	0.195	0.199	0.177	0.172	0.176
2	0.213	0.208	0.213	0.204	0.198	0.200
3	0.211	0.206	0.212	0.203	0.197	0.199
4	0.202	0.197	0.202	0.197	0.191	0.194
5	0.197	0.195	0.199	0.232	0.220	0.221

Table S2. The selected optimized bond lengths (in angstrom) and bond angles (in degree) of molecules 1 and 5 in the neutral and ionic states, respectively, together with experimental values[31]

Compds.	Bond Parameters	Neutral	Expt.	Cationic	Δ(C-N)	Anionic	Δ(A-N)
1	R(C1-C2)	1.44	1.44	1.43	-0.01	1.42	-0.02
	R(C3-C6)	1.44	1.44	1.42	-0.02	1.43	-0.01
	R(C4-C5)	1.49	1.49	1.46	-0.03	1.46	-0.03
	R(C5-C6)	1.42	1.41	1.45	0.03	1.43	0.01
	θ(C6-C7-C8)	114.2	114.5	113.2	-1.0	114.6	0.4
	θ(C5-C4-C11)	133.1	133.3	132.2	-0.9	133.8	0.7
2	R(C1-C2)	1.46	1.47	1.46	0.00	1.45	-0.01
	R(C3-C6)	1.44	1.44	1.42	-0.02	1.43	-0.01
	R(C4-C5)	1.48	1.49	1.46	-0.02	1.46	-0.02
	R(C5-C6)	1.42	1.41	1.45	0.03	1.43	0.01
	R(C13-Si14)	1.84	1.84	1.87	0.03	1.82	-0.02
	θ(C1-C2-C12)	119.2	120.1	119.7	0.5	119.5	0.3
	θ(C6-C7-C8)	114.6	114.7	113.7	-0.9	115.1	0.5
	θ(C5-C4-C11)	132.6	132.8	132.0	-0.6	133.1	0.5
3	R(C1-C2)	1.47	1.46	1.46	-0.01	1.45	-0.02
	R(C3-C6)	1.44	1.45	1.42	-0.02	1.43	-0.01
	R(C4-C5)	1.48	1.48	1.46	-0.02	1.46	-0.02
	R(C5-C6)	1.42	1.41	1.45	0.03	1.43	0.01
	R(C13-Si14)	1.85	1.83	1.87	0.02	1.82	-0.03
	θ(C1-C2-C12)	118.9	119.0	119.5	0.6	119.2	0.3
	θ(C6-C7-C8)	114.6	114.9	113.7	-0.9	115.1	0.5
	θ(C5-C4-C11)	132.7	132.6	132.1	-0.6	133.2	0.5
4	R(C1-C2)	1.47	1.43	1.46	-0.01	1.45	-0.02
	R(C3-C6)	1.44	1.44	1.42	-0.02	1.43	-0.01
	R(C4-C5)	1.48	1.48	1.46	-0.02	1.46	-0.02
	R(C5-C6)	1.42	1.40	1.45	0.03	1.43	0.01
	R(C13-Si14)	1.85	1.83	1.87	0.02	1.83	-0.02
	θ(C1-C2-C12)	119.0	123.4	119.5	0.5	119.3	0.3
	θ(C6-C7-C8)	114.6	117.0	113.7	-0.9	115.1	0.5
	θ(C5-C4-C11)	132.7	129.4	132.1	-0.6	133.2	0.5
5	R(C1-C2)	1.46	1.45	1.45	-0.01	1.44	-0.02
	R(C3-C6)	1.44	1.44	1.42	-0.02	1.43	-0.01
	R(C4-C5)	1.48	1.49	1.46	-0.02	1.46	-0.02
	R(C5-C6)	1.42	1.41	1.45	0.03	1.43	0.01
	θ(C1-C2-C12)	120.1	120.9	120.8	0.7	121.0	0.9
	θ(C6-C7-C8)	115.1	115.4	114.4	-0.7	115.5	0.4
	θ(C5-C4-C11)	132.7	133.1	132.0	-0.7	133.1	0.4

Table S3. Selected transfer integrals of hole (V_{hole}) and electron ($V_{electron}$) for the different hopping pathways of all the investigated molecules.

Compds.	Pathway	Distance(Å)	V_{hole} (meV)	$V_{electron}$ (meV)
1	7, 8	12.57	-7.7×10^{-2}	0.1
	9	11.73	9.9×10^{-3}	3.8×10^{-4}
	10	11.15	3.3	-3.7
	11	11.91	2.7×10^{-2}	-0.3
	12	12.28	-2.5×10^{-3}	9.1×10^{-4}
	13, 14	10.96	-0.5	-1.1
2	5, 6	19.63	3.4×10^{-2}	-2.7×10^{-2}
	7, 8	19.98	-4.3×10^{-2}	9.5×10^{-2}
	9, 10	13.66	-6.5×10^{-4}	8.5×10^{-2}
3	3, 4, 5, 6	21.58	9.3×10^{-4}	-4.4×10^{-3}
	7, 8	21.24	1.2×10^{-3}	-4.3×10^{-3}
4	5	12.98	5.4×10^{-3}	3.3×10^{-3}
	6	17.38	-1.1	0.2
	7	19.23	-2.3×10^{-3}	9.8×10^{-4}
	8	10.31	0.2	1.1
	9, 10	17.02	1.2×10^{-3}	5.3×10^{-2}
	11, 12	23.12	3.7×10^{-2}	-4.9×10^{-2}
	13	18.93	1.5×10^{-2}	-1.7×10^{-2}
	14	13.41	0.2	-0.9
	15	19.28	-8.6×10^{-3}	-8.7×10^{-3}
	16	16.07	2.0×10^{-5}	3.3×10^{-4}
5	5, 6	13.34	2.8×10^{-4}	-4.1×10^{-5}
	13, 14	15.61	-7.2×10^{-2}	0.1

Table S4. The relative probability of the charge hopping (P_i) and the diffusion coefficient (D) for the different hopping pathways of molecules 1 to 5.

Compd.	Pathway	$P_{i,hole}$	D_{hole}	$P_{i,electron}$	$D_{electron}$
1	1, 2	0.50	3.72×10^{-2}	0.49	4.61×10^{-3}
	3, 4	1.18×10^{-4}	2.08×10^{-8}	9.78×10^{-4}	1.86×10^{-7}
	5, 6	5.49×10^{-6}	4.12×10^{-11}	6.82×10^{-3}	8.25×10^{-6}
	7, 8	3.22×10^{-7}	1.60×10^{-13}	7.98×10^{-6}	1.27×10^{-11}
	9	5.35×10^{-9}	3.82×10^{-17}	7.94×10^{-11}	1.10×10^{-21}
	10	5.82×10^{-4}	4.10×10^{-7}	7.52×10^{-3}	8.88×10^{-6}
	11	4.09×10^{-8}	2.31×10^{-15}	6.75×10^{-5}	8.15×10^{-10}
	12	3.58×10^{-10}	1.88×10^{-19}	4.63×10^{-10}	4.08×10^{-20}
	13, 14	1.62×10^{-5}	3.08×10^{-10}	6.41×10^{-4}	6.22×10^{-8}
2	1, 2	0.50	1.57×10^{-2}	0.50	6.48×10^{-3}
	3, 4	1.49×10^{-5}	3.97×10^{-10}	9.75×10^{-5}	7.05×10^{-9}
	5, 6	1.14×10^{-7}	2.26×10^{-14}	2.06×10^{-7}	3.05×10^{-14}
	7, 8	1.85×10^{-7}	6.12×10^{-14}	2.48×10^{-6}	4.56×10^{-12}
	9, 10	4.35×10^{-11}	1.58×10^{-21}	1.99×10^{-6}	1.38×10^{-12}
	11, 12	4.25×10^{-5}	1.39×10^{-9}	9.66×10^{-4}	2.98×10^{-7}
	13, 14	1.73×10^{-4}	2.21×10^{-8}	6.31×10^{-5}	1.22×10^{-9}
3	1, 2	0.50	1.58×10^{-2}	0.50	1.16×10^{-2}
	3, 4, 5, 6	9.36×10^{-11}	1.78×10^{-20}	3.15×10^{-9}	1.49×10^{-17}
	7, 8	1.44×10^{-10}	4.09×10^{-20}	2.89×10^{-9}	1.22×10^{-17}
	9, 10	1.86×10^{-5}	4.30×10^{-10}	1.0×10^{-3}	9.65×10^{-7}
	11, 12	1.29×10^{-5}	1.93×10^{-10}	8.79×10^{-5}	6.70×10^{-9}
	13, 14	7.75×10^{-5}	7.33×10^{-9}	2.89×10^{-3}	7.58×10^{-6}
4	1	0.27	7.06×10^{-3}	0.44	1.77×10^{-2}
	2	0.69	4.78×10^{-2}	0.55	2.89×10^{-2}
	3, 4	2.07×10^{-2}	1.50×10^{-4}	2.74×10^{-3}	2.47×10^{-6}
	5	7.92×10^{-9}	2.00×10^{-17}	3.35×10^{-9}	3.37×10^{-18}
	6	3.54×10^{-4}	7.16×10^{-8}	7.87×10^{-6}	3.32×10^{-11}
	7	1.41×10^{-9}	1.39×10^{-18}	3.00×10^{-10}	5.92×10^{-20}
	8	6.74×10^{-6}	9.16×10^{-12}	3.48×10^{-4}	2.29×10^{-8}
	9, 10	3.76×10^{-10}	7.74×10^{-20}	8.94×10^{-7}	4.11×10^{-13}

	11, 12	3.79×10^{-7}	1.46×10^{-13}	7.44×10^{-7}	5.26×10^{-13}
	13	6.37×10^{-8}	2.75×10^{-15}	9.30×10^{-8}	5.50×10^{-15}
	14	9.51×10^{-6}	3.08×10^{-11}	2.73×10^{-4}	2.39×10^{-8}
	15	2.04×10^{-8}	2.94×10^{-16}	2.35×10^{-8}	3.66×10^{-16}
	16	1.05×10^{-13}	5.44×10^{-27}	3.35×10^{-11}	5.16×10^{-22}
5	1, 2	0.19	4.97×10^{-4}	0.45	2.50×10^{-3}
	3, 4	1.93×10^{-3}	2.73×10^{-7}	4.65×10^{-3}	1.47×10^{-6}
	5, 6	1.07×10^{-10}	8.35×10^{-22}	1.62×10^{-12}	1.78×10^{-25}
	7, 8	7.92×10^{-3}	3.76×10^{-6}	2.89×10^{-5}	4.59×10^{-11}
	9,10,11,12	0.15	1.64×10^{-3}	2.46×10^{-2}	4.07×10^{-5}
	13, 14	6.92×10^{-6}	4.82×10^{-12}	1.24×10^{-5}	1.43×10^{-11}

Table S5. The transfer integrals and charge mobilities of hole (V_{hole}) and electron ($V_{electron}$) for the different hopping pathways of molecule 2 based on B3LYP/6-31G (d, p) level.

Compd.	Pathway	Distance (Å)	V_{hole} (meV)	$V_{electron}$ (meV)	$\mu_{h,ave.}$ ($cm^2V^{-1}s^{-1}$)	$\mu_{e,ave.}$ ($cm^2V^{-1}s^{-1}$)
2	1, 2	3.74	64.4	-44.4	0.17	0.09
	3, 4	19.98	-0.3	0.5		
	5, 6	19.63	3.0×10^{-2}	-2.4×10^{-2}		
	7, 8	19.98	-4.2×10^{-2}	0.1		
	9, 10	13.66	5.1×10^{-3}	9.0×10^{-2}		
	11, 12	13.11	-0.9	1.9		
	13, 14	12.86	1.5	-0.4		

Cartesian coordinates of optimized S_1 geometry

Molecule 1 at B3LYP/6-31+G(d, p) level

C	0.69063400	-2.67570400	-0.09419000
C	1.98901600	-3.15316300	-0.01193300
H	2.21793200	-4.20768400	-0.13780400
C	3.04415300	-2.24730100	0.28953700
C	4.36580900	-2.72809900	0.50902600
H	4.55650300	-3.79007600	0.37677400
C	5.38176900	-1.88647500	0.91519800
H	6.37901200	-2.27984400	1.08948600
C	5.11136700	-0.51727900	1.14251800
H	5.89149400	0.13588600	1.52175300
C	3.84654600	-0.00983500	0.89733400
H	3.64641700	1.03123900	1.11751100
C	2.79317700	-0.82856100	0.42266000
C	1.45705200	-0.32466500	0.15887400
C	1.00283700	1.01981400	-0.03900800
C	1.61679200	2.27797700	-0.36483800
C	2.93483500	2.63393700	-0.74920400
H	3.71087600	1.88341400	-0.82971200
C	3.22637500	3.95451700	-1.06049800
H	4.23403400	4.22420000	-1.36111400
C	2.22827700	4.95283400	-1.00050900
H	2.48535400	5.98089800	-1.23775100
C	0.91023300	4.62747000	-0.66801300
H	0.14384300	5.39706100	-0.65910000
C	0.59053600	3.30272800	-0.37321200
C	-0.69063400	2.67570400	-0.09419000
C	-1.98901600	3.15316300	-0.01193400
H	-2.21793200	4.20768400	-0.13780500
C	-3.04415300	2.24730200	0.28953700
C	-4.36580900	2.72809900	0.50902600
H	-4.55650300	3.79007600	0.37677400
C	-5.38176900	1.88647500	0.91519800
H	-6.37901200	2.27984400	1.08948500
C	-5.11136700	0.51728000	1.14251800
H	-5.89149400	-0.13588500	1.52175200
C	-3.84654600	0.00983500	0.89733500
H	-3.64641700	-1.03123800	1.11751200
C	-2.79317700	0.82856100	0.42266100

C	-1.45705200	0.32466500	0.15887400
C	-0.43319200	1.28286900	0.04625000
C	-1.00283700	-1.01981400	-0.03900700
C	0.43319200	-1.28286900	0.04625000
C	-1.61679200	-2.27797700	-0.36483800
C	-2.93483500	-2.63393700	-0.74920400
H	-3.71087600	-1.88341500	-0.82971200
C	-3.22637400	-3.95451700	-1.06049800
H	-4.23403400	-4.22420000	-1.36111500
C	-2.22827700	-4.95283400	-1.00050900
H	-2.48535300	-5.98089800	-1.23775200
C	-0.91023300	-4.62747000	-0.66801300
H	-0.14384300	-5.39706100	-0.65910000
C	-0.59053600	-3.30272800	-0.37321200

Molecule 1 at PBE0/6-31+G(d, p) level

C	0.66796600	-2.67185400	-0.08908300
C	1.95955500	-3.15683400	-0.00803700
H	2.18277800	-4.21300700	-0.13465600
C	3.01660900	-2.25841700	0.29119900
C	4.33188700	-2.74526200	0.50831000
H	4.51629200	-3.80887400	0.37735700
C	5.35016000	-1.91024200	0.90961500
H	6.34574400	-2.30888100	1.08268300
C	5.08847700	-0.54278400	1.13555600
H	5.87278700	0.10621700	1.51401400
C	3.82992800	-0.03040600	0.89250900
H	3.63153300	1.01234800	1.11312400
C	2.77607900	-0.84437400	0.42185800
C	1.44940500	-0.33454600	0.16148200
C	1.00618800	1.00829300	-0.03719000
C	1.62783200	2.25616000	-0.36377300
C	2.94464800	2.59560300	-0.75254500
H	3.71185100	1.83483900	-0.83816200
C	3.24661300	3.90984700	-1.06354700
H	4.25552600	4.16999500	-1.36924200
C	2.26127000	4.91474300	-0.99938400
H	2.52791600	5.94047000	-1.23760900
C	0.94444200	4.60389600	-0.66412400
H	0.18482200	5.38061300	-0.65302100
C	0.61515300	3.28552800	-0.36937000
C	-0.66796600	2.67185400	-0.08908200
C	-1.95955500	3.15683400	-0.00803600

H	-2.18277800	4.21300700	-0.13465400
C	-3.01660900	2.25841700	0.29120000
C	-4.33188700	2.74526200	0.50831000
H	-4.51629200	3.80887400	0.37735800
C	-5.35016000	1.91024200	0.90961500
H	-6.34574400	2.30888000	1.08268200
C	-5.08847700	0.54278300	1.13555400
H	-5.87278700	-0.10621800	1.51401100
C	-3.82992800	0.03040500	0.89250800
H	-3.63153300	-1.01234900	1.11312300
C	-2.77607900	0.84437400	0.42185900
C	-1.44940500	0.33454600	0.16148200
C	-0.42151200	1.28148300	0.05077600
C	-1.00618800	-1.00829300	-0.03719000
C	0.42151300	-1.28148300	0.05077600
C	-1.62783100	-2.25615900	-0.36377300
C	-2.94464800	-2.59560300	-0.75254500
H	-3.71185100	-1.83483800	-0.83816100
C	-3.24661300	-3.90984700	-1.06354600
H	-4.25552700	-4.16999400	-1.36924000
C	-2.26127100	-4.91474300	-0.99938300
H	-2.52791700	-5.94047000	-1.23760700
C	-0.94444200	-4.60389500	-0.66412400
H	-0.18482200	-5.38061300	-0.65302100
C	-0.61515300	-3.28552800	-0.36937100

Molecule 1 at BMK/6-31+G(d, p) level

C	0.67319800	-2.68790100	-0.08536900
C	1.96741900	-3.17748700	-0.00194700
H	2.18919700	-4.23662900	-0.12534400
C	3.03293000	-2.27213800	0.29494500
C	4.35604400	-2.76505800	0.51239700
H	4.53695400	-3.83183900	0.38618000
C	5.38122500	-1.92582500	0.90556900
H	6.37875200	-2.32481000	1.07805300
C	5.12103600	-0.54621600	1.12459500
H	5.91032500	0.10407300	1.49584600
C	3.85822200	-0.02956100	0.88394700
H	3.66085400	1.01546200	1.10052000
C	2.79349700	-0.85119000	0.41983100
C	1.45827000	-0.33828300	0.16114500
C	1.01364400	1.01479400	-0.03623800
C	1.63853400	2.27066400	-0.36290500

C	2.96291100	2.61559000	-0.75353200
H	3.73261800	1.85538700	-0.84155100
C	3.26381500	3.93820100	-1.06319800
H	4.27447500	4.20019300	-1.36852100
C	2.27212100	4.94805500	-0.99708000
H	2.53748600	5.97645000	-1.23399300
C	0.94851700	4.63138700	-0.66019500
H	0.18429200	5.40667200	-0.64685400
C	0.62195400	3.30582300	-0.36662000
C	-0.67319800	2.68790000	-0.08537100
C	-1.96741800	3.17748700	-0.00194700
H	-2.18919500	4.23662900	-0.12534300
C	-3.03293000	2.27213800	0.29494500
C	-4.35604300	2.76506000	0.51239800
H	-4.53695200	3.83184200	0.38618200
C	-5.38122400	1.92582700	0.90556800
H	-6.37875100	2.32481300	1.07805300
C	-5.12103600	0.54621800	1.12459400
H	-5.91032700	-0.10407000	1.49584400
C	-3.85822300	0.02956300	0.88394500
H	-3.66085600	-1.01546100	1.10051800
C	-2.79349700	0.85119000	0.41983100
C	-1.45827100	0.33828300	0.16114400
C	-0.42569100	1.28948700	0.05059800
C	-1.01364600	-1.01479600	-0.03623600
C	0.42569000	-1.28948800	0.05060100
C	-1.63853500	-2.27066400	-0.36290300
C	-2.96291200	-2.61559200	-0.75353100
H	-3.73262000	-1.85538900	-0.84154900
C	-3.26381500	-3.93820200	-1.06319800
H	-4.27447400	-4.20019600	-1.36852100
C	-2.27211900	-4.94805600	-0.99708000
H	-2.53748300	-5.97645000	-1.23399400
C	-0.94851600	-4.63138800	-0.66019500
H	-0.18429000	-5.40667300	-0.64685500
C	-0.62195300	-3.30582400	-0.36661900

Molecule 1 at M062X/6-31+G(d, p) level

C	0.63484900	-2.68241100	-0.07886500
C	1.91709600	-3.18277600	0.00137200
H	2.12788600	-4.24154700	-0.12302400
C	2.98839700	-2.29242200	0.29416300
C	4.30070700	-2.79534200	0.50858700

H	4.47068100	-3.86141500	0.38307500
C	5.32847600	-1.96954900	0.89741200
H	6.32012000	-2.37635000	1.06801700
C	5.08271300	-0.59405500	1.11728700
H	5.87655700	0.04579200	1.48892000
C	3.83148000	-0.06912500	0.88024900
H	3.63958100	0.97522100	1.09879200
C	2.76611100	-0.87924500	0.41750100
C	1.44533900	-0.35452100	0.16285300
C	1.02157300	0.99696900	-0.03452600
C	1.65954100	2.23724700	-0.36144100
C	2.98035800	2.55815000	-0.75916900
H	3.73459900	1.78618900	-0.85632000
C	3.29763600	3.87000800	-1.06627100
H	4.30720000	4.11679700	-1.37781100
C	2.32742400	4.88956900	-0.99249200
H	2.60735800	5.91123900	-1.22878800
C	1.00734800	4.59520800	-0.65201300
H	0.25653600	5.37972400	-0.63469100
C	0.66442300	3.28065700	-0.36033200
C	-0.63484900	2.68241100	-0.07886500
C	-1.91709600	3.18277600	0.00137200
H	-2.12788600	4.24154700	-0.12302300
C	-2.98839700	2.29242200	0.29416400
C	-4.30070600	2.79534300	0.50858700
H	-4.47068100	3.86141500	0.38307600
C	-5.32847600	1.96954900	0.89741200
H	-6.32012000	2.37635000	1.06801700
C	-5.08271300	0.59405500	1.11728600
H	-5.87655700	-0.04579200	1.48891900
C	-3.83148000	0.06912400	0.88024900
H	-3.63958100	-0.97522100	1.09879100
C	-2.76611100	0.87924500	0.41750100
C	-1.44533900	0.35452100	0.16285200
C	-0.40642900	1.28737700	0.05599000
C	-1.02157300	-0.99697000	-0.03452600
C	0.40642900	-1.28737700	0.05599000
C	-1.65954100	-2.23724700	-0.36144100
C	-2.98035800	-2.55815000	-0.75916900
H	-3.73459900	-1.78618900	-0.85632000
C	-3.29763600	-3.87000800	-1.06627100
H	-4.30720000	-4.11679700	-1.37781100
C	-2.32742400	-4.88956900	-0.99249200
H	-2.60735800	-5.91123900	-1.22878800

C	-1.00734800	-4.59520800	-0.65201300
H	-0.25653600	-5.37972400	-0.63469200
C	-0.66442300	-3.28065700	-0.36033200

Molecule 1 at CAM-B3LYP/6-31+G(d, p) level

C	0.66300600	-2.67088700	-0.08577800
C	1.94591900	-3.15864900	0.00283300
H	2.16473800	-4.21547700	-0.11656600
C	3.00794800	-2.26239400	0.29867600
C	4.31979600	-2.75745700	0.52139400
H	4.49563500	-3.82243400	0.39982500
C	5.34075000	-1.92845100	0.91268400
H	6.33313300	-2.33016100	1.09014500
C	5.08685800	-0.55604600	1.12273000
H	5.87586900	0.09094900	1.49202700
C	3.83633900	-0.03903400	0.87735300
H	3.64696100	1.00542700	1.08645800
C	2.77398700	-0.85200100	0.41662500
C	1.44943500	-0.33839400	0.15500000
C	1.00995000	1.00698200	-0.04426500
C	1.63206500	2.25573400	-0.36849200
C	2.94745700	2.59777800	-0.75701700
H	3.71454400	1.84020400	-0.84813700
C	3.24947600	3.91220400	-1.06098500
H	4.25800500	4.17183400	-1.36519400
C	2.26786400	4.91647800	-0.99192200
H	2.53385000	5.94220900	-1.22592900
C	0.95364000	4.60232200	-0.65592100
H	0.19338900	5.37703900	-0.63937400
C	0.62694600	3.28526200	-0.36723500
C	-0.66300600	2.67088700	-0.08577900
C	-1.94591900	3.15864900	0.00283300
H	-2.16473700	4.21547600	-0.11656700
C	-3.00794800	2.26239400	0.29867600
C	-4.31979600	2.75745700	0.52139400
H	-4.49563400	3.82243400	0.39982500
C	-5.34075100	1.92845100	0.91268400
H	-6.33313300	2.33016100	1.09014500
C	-5.08685800	0.55604600	1.12273000
H	-5.87587000	-0.09094900	1.49202600
C	-3.83633900	0.03903500	0.87735300
H	-3.64696200	-1.00542700	1.08645700
C	-2.77398700	0.85200100	0.41662500

C	-1.44943500	0.33839400	0.15500000
C	-0.42105100	1.28052000	0.04544600
C	-1.00995000	-1.00698200	-0.04426500
C	0.42105100	-1.28052000	0.04544500
C	-1.63206500	-2.25573400	-0.36849100
C	-2.94745700	-2.59777900	-0.75701700
H	-3.71454400	-1.84020500	-0.84813700
C	-3.24947600	-3.91220400	-1.06098500
H	-4.25800400	-4.17183500	-1.36519500
C	-2.26786400	-4.91647800	-0.99192200
H	-2.53384900	-5.94220900	-1.22593000
C	-0.95364000	-4.60232200	-0.65592100
H	-0.19338800	-5.37703900	-0.63937500
C	-0.62694600	-3.28526200	-0.36723400

Molecule 2 at B3LYP/6-31+G(d, p) level

Si	8.07822500	-0.14479500	0.47551100
Si	-8.07751500	0.14714600	0.47616900
C	8.28084100	-1.25630400	1.98968000
H	7.77455000	-2.21725400	1.84664500
C	8.78158600	-0.99215600	-1.06007000
H	8.65660200	-0.36480200	-1.94934000
C	8.92290200	1.52083600	0.75594600
H	9.99822300	1.37932000	0.91667900
C	6.27417400	0.15718400	0.20925100
C	5.07523900	0.35575000	0.03366900
C	3.69549700	0.60914700	-0.17019500
C	3.24598500	1.94626100	-0.50784300
C	4.18241900	2.98458700	-0.74973000
H	5.23714300	2.77244600	-0.61137700
C	3.78224800	4.23386100	-1.18775700
H	4.52464800	5.00361400	-1.37706900
C	2.41784900	4.49282700	-1.42679000
H	2.10374500	5.45091700	-1.82942700
C	1.47696100	3.51212300	-1.15970800
H	0.43564000	3.70475700	-1.38483100
C	1.84505900	2.24406200	-0.65284200
C	0.86281100	1.20784200	-0.37338000
C	1.35533600	-0.10295600	-0.25366400
C	0.54435900	-1.31831400	-0.17078800
C	1.45510000	-2.37699700	0.16590000
C	1.24747300	-3.72372200	0.55156800
H	0.24746900	-4.13332100	0.61508900

C	2.33548300	-4.51747700	0.88483000
H	2.17661400	-5.54775100	1.18726100
C	3.64688100	-3.99693500	0.84292900
H	4.48451200	-4.63997300	1.09634500
C	3.88239200	-2.66070600	0.50862000
H	4.89062900	-2.26495000	0.51503100
C	2.80054200	-1.83585300	0.19140300
C	2.73102400	-0.41069200	-0.09685500
C	-0.54452900	1.31724100	-0.17081800
C	-1.45548100	2.37591800	0.16549600
C	-1.24823300	3.72276500	0.55091100
H	-0.24832300	4.13253300	0.61481300
C	-2.33657800	4.51646500	0.88331700
H	-2.17797600	5.54686700	1.18546200
C	-3.64792500	3.99584300	0.84069700
H	-4.48582900	4.63890900	1.09310000
C	-3.88313100	2.65942900	0.50677400
H	-4.89150900	2.26403800	0.51223100
C	-2.80090600	1.83468300	0.19055600
C	-2.73110800	0.40951500	-0.09732700
C	-3.69566700	-0.61013200	-0.17128800
C	-3.24617000	-1.94734200	-0.50862400
C	-4.18252000	-2.98556200	-0.75118900
H	-5.23731600	-2.77327100	-0.61363500
C	-3.78225300	-4.23480300	-1.18917200
H	-4.52462300	-5.00444700	-1.37905100
C	-2.41775600	-4.49383900	-1.42759400
H	-2.10354100	-5.45190200	-1.83020900
C	-1.47693600	-3.51320000	-1.16007300
H	-0.43554800	-3.70586800	-1.38485400
C	-1.84517000	-2.24511200	-0.65335400
C	-0.86294500	-1.20893700	-0.37361900
C	-1.35542300	0.10184000	-0.25384400
C	-5.07519500	-0.35618900	0.03316500
C	-6.27391900	-0.15629300	0.20857200
C	-9.00222400	-0.29038000	-1.11227800
H	-8.65930100	0.32458200	-1.95144500
C	-8.66452900	-0.94540000	1.90129900
H	-8.12461500	-0.71272000	2.82558000
C	-8.31575400	1.97237900	0.89960600
H	-9.37772200	2.18771100	1.06695100
H	8.79434800	2.18055000	-0.10915600
H	8.51286200	2.02935600	1.63528000
H	9.85274400	-1.18789800	-0.93023900

H	8.28250700	-1.94915200	-1.24773900
H	7.86424500	-0.78353700	2.88570800
H	9.34269900	-1.45791300	2.17451500
H	-7.96485900	2.61722300	0.08642900
H	-7.76908900	2.24279400	1.80966000
H	-8.85308600	-1.34229800	-1.37946600
H	-10.07837200	-0.12234100	-0.98534900
H	-9.73448500	-0.79040500	2.08463800
H	-8.50976700	-2.00624600	1.67591500

Molecule 2 at PBE0/6-31+G(d, p) level

Si	8.05387300	-0.12849600	0.46332100
Si	-8.04730000	0.16132100	0.46512200
C	8.24730900	-1.25492400	1.95725900
H	7.73794300	-2.21147000	1.79931500
C	8.74960900	-0.95361100	-1.07753800
H	8.62344300	-0.31451800	-1.95761800
C	8.89055300	1.52839400	0.76304000
H	9.96553100	1.38634900	0.92224100
C	6.25212600	0.17713300	0.20053800
C	5.05335100	0.37458700	0.02898600
C	3.67506200	0.62123900	-0.17024700
C	3.22012600	1.95126600	-0.50101200
C	4.14979800	2.99140100	-0.73602500
H	5.20611300	2.78084000	-0.59781700
C	3.74336400	4.23727400	-1.16557900
H	4.48132500	5.01259900	-1.35065900
C	2.38080400	4.48919200	-1.40396600
H	2.06218300	5.44748400	-1.80320200
C	1.44748900	3.50519000	-1.14347800
H	0.40361700	3.68996300	-1.37009600
C	1.82370700	2.24093000	-0.64405600
C	0.85173700	1.20252000	-0.37143700
C	1.34842000	-0.10235000	-0.25402100
C	0.54836300	-1.31787400	-0.16816900
C	1.46239600	-2.36745400	0.16719400
C	1.26105900	-3.70987300	0.55657900
H	0.26157400	-4.12306200	0.62579100
C	2.35182000	-4.49402900	0.88810000
H	2.19961600	-5.52427600	1.19494600
C	3.65664600	-3.96801600	0.84165200
H	4.49815600	-4.60644900	1.09527900
C	3.88450100	-2.63495500	0.50526200

H	4.89070100	-2.23088700	0.50894300
C	2.79894000	-1.82126500	0.18922500
C	2.72132800	-0.40138600	-0.09909200
C	-0.55118200	1.30295000	-0.16976600
C	-1.46560200	2.35288100	0.16373400
C	-1.26484800	3.69590300	0.55133700
H	-0.26549400	4.10933000	0.62099400
C	-2.35609100	4.48048600	0.88037600
H	-2.20428400	5.51124400	1.18571500
C	-3.66086200	3.95440000	0.83302300
H	-4.50285600	4.59320600	1.08419000
C	-3.88830000	2.62074200	0.49864500
H	-4.89476300	2.21724700	0.50133500
C	-2.80216700	1.80662000	0.18539500
C	-2.72399600	0.38637300	-0.10077500
C	-3.67771100	-0.63628900	-0.17136800
C	-3.22286000	-1.96659200	-0.50049800
C	-4.15258400	-3.00659700	-0.73558900
H	-5.20896300	-2.79548400	-0.59876100
C	-3.74610700	-4.25287500	-1.16386500
H	-4.48406300	-5.02815700	-1.34912800
C	-2.38338000	-4.50523900	-1.40092500
H	-2.06465800	-5.46392000	-1.79914300
C	-1.45003200	-3.52120300	-1.14064600
H	-0.40605600	-3.70640200	-1.36645600
C	-1.82634700	-2.25639900	-0.64266400
C	-0.85445200	-1.21772800	-0.37060300
C	-1.35108100	0.08727100	-0.25469100
C	-5.05534500	-0.38687200	0.02832200
C	-6.25243400	-0.18043700	0.20079800
C	-8.97531400	-0.27982100	-1.11026600
H	-8.61848700	0.31482800	-1.95757600
C	-8.64896100	-0.89250000	1.90199900
H	-8.10069700	-0.65688200	2.81999900
C	-8.23457600	1.99115500	0.85777500
H	-9.28979300	2.23682000	1.02292600
H	8.76006900	2.19659800	-0.09464600
H	8.47822500	2.02400600	1.64805100
H	9.82021900	-1.15152600	-0.95066100
H	8.24862300	-1.90716000	-1.27467600
H	7.83005700	-0.79125700	2.85712100
H	9.30782700	-1.46195400	2.14090000
H	-7.86774300	2.61157600	0.03320500
H	-7.67891800	2.25955700	1.76254200

H	-8.84746200	-1.33854400	-1.35900300
H	-10.04703700	-0.08700700	-0.98555900
H	-9.71430300	-0.71114300	2.08501600
H	-8.51732500	-1.95881800	1.69050600

Molecule 2 at BMK/6-31+G(d, p) level

Si	8.08403300	-0.12524200	0.45221100
Si	-8.07697400	0.16699100	0.45146700
C	8.31815700	-1.01844100	2.08607500
H	7.80528100	-1.98926400	2.08352700
C	8.72955900	-1.16822400	-0.96848300
H	8.57646900	-0.66161600	-1.93050700
C	8.93004900	1.54910800	0.48364000
H	10.01151900	1.42436900	0.63455300
C	6.28062200	0.15494300	0.19716700
C	5.08349300	0.35461400	0.02741200
C	3.69487300	0.61186000	-0.17125100
C	3.24360200	1.95327900	-0.50005900
C	4.18238900	2.99838400	-0.73652600
H	5.24034200	2.78614100	-0.60258300
C	3.77461600	4.25135100	-1.16117100
H	4.51451400	5.02732600	-1.34678400
C	2.40185700	4.50992600	-1.39471300
H	2.08485200	5.47262000	-1.78975800
C	1.46255400	3.52435900	-1.13450800
H	0.41698400	3.71109500	-1.35762700
C	1.84071500	2.24847200	-0.63827600
C	0.86042300	1.20550700	-0.36515200
C	1.35614700	-0.10712000	-0.24754700
C	0.54755500	-1.33132200	-0.16253800
C	1.46656100	-2.38885100	0.17216400
C	1.26457100	-3.74026000	0.56152900
H	0.26387500	-4.15438400	0.63289500
C	2.36191200	-4.52935000	0.89036500
H	2.20879200	-5.56213600	1.19524200
C	3.67484300	-4.00213800	0.84213200
H	4.51796400	-4.64272400	1.09306700
C	3.90304300	-2.66085000	0.50590200
H	4.91060200	-2.25457100	0.50724400
C	2.81106000	-1.84395500	0.19240500
C	2.73616000	-0.41085200	-0.09600300
C	-0.55097000	1.31187900	-0.16408500
C	-1.46976400	2.36995800	0.16980400

C	-1.26690800	3.72168400	0.55723100
H	-0.26599700	4.13559600	0.62699700
C	-2.36373300	4.51151100	0.88605300
H	-2.21006500	5.54465600	1.18945600
C	-3.67680600	3.98471100	0.83947100
H	-4.51935300	4.62598700	1.09019300
C	-3.90602900	2.64303500	0.50506200
H	-4.91439700	2.23784600	0.50764800
C	-2.81443600	1.82533800	0.19152500
C	-2.73934400	0.39178200	-0.09500500
C	-3.69827500	-0.63068900	-0.16953600
C	-3.24753300	-1.97273100	-0.49567400
C	-4.18673300	-3.01784300	-0.73026700
H	-5.24457600	-2.80468900	-0.59695600
C	-3.77947000	-4.27173500	-1.15255300
H	-4.51961500	-5.04780800	-1.33673300
C	-2.40676700	-4.53119300	-1.38561600
H	-2.09015700	-5.49474400	-1.77887100
C	-1.46705600	-3.54547700	-1.12751100
H	-0.42162700	-3.73299400	-1.35054600
C	-1.84467900	-2.26848600	-0.63361100
C	-0.86406800	-1.22522900	-0.36274300
C	-1.35952700	0.08762500	-0.24661800
C	-5.08620200	-0.36921200	0.02749000
C	-6.28152800	-0.15876200	0.19627400
C	-8.98682700	-0.26637200	-1.13181900
H	-8.62658700	0.34092000	-1.97261800
C	-8.67563900	-0.90404200	1.87148200
H	-8.13204100	-0.67180500	2.79672700
C	-8.28208700	1.98678700	0.85940900
H	-9.34355400	2.22198800	1.02042500
H	8.77743200	2.08652900	-0.46165600
H	8.54110400	2.17226200	1.29973800
H	9.80636200	-1.35130400	-0.84539600
H	8.22029100	-2.14016700	-1.00862400
H	7.92221200	-0.42435600	2.92021400
H	9.38681500	-1.19778500	2.27023900
H	-7.91424700	2.61927900	0.04057100
H	-7.73291100	2.25084300	1.77292200
H	-8.84782700	-1.32467000	-1.38938000
H	-10.06392500	-0.08236000	-1.01308900
H	-9.74636200	-0.73262800	2.05106800
H	-8.53326100	-1.96981100	1.64893100

Molecule 2 at M062X/6-31+G(d, p) level

Si	-8.03773700	0.08001600	0.45878300
Si	8.01076400	-0.19752500	0.46522300
C	-8.19326300	1.18434500	1.96893100
H	-7.66524800	2.13080800	1.81655600
C	-8.71015600	0.94594000	-1.06484500
H	-8.59914900	0.31763200	-1.95341600
C	-8.89771900	-1.56482300	0.73215000
H	-9.96942400	-1.40873700	0.89300100
C	-6.23563700	-0.25427500	0.18598100
C	-5.04097800	-0.45019100	0.01695300
C	-3.65018700	-0.68117800	-0.17987300
C	-3.17105300	-2.00484100	-0.49786900
C	-4.08185900	-3.06850300	-0.72148500
H	-5.14223400	-2.87995800	-0.58498600
C	-3.64626000	-4.30722800	-1.13566600
H	-4.36431500	-5.10173200	-1.31194200
C	-2.27428100	-4.53164500	-1.37358200
H	-1.93719200	-5.48613800	-1.76425600
C	-1.36344100	-3.52700600	-1.12668400
H	-0.31568900	-3.68548600	-1.35509400
C	-1.77138500	-2.26519600	-0.63738700
C	-0.82197100	-1.20383100	-0.37454300
C	-1.34494600	0.09071600	-0.26020300
C	-0.57248600	1.32900500	-0.17105500
C	-1.51282900	2.35786200	0.16452700
C	-1.34086100	3.70301900	0.56389100
H	-0.35080500	4.13557600	0.64542400
C	-2.45142300	4.46112700	0.89186500
H	-2.32320500	5.49164400	1.20569600
C	-3.74528700	3.90873400	0.83394600
H	-4.60086600	4.52771000	1.08506700
C	-3.94254000	2.57171300	0.49092600
H	-4.93943600	2.14591900	0.48701000
C	-2.83615300	1.78547300	0.17859500
C	-2.72511400	0.35962600	-0.11000600
C	0.58373100	-1.27622200	-0.17736200
C	1.52513700	-2.30642500	0.15157700
C	1.35543300	-3.65381100	0.54470100
H	0.36597500	-4.08763600	0.62676300

C	2.46747200	-4.41295600	0.86559000
H	2.34058400	-5.44519100	1.17429800
C	3.76098500	-3.85957500	0.80679900
H	4.61831500	-4.47890500	1.05174200
C	3.95608900	-2.52070200	0.47044300
H	4.95254800	-2.09430800	0.46583000
C	2.84828500	-1.73351800	0.16525500
C	2.73597100	-0.30660600	-0.11648200
C	3.66125100	0.73430400	-0.18414300
C	3.18212900	2.05881600	-0.49599800
C	4.09318200	3.12233100	-0.71824200
H	5.15365200	2.93191300	-0.58561900
C	3.65750500	4.36281900	-1.12692000
H	4.37557900	5.15746200	-1.30245300
C	2.28498800	4.58890000	-1.36040400
H	1.94755500	5.54505700	-1.74668900
C	1.37396400	3.58396400	-1.11514100
H	0.32582200	3.74414200	-1.34061100
C	1.78211500	2.31998800	-0.63164700
C	0.83282700	1.25770200	-0.37116100
C	1.35573500	-0.03737700	-0.26292200
C	5.05040300	0.49312600	0.01130000
C	6.23901100	0.26517900	0.18293700
C	8.98395300	0.19010200	-1.09160700
H	8.59267700	-0.36889500	-1.94664800
C	8.66062200	0.79252300	1.92051100
H	8.08049900	0.58518800	2.82444900
C	8.04332300	-2.03824900	0.83677700
H	9.07103500	-2.36996000	1.01769300
H	-8.77387700	-2.21850100	-0.13650400
H	-8.49054200	-2.07696100	1.60891700
H	-9.77393100	1.16977000	-0.93287800
H	-8.18147100	1.88743200	-1.24222600
H	-7.77497000	0.69705500	2.85451700
H	-9.24666500	1.40947200	2.16573000
H	7.64296300	-2.61413300	-0.00361300
H	7.44955600	-2.26786400	1.72722400
H	8.93468500	1.25739000	-1.32705200
H	10.03581100	-0.08221600	-0.95552100
H	9.70617800	0.53252500	2.11615300
H	8.60751500	1.86612500	1.71678300

Molecule 2 at CAM-B3LYP/6-31+G(d, p) level

Si	8.04957800	-0.12349700	0.43634900
Si	-8.04281600	0.15973600	0.43645600
C	8.25050900	-1.22494300	1.94385700
H	7.73817100	-2.18194800	1.80569400
C	8.73010100	-0.97217600	-1.09443800
H	8.59973900	-0.34720100	-1.98295500
C	8.89140300	1.53267500	0.70472600
H	9.96641900	1.39269400	0.85908900
C	6.24524900	0.18255100	0.18186800
C	5.05358300	0.38118000	0.01862500
C	3.66620600	0.62932500	-0.17222000
C	3.20979400	1.95855300	-0.49787100
C	4.13856200	3.00057500	-0.73804800
H	5.19444500	2.79170300	-0.60887000
C	3.72996500	4.24340800	-1.15876100
H	4.46461500	5.01938800	-1.34803800
C	2.36385400	4.49579900	-1.38311300
H	2.04272700	5.45523400	-1.77490600
C	1.43583600	3.51470400	-1.11960100
H	0.39234600	3.70165500	-1.33551100
C	1.81606100	2.24630700	-0.62856300
C	0.84748800	1.20580900	-0.35328700
C	1.34736400	-0.09550900	-0.23714800
C	0.55215200	-1.31816500	-0.14908700
C	1.47355400	-2.36331300	0.18447000
C	1.28101800	-3.70562000	0.57452500
H	0.28616000	-4.12412500	0.64879800
C	2.37518300	-4.48494500	0.90009300
H	2.22721300	-5.51505500	1.20631600
C	3.67555500	-3.95624700	0.84800100
H	4.52044800	-4.58985900	1.09774600
C	3.89334900	-2.62381000	0.50963800
H	4.89632200	-2.21634800	0.50768400
C	2.80442400	-1.81693900	0.19912000
C	2.72107000	-0.39001800	-0.09073200
C	-0.55505900	1.30163000	-0.15014900
C	-1.47650100	2.34715300	0.18234500
C	-1.28404800	3.69001800	0.57050500
H	-0.28920600	4.10865600	0.64425000

C	-2.37831200	4.46979500	0.89475100
H	-2.23037200	5.50037300	1.19942100
C	-3.67870100	3.94108400	0.84303800
H	-4.52375500	4.57509200	1.09127500
C	-3.89653100	2.60810100	0.50677300
H	-4.89983700	2.20141500	0.50482600
C	-2.80740600	1.80074500	0.19782200
C	-2.72376500	0.37348000	-0.09006200
C	-3.66901700	-0.64581700	-0.17064900
C	-3.21299400	-1.97539600	-0.49470400
C	-4.14204000	-3.01730700	-0.73403100
H	-5.19787500	-2.80780600	-0.60547200
C	-3.73377800	-4.26065000	-1.15349900
H	-4.46859400	-5.03660900	-1.34220900
C	-2.36769200	-4.51357500	-1.37751000
H	-2.04680200	-5.47348000	-1.76834900
C	-1.43940100	-3.53243300	-1.11509600
H	-0.39599800	-3.71989200	-1.33098600
C	-1.81927000	-2.26338600	-0.62545100
C	-0.85049600	-1.22262500	-0.35165600
C	-1.35019700	0.07883900	-0.23653500
C	-5.05567700	-0.39440100	0.02027800
C	-6.24558800	-0.18595200	0.18378500
C	-8.95726700	-0.26779200	-1.14675400
H	-8.59163600	0.32940200	-1.98741300
C	-8.65662200	-0.89919000	1.86017300
H	-8.11423600	-0.67241700	2.78288300
C	-8.22855400	1.98451400	0.83842900
H	-9.28299600	2.23415400	0.99624400
H	8.75729800	2.18874200	-0.16065000
H	8.48711000	2.04332000	1.58383700
H	9.80013400	-1.17251300	-0.97497100
H	8.22549500	-1.92615500	-1.27481600
H	7.84066600	-0.74763000	2.83895800
H	9.31024800	-1.43276900	2.12552000
H	-7.85300600	2.60961900	0.02253100
H	-7.68050300	2.24668800	1.74858300
H	-8.83167100	-1.32439300	-1.40184100
H	-10.02877700	-0.07249900	-1.03278700
H	-9.72149300	-0.71689900	2.03935700
H	-8.52765100	-1.96408900	1.64434100

Molecule 3 at B3LYP/6-31+G(d, p) level

Si	8.09009600	0.71657700	0.38767800
C	8.81570700	1.71335000	-1.04804400
H	8.61279800	1.24049700	-2.01450600
H	9.90111200	1.81979400	-0.94064100
H	8.38042200	2.71858600	-1.06781900
C	8.45053200	1.60800000	2.01765000
H	7.98893700	1.09851200	2.86962400
H	8.05659300	2.62979300	1.98350000
H	9.52954000	1.66995500	2.20008400
C	8.77319600	-1.08221700	0.40680300
C	10.31626300	-1.04287900	0.49575200
H	10.71631700	-2.06627600	0.52232000
H	10.66503500	-0.53397500	1.40182800
H	10.76575900	-0.53998800	-0.36791600
C	8.36504500	-1.82239500	-0.88549400
H	8.76017300	-2.84817600	-0.87412700
H	8.75991000	-1.33049500	-1.78180800
H	7.27682900	-1.88809900	-0.99303600
C	8.22253700	-1.84914800	1.62875300
H	8.59625300	-2.88293700	1.62601600
H	7.12785500	-1.89500600	1.62648200
H	8.53438900	-1.39142000	2.57419700
C	6.25404800	0.67646000	0.15834200
C	5.03900500	0.73940700	-0.01013800
C	3.64246500	0.87847900	-0.21542300
C	3.09465800	2.17960600	-0.55379500
C	3.95050800	3.28539700	-0.79579900
H	5.01793400	3.15339100	-0.65712300
C	3.45863500	4.50111400	-1.23501800
H	4.14199500	5.32376200	-1.42423800
C	2.07919200	4.65774900	-1.47568300
H	1.69483500	5.58937200	-1.87946700
C	1.21424800	3.60958900	-1.20851700
H	0.16165200	3.72330900	-1.43476700
C	1.67562100	2.37301700	-0.70025500
C	0.77209900	1.26780400	-0.42073500
C	-0.63949100	1.27404300	-0.21841900
C	-1.62502900	2.26363400	0.11720900
C	-1.51761400	3.62241400	0.50174300
H	-0.55064200	4.10482100	0.56560100
C	-2.66155300	4.33422400	0.83294500
H	-2.57933300	5.37369600	1.13438100
C	1.35978200	-0.00279300	-0.30074100
C	2.75461900	-0.20886200	-0.14401300

C	2.92684400	-1.62535500	0.14202600
C	4.06625500	-2.36877200	0.45583800
H	5.04178700	-1.89882400	0.45901800
C	3.93122200	-3.71891100	0.78920900
H	4.81446300	-4.29884200	1.03975200
Si	-8.09009600	-0.71657700	0.38767700
C	-8.81570700	-1.71334800	-1.04804500
H	-8.61279700	-1.24049600	-2.01450600
H	-9.90111300	-1.81979200	-0.94064200
H	-8.38042300	-2.71858500	-1.06782000
C	-8.45053200	-1.60800200	2.01764900
H	-7.98893800	-1.09851300	2.86962300
H	-8.05659100	-2.62979300	1.98349900
H	-9.52954000	-1.66995900	2.20008300
C	-8.77319600	1.08221700	0.40680400
C	-10.31626300	1.04287900	0.49575400
H	-10.71631700	2.06627600	0.52232200
H	-10.66503500	0.53397400	1.40182900
H	-10.76576000	0.53998800	-0.36791400
C	-8.36504500	1.82239600	-0.88549200
H	-8.76017300	2.84817700	-0.87412500
H	-8.75991000	1.33049700	-1.78180700
H	-7.27682900	1.88810000	-0.99303500
C	-8.22253700	1.84914800	1.62875400
H	-8.59625300	2.88293600	1.62601800
H	-7.12785500	1.89500500	1.62648300
H	-8.53438800	1.39141900	2.57419800
C	-6.25404800	-0.67646000	0.15834200
C	-5.03900500	-0.73940700	-0.01013800
C	-3.64246500	-0.87847900	-0.21542400
C	-3.09465800	-2.17960600	-0.55379600
C	-3.95050800	-3.28539700	-0.79580000
H	-5.01793300	-3.15339200	-0.65712400
C	-3.45863400	-4.50111400	-1.23501900
H	-4.14199400	-5.32376200	-1.42423800
C	-2.07919200	-4.65774900	-1.47568300
H	-1.69483400	-5.58937200	-1.87946700
C	-1.21424700	-3.60958900	-1.20851700
H	-0.16165200	-3.72330800	-1.43476700
C	-1.67562100	-2.37301700	-0.70025600
C	-0.77209900	-1.26780400	-0.42073600
C	0.63949100	-1.27404300	-0.21841900
C	1.62502900	-2.26363400	0.11721000
C	1.51761400	-3.62241400	0.50174400

H	0.55064100	-4.10482000	0.56560200
C	2.66155300	-4.33422400	0.83294500
H	2.57933300	-5.37369600	1.13438200
C	-1.35978200	0.00279300	-0.30074100
C	-2.75461900	0.20886200	-0.14401400
C	-2.92684400	1.62535500	0.14202400
C	-4.06625500	2.36877200	0.45583700
H	-5.04178700	1.89882400	0.45901700
C	-3.93122200	3.71891100	0.78920800
H	-4.81446300	4.29884200	1.03975100

Molecule 3 at PBE0/6-31+G(d, p) level

Si	-8.06663000	-0.71543000	0.37417900
C	-8.79056800	-1.68731600	-1.06780700
H	-8.57785200	-1.20581800	-2.02754200
H	-9.87707200	-1.78342600	-0.96469500
H	-8.36469300	-2.69602800	-1.09477700
C	-8.44747400	-1.60058400	1.99256200
H	-7.97537800	-1.10330900	2.84562000
H	-8.07747400	-2.63075400	1.95531100
H	-9.52805100	-1.63715400	2.17106800
C	-8.71074500	1.08505100	0.39592700
C	-10.24473500	1.06902100	0.46076300
H	-10.62891700	2.09843400	0.49092900
H	-10.61477500	0.55736600	1.35693400
H	-10.68810100	0.58113400	-0.41472800
C	-8.26838300	1.81606600	-0.87765500
H	-8.64025300	2.85054000	-0.86725500
H	-8.66035200	1.33678200	-1.78211000
H	-7.17705100	1.85659600	-0.96804900
C	-8.16425300	1.82130100	1.62545600
H	-8.50938700	2.86503500	1.62478700
H	-7.06848100	1.83632500	1.64325700
H	-8.50569600	1.36411000	2.56094600
C	-6.23120700	-0.69418800	0.15721900
C	-5.01683000	-0.75969000	-0.00898300
C	-3.62261400	-0.89368600	-0.21052100
C	-3.07100100	-2.18797500	-0.54068400
C	-3.92098500	-3.29449500	-0.77473100
H	-4.98977700	-3.16304100	-0.63604400
C	-3.42421600	-4.50707200	-1.20473300
H	-4.10341100	-5.33456900	-1.38895200
C	-2.04731500	-4.65802900	-1.44507000

H	-1.65927500	-5.59012000	-1.84487300
C	-1.18926100	-3.60755400	-1.18574100
H	-0.13489400	-3.71428300	-1.41379500
C	-1.65722500	-2.37465600	-0.68560100
C	-0.76306300	-1.26846800	-0.41395000
C	0.64348900	-1.26699500	-0.21307200
C	1.63149100	-2.24832100	0.11913400
C	1.53075600	-3.60301400	0.50538700
H	0.56473200	-4.08911500	0.57601800
C	2.67731800	-4.30585900	0.83142000
H	2.60202000	-5.34531700	1.13563400
C	-1.35353400	-0.00348800	-0.29733000
C	-2.74481500	0.19504500	-0.14334600
C	-2.92421200	1.60620800	0.13970900
C	-4.06696200	2.33902300	0.44823900
H	-5.03955100	1.86036300	0.44692600
C	-3.94020100	3.68598900	0.78140200
H	-4.82764500	4.26155600	1.02897100
Si	8.06663000	0.71542900	0.37417900
C	8.79057000	1.68731100	-1.06780900
H	8.57785200	1.20581200	-2.02754300
H	9.87707400	1.78341800	-0.96469800
H	8.36469700	2.69602300	-1.09478000
C	8.44747500	1.60058600	1.99256000
H	7.97538000	1.10331200	2.84562000
H	8.07747500	2.63075500	1.95530800
H	9.52805200	1.63715600	2.17106600
C	8.71074300	-1.08505300	0.39593100
C	10.24473300	-1.06902500	0.46076400
H	10.62891400	-2.09843800	0.49093100
H	10.61477500	-0.55736800	1.35693300
H	10.68809700	-0.58114100	-0.41473000
C	8.26837600	-1.81607200	-0.87764800
H	8.64024600	-2.85054600	-0.86724600
H	8.66034300	-1.33679100	-1.78210500
H	7.17704400	-1.85660100	-0.96803800
C	8.16425300	-1.82129900	1.62546400
H	8.50938600	-2.86503300	1.62479700
H	7.06848100	-1.83632200	1.64326700
H	8.50569900	-1.36410500	2.56095100
C	6.23120700	0.69418800	0.15721800
C	5.01683100	0.75969100	-0.00898500
C	3.62261500	0.89368800	-0.21052400
C	3.07100100	2.18797600	-0.54068700

C	3.92098500	3.29449700	-0.77473400
H	4.98977700	3.16304200	-0.63604900
C	3.42421500	4.50707400	-1.20473700
H	4.10341000	5.33457000	-1.38895600
C	2.04731400	4.65803000	-1.44507200
H	1.65927400	5.59012100	-1.84487400
C	1.18926100	3.60755500	-1.18574200
H	0.13489300	3.71428400	-1.41379500
C	1.65722500	2.37465800	-0.68560300
C	0.76306300	1.26846900	-0.41395100
C	-0.64348900	1.26699600	-0.21307100
C	-1.63149000	2.24832200	0.11913600
C	-1.53075400	3.60301500	0.50539000
H	-0.56473000	4.08911700	0.57601900
C	-2.67731600	4.30586000	0.83142500
H	-2.60201700	5.34531800	1.13563900
C	1.35353500	0.00348900	-0.29733200
C	2.74481600	-0.19504300	-0.14335000
C	2.92421400	-1.60620700	0.13970500
C	4.06696400	-2.33902200	0.44823200
H	5.03955200	-1.86036200	0.44691700
C	3.94020300	-3.68598800	0.78139500
H	4.82764700	-4.26155500	1.02896200

Molecule 3 at BMK/6-31+G(d, p) level

Si	-8.07665800	-0.70515900	0.29606000
C	-8.87222900	-1.26901600	-1.30953800
H	-8.59742300	-0.61386800	-2.14643500
H	-9.96749500	-1.27273200	-1.21952200
H	-8.54974500	-2.28915400	-1.55721600
C	-8.50506500	-1.89879400	1.68170400
H	-8.02361800	-1.60985000	2.62503100
H	-8.17174200	-2.91390400	1.42792300
H	-9.59147100	-1.92974900	1.84441200
C	-8.59394100	1.06838300	0.73275700
C	-10.12878900	1.11578200	0.95304500
H	-10.43739500	2.14357800	1.20065300
H	-10.44110700	0.46620800	1.78230500
H	-10.67955200	0.81169900	0.05219900
C	-8.22495300	2.03543600	-0.42004200
H	-8.51317900	3.06437700	-0.15316400
H	-8.74649900	1.77358300	-1.35075400
H	-7.14535800	2.03030100	-0.62528700

C	-7.88880400	1.53153000	2.03219300
H	-8.19108400	2.56226700	2.27564200
H	-6.79497800	1.51640900	1.92841300
H	-8.15561100	0.89495700	2.88691600
C	-6.24777200	-0.74075500	0.06420300
C	-5.03517100	-0.81838500	-0.09690800
C	-3.62770900	-0.94849000	-0.29059500
C	-3.05754700	-2.24538300	-0.61462600
C	-3.89881300	-3.37104300	-0.84784400
H	-4.97137000	-3.25289200	-0.71473500
C	-3.38060900	-4.58412100	-1.26781900
H	-4.04803300	-5.42386100	-1.45042300
C	-1.99012500	-4.71962700	-1.50023600
H	-1.58794500	-5.65145000	-1.89170900
C	-1.14293700	-3.65306500	-1.24319700
H	-0.08482900	-3.74635000	-1.46563600
C	-1.63374300	-2.41451500	-0.75103200
C	-0.75017200	-1.28777400	-0.48017300
C	0.66509100	-1.26712900	-0.27958900
C	1.67492200	-2.23847500	0.05494200
C	1.59591500	-3.60158000	0.44785000
H	0.63655500	-4.10337200	0.52331400
C	2.76010100	-4.28848900	0.77662700
H	2.70037900	-5.32986700	1.08471800
C	-1.36095100	-0.02456700	-0.36452300
C	-2.76306000	0.15479900	-0.21529600
C	-2.96509900	1.57529700	0.07169800
C	-4.12555300	2.29115600	0.38365300
H	-5.09221200	1.79561500	0.38044900
C	-4.02069300	3.64633100	0.72356700
H	-4.91899300	4.20741500	0.97312500
Si	8.07665800	0.70515900	0.29606100
C	8.87222600	1.26902000	-1.30953700
H	8.59741400	0.61387700	-2.14643600
H	9.96749200	1.27273100	-1.21952400
H	8.54974600	2.28916100	-1.55720800
C	8.50506800	1.89879000	1.68170800
H	8.02362600	1.60984100	2.62503600
H	8.17174000	2.91390000	1.42793200
H	9.59147400	1.92974800	1.84441000
C	8.59394200	-1.06838500	0.73275300
C	10.12879000	-1.11578400	0.95303800
H	10.43739600	-2.14358100	1.20064400
H	10.44111000	-0.46621200	1.78229900

H	10.67955100	-0.81169800	0.05219200
C	8.22495200	-2.03543400	-0.42004800
H	8.51317900	-3.06437600	-0.15317400
H	8.74649600	-1.77357800	-1.35076100
H	7.14535700	-2.03029900	-0.62529200
C	7.88880700	-1.53153500	2.03218900
H	8.19108600	-2.56227400	2.27563300
H	6.79498100	-1.51641200	1.92841200
H	8.15561700	-0.89496600	2.88691300
C	6.24777100	0.74075500	0.06420700
C	5.03517100	0.81838500	-0.09690600
C	3.62770900	0.94849000	-0.29059300
C	3.05754700	2.24538300	-0.61462400
C	3.89881300	3.37104400	-0.84784100
H	4.97137000	3.25289200	-0.71473100
C	3.38060900	4.58412200	-1.26781600
H	4.04803300	5.42386100	-1.45042000
C	1.99012500	4.71962700	-1.50023400
H	1.58794500	5.65145100	-1.89170700
C	1.14293700	3.65306500	-1.24319600
H	0.08482900	3.74635000	-1.46563500
C	1.63374300	2.41451500	-0.75103100
C	0.75017200	1.28777400	-0.48017200
C	-0.66509100	1.26713000	-0.27958900
C	-1.67492300	2.23847500	0.05494000
C	-1.59591600	3.60158100	0.44784700
H	-0.63655500	4.10337300	0.52331200
C	-2.76010200	4.28849000	0.77662300
H	-2.70038000	5.32986800	1.08471300
C	1.36095100	0.02456800	-0.36452200
C	2.76306000	-0.15479900	-0.21529400
C	2.96509900	-1.57529600	0.07170100
C	4.12555300	-2.29115500	0.38365600
H	5.09221100	-1.79561500	0.38045200
C	4.02069300	-3.64633000	0.72357200
H	4.91899300	-4.20741400	0.97313100

Molecule 3 at M062X/6-31+G(d, p) level

Si	-8.04509000	-0.72715000	0.38933300
C	-8.83480400	-1.70179000	-1.00966300
H	-8.64748800	-1.23453300	-1.98095500
H	-9.91744800	-1.77361000	-0.86312600
H	-8.42771900	-2.71731200	-1.03648400

C	-8.43921100	-1.52914800	2.04240300
H	-7.89333000	-1.04746700	2.85864200
H	-8.15975000	-2.58699700	2.02322900
H	-9.51101500	-1.46522800	2.25788800
C	-8.58416500	1.09538900	0.35977800
C	-10.11954700	1.16485100	0.36379400
H	-10.44612400	2.21326300	0.38707500
H	-10.55059900	0.66702400	1.24022500
H	-10.54828300	0.70542700	-0.53377800
C	-8.05372300	1.78494900	-0.90519300
H	-8.38018100	2.83364700	-0.92551700
H	-8.42683900	1.30481500	-1.81699900
H	-6.95899500	1.77401800	-0.94660400
C	-8.04295700	1.81590200	1.60324400
H	-8.29856700	2.88345600	1.56127200
H	-6.95201000	1.73730200	1.68097300
H	-8.47215800	1.40792300	2.52492700
C	-6.20654400	-0.78581900	0.15151600
C	-4.99787000	-0.86257400	-0.01772600
C	-3.59292100	-0.98196500	-0.21866400
C	-3.01482900	-2.26675500	-0.53442700
C	-3.84181800	-3.39721000	-0.75589400
H	-4.91344500	-3.28998300	-0.62007700
C	-3.31348700	-4.59998800	-1.16826400
H	-3.96937200	-5.44685400	-1.34316100
C	-1.92875200	-4.72015500	-1.40656300
H	-1.52032100	-5.64696700	-1.79576100
C	-1.09704200	-3.64835500	-1.16244500
H	-0.04052900	-3.72664200	-1.39187600
C	-1.59938800	-2.42038200	-0.67534700
C	-0.73189500	-1.28996600	-0.41638100
C	0.67498500	-1.25599800	-0.21960700
C	1.69170700	-2.21183600	0.11104800
C	1.62960100	-3.56855100	0.50446700
H	0.67816600	-4.08066100	0.58478900
C	2.79800300	-4.23687300	0.82869200
H	2.75206000	-5.27578900	1.13753700
C	-1.35109100	-0.03836400	-0.30531500
C	-2.74743100	0.12473800	-0.15536600
C	-2.96549500	1.53815000	0.12682400
C	-4.13040300	2.23385400	0.43524200
H	-5.08659300	1.72438600	0.43159100
C	-4.04425500	3.58329300	0.77295000
H	-4.94827000	4.13126400	1.02095400

Si	8.04509000	0.72715000	0.38933200
C	8.83480700	1.70178500	-1.00966500
H	8.64749200	1.23452500	-1.98095600
H	9.91745000	1.77360500	-0.86312700
H	8.42772300	2.71730800	-1.03649100
C	8.43920900	1.52915300	2.04240000
H	7.89332600	1.04747500	2.85864000
H	8.15974800	2.58700300	2.02322200
H	9.51101200	1.46523300	2.25788800
C	8.58416300	-1.09538900	0.35978400
C	10.11954600	-1.16485200	0.36380300
H	10.44612200	-2.21326400	0.38708800
H	10.55059600	-0.66702200	1.24023200
H	10.54828300	-0.70543100	-0.53377000
C	8.05372300	-1.78495200	-0.90518500
H	8.38018000	-2.83365100	-0.92550600
H	8.42684000	-1.30482200	-1.81699300
H	6.95899500	-1.77402100	-0.94659800
C	8.04295400	-1.81589700	1.60325200
H	8.29856300	-2.88345100	1.56128400
H	6.95200600	-1.73729700	1.68097900
H	8.47215300	-1.40791600	2.52493400
C	6.20654400	0.78581900	0.15151300
C	4.99787000	0.86257500	-0.01773100
C	3.59292100	0.98196500	-0.21866800
C	3.01482900	2.26675500	-0.53443000
C	3.84181800	3.39721000	-0.75589900
H	4.91344500	3.28998300	-0.62008200
C	3.31348600	4.59998800	-1.16826800
H	3.96937200	5.44685400	-1.34316600
C	1.92875100	4.72015500	-1.40656700
H	1.52032000	5.64696700	-1.79576400
C	1.09704200	3.64835500	-1.16244800
H	0.04052800	3.72664100	-1.39187800
C	1.59938800	2.42038200	-0.67534900
C	0.73189500	1.28996600	-0.41638200
C	-0.67498500	1.25599800	-0.21960600
C	-1.69170600	2.21183600	0.11105200
C	-1.62959900	3.56855000	0.50447100
H	-0.67816500	4.08066000	0.58479300
C	-2.79800100	4.23687200	0.82869900
H	-2.75205800	5.27578700	1.13754600
C	1.35109200	0.03836400	-0.30531700
C	2.74743100	-0.12473800	-0.15537000

C	2.96549600	-1.53815000	0.12681900
C	4.13040400	-2.23385400	0.43523500
H	5.08659400	-1.72438600	0.43158300
C	4.04425700	-3.58329400	0.77294100
H	4.94827200	-4.13126600	1.02094200

Molecule 3 at CAM-B3LYP/6-31+G(d, p) level

Si	-8.06096000	-0.71896400	0.35016500
C	-8.77916100	-1.69109000	-1.09047200
H	-8.56167600	-1.21397100	-2.05024300
H	-9.86533700	-1.78617100	-0.99486700
H	-8.35550000	-2.69979400	-1.11383100
C	-8.44924200	-1.59838800	1.96622500
H	-7.98105700	-1.10132000	2.82030700
H	-8.08036000	-2.62812200	1.93372300
H	-9.52909800	-1.63469800	2.14245700
C	-8.70179300	1.07835500	0.36477000
C	-10.23929400	1.06921800	0.42332800
H	-10.61900500	2.09872100	0.44994200
H	-10.61467800	0.56083900	1.31772100
H	-10.68044000	0.58160400	-0.45194800
C	-8.25591300	1.81271800	-0.90954500
H	-8.63193200	2.84406200	-0.90108200
H	-8.64105800	1.33195500	-1.81473900
H	-7.16576300	1.85850600	-0.99491300
C	-8.16218700	1.82429900	1.59549700
H	-8.51122800	2.86506100	1.58852800
H	-7.06792400	1.84442800	1.61759700
H	-8.50494400	1.37044300	2.53074400
C	-6.22301100	-0.70408400	0.14187300
C	-5.01561300	-0.77243200	-0.01455300
C	-3.61190600	-0.90679600	-0.20642200
C	-3.05734900	-2.19943700	-0.53132900
C	-3.90491000	-3.30895000	-0.77008400
H	-4.97326500	-3.18057900	-0.64014600
C	-3.40468800	-4.51775700	-1.19109300
H	-4.07946400	-5.34661600	-1.37915100
C	-2.02404200	-4.66709500	-1.41772100
H	-1.63226900	-5.59969900	-1.81000200
C	-1.17236100	-3.61873900	-1.15576200
H	-0.11813300	-3.72629500	-1.37342700
C	-1.64614100	-2.38255000	-0.66413700
C	-0.75694400	-1.27328900	-0.39016900

C	0.64900100	-1.26536900	-0.18836400
C	1.64527600	-2.24030200	0.14251500
C	1.55505400	-3.59443800	0.52930200
H	0.59474800	-4.08699900	0.60420800
C	2.70541700	-4.29040200	0.85038500
H	2.63567200	-5.32951700	1.15390000
C	-1.35194000	-0.01286500	-0.27464300
C	-2.74388900	0.17918700	-0.12863200
C	-2.93139500	1.59655200	0.15655800
C	-4.07785000	2.32043500	0.46091600
H	-5.04621600	1.83744500	0.45498200
C	-3.96273200	3.66613300	0.79608300
H	-4.85378400	4.23523800	1.04077700
Si	8.06096000	0.71896500	0.35016100
C	8.77916100	1.69108000	-1.09048400
H	8.56167300	1.21395500	-2.05025200
H	9.86533700	1.78616100	-0.99488100
H	8.35550000	2.69978400	-1.11384800
C	8.44924400	1.59839900	1.96621400
H	7.98106100	1.10133700	2.82030000
H	8.08036200	2.62813200	1.93370600
H	9.52910000	1.63471100	2.14244400
C	8.70179300	-1.07835500	0.36477700
C	10.23929400	-1.06921900	0.42333400
H	10.61900400	-2.09872100	0.44995400
H	10.61467900	-0.56083300	1.31772300
H	10.68043900	-0.58161100	-0.45194700
C	8.25591100	-1.81272600	-0.90953300
H	8.63192900	-2.84407000	-0.90106200
H	8.64105500	-1.33197000	-1.81472900
H	7.16576000	-1.85851500	-0.99489800
C	8.16218800	-1.82429000	1.59551000
H	8.51122800	-2.86505200	1.58854800
H	7.06792500	-1.84441900	1.61761100
H	8.50494600	-1.37042800	2.53075300
C	6.22301100	0.70408300	0.14187100
C	5.01561300	0.77243200	-0.01455500
C	3.61190600	0.90679600	-0.20642400
C	3.05734900	2.19943700	-0.53133000
C	3.90491000	3.30895100	-0.77008500
H	4.97326500	3.18057900	-0.64014700
C	3.40468800	4.51775800	-1.19109200
H	4.07946300	5.34661700	-1.37915000
C	2.02404100	4.66709600	-1.41772000

H	1.63226800	5.59970000	-1.81000000
C	1.17236000	3.61873900	-1.15576100
H	0.11813200	3.72629500	-1.37342700
C	1.64614100	2.38255000	-0.66413800
C	0.75694400	1.27328900	-0.39016900
C	-0.64900100	1.26536900	-0.18836400
C	-1.64527600	2.24030200	0.14251700
C	-1.55505300	3.59443800	0.52930400
H	-0.59474800	4.08699800	0.60421000
C	-2.70541700	4.29040100	0.85038900
H	-2.63567100	5.32951600	1.15390500
C	1.35194000	0.01286500	-0.27464400
C	2.74388900	-0.17918700	-0.12863300
C	2.93139500	-1.59655200	0.15655500
C	4.07785000	-2.32043600	0.46091200
H	5.04621600	-1.83744600	0.45497800
C	3.96273200	-3.66613300	0.79607900
H	4.85378400	-4.23523900	1.04077200

Molecule 4 at B3LYP/6-31+G(d, p) level

Si	8.10416900	-0.14337900	0.28493000
Si	-8.09800000	0.06822400	0.35618500
C	8.33925800	-1.23097000	1.85387900
H	8.16920400	-2.25923000	1.50036500
C	9.77890600	-1.16869000	2.40875300
H	10.53351600	-1.41067500	1.65355100
H	10.01360200	-0.17308800	2.80288300
H	9.90179500	-1.88115400	3.23493100
C	7.31820800	-0.96687100	2.97875700
H	6.28664900	-1.06861500	2.62885300
H	7.46573000	-1.67777000	3.80272600
H	7.42573900	0.04050600	3.39671800
C	8.70356100	-1.05977700	-1.29291200
H	8.41529600	-0.38958700	-2.11643000
C	10.23220300	-1.25209700	-1.36441300
H	10.78080200	-0.31265300	-1.23601900
H	10.58563100	-1.95111100	-0.59749100
H	10.52094900	-1.67034200	-2.33764100
C	7.97760100	-2.39989700	-1.52142800
H	6.88904300	-2.28060300	-1.52933200
H	8.26998500	-2.83851600	-2.48460300
H	8.22927800	-3.13203000	-0.74440900
C	8.97810200	1.55625300	0.42752300

H	10.03755900	1.32190900	0.61220200
C	8.47510000	2.40321700	1.61383100
H	8.60920800	1.89664100	2.57483200
H	9.02061700	3.35481500	1.66586800
H	7.40988200	2.64089800	1.51023900
C	8.90291600	2.36800700	-0.88163800
H	9.34114000	1.83395700	-1.73109000
H	7.86536600	2.60949600	-1.14175500
H	9.44273500	3.31837200	-0.77680500
C	6.29440200	0.16564300	0.04667800
C	5.09636700	0.37298800	-0.12604000
C	3.71705900	0.63463900	-0.32618900
C	3.27624100	1.97142400	-0.67702200
C	4.21951500	2.99959500	-0.93488100
H	5.27283300	2.78005500	-0.79903500
C	3.82802500	4.24735400	-1.38459000
H	4.57607600	5.00857700	-1.58572800
C	2.46468600	4.51526100	-1.61990900
H	2.15659700	5.47154500	-2.03139200
C	1.51720000	3.54527900	-1.33779200
H	0.47642200	3.74389200	-1.56018000
C	1.87721900	2.27959700	-0.81914700
C	0.88775400	1.25470300	-0.52547700
C	1.37034100	-0.05848500	-0.39315900
C	0.54910900	-1.26579700	-0.29625000
C	1.45164700	-2.32886900	0.04861600
C	1.23316500	-3.66965900	0.44857400
H	0.22968900	-4.06966600	0.51858400
C	2.31492800	-4.46966000	0.78739800
H	2.14776600	-5.49531700	1.10085500
C	3.63057400	-3.96109500	0.73668600
H	4.46343100	-4.60860600	0.99439700
C	3.87665400	-2.63051700	0.38760300
H	4.88828600	-2.24393700	0.38628700
C	2.80162300	-1.79925600	0.06458500
C	2.74398600	-0.37622900	-0.23792300
C	-0.51789400	1.37775800	-0.31950100
C	-1.41829200	2.44724700	0.00973000
C	-1.19875800	3.79591400	0.38201500
H	-0.19533000	4.19815000	0.43848200
C	-2.27927800	4.60151900	0.71129400
H	-2.11118700	5.63329000	1.00345300
C	-3.59493500	4.09112100	0.67858200
H	-4.42683800	4.74282000	0.92843700

C	-3.84107500	2.75375500	0.35738200
H	-4.85140100	2.36461100	0.37021100
C	-2.76771800	1.91742100	0.04437600
C	-2.71277600	0.48916300	-0.23025500
C	-3.68686000	-0.52276600	-0.29167600
C	-3.24701000	-1.86663300	-0.61951400
C	-4.19027000	-2.90120700	-0.85134200
H	-5.24306900	-2.68144300	-0.71303000
C	-3.80022600	-4.15685300	-1.28005800
H	-4.54895200	-4.92231700	-1.46168900
C	-2.43839500	-4.42804800	-1.51950400
H	-2.13191800	-5.39161000	-1.91487800
C	-1.49049500	-3.45173400	-1.26190800
H	-0.45084900	-3.65318100	-1.48709700
C	-1.84870100	-2.17683600	-0.76512900
C	-0.85759000	-1.14661800	-0.49694500
C	-1.33978200	0.16870800	-0.38799400
C	-5.06686800	-0.26692200	-0.08399100
C	-6.27074000	-0.09561500	0.09087400
C	-8.93250200	-0.32538000	-1.32785300
H	-8.49371100	0.42811300	-1.99973500
C	-8.58045100	-1.70588700	-1.91552600
H	-7.49924300	-1.87572100	-1.94664800
H	-9.03110800	-2.51851300	-1.33535100
H	-8.95928500	-1.79254100	-2.94250000
C	-10.45982600	-0.10700600	-1.32984300
H	-10.74319200	0.88614300	-0.96470600
H	-10.85917700	-0.20781600	-2.34760200
H	-10.97288100	-0.84857200	-0.70721400
C	-8.53274100	-1.08365500	1.82998600
H	-7.88780600	-0.70193400	2.63622600
C	-8.15836000	-2.56416400	1.62211800
H	-7.11899400	-2.68467800	1.29947600
H	-8.28206900	-3.12534400	2.55778000
H	-8.79980500	-3.04068400	0.87268400
C	-9.99278900	-0.95502500	2.31181800
H	-10.27570300	0.08168200	2.52379600
H	-10.69779400	-1.34659200	1.56991400
H	-10.14254300	-1.53028900	3.23494200
C	-8.48790300	1.88145600	0.84188500
H	-9.57634300	1.90764800	1.00347000
C	-8.16637200	2.88829000	-0.28088500
H	-8.71919100	2.67475300	-1.20158500
H	-8.42778400	3.90857200	0.02930600

H	-7.09872600	2.88628300	-0.53026600
C	-7.81724600	2.30497000	2.16428400
H	-8.11230600	1.66623000	3.00330600
H	-6.72404900	2.26743200	2.09060700
H	-8.09292100	3.33554100	2.42400500

Molecule 4 at PBE0/6-31+G(d, p) level

Si	8.08067700	-0.14840600	0.27242300
Si	-8.07267500	0.06880400	0.34478800
C	8.31563700	-1.19709600	1.85484600
H	8.19536100	-2.23810300	1.51707100
C	9.73045700	-1.05790600	2.43199600
H	10.51156200	-1.27542400	1.69620100
H	9.90900200	-0.04515800	2.81181200
H	9.87110200	-1.74817500	3.27375200
C	7.26363300	-0.94511200	2.93965500
H	6.24596200	-1.10077600	2.56875600
H	7.42039300	-1.62180800	3.78995600
H	7.31742300	0.07919300	3.32584400
C	8.66765500	-1.09557800	-1.27694700
H	8.41716900	-0.42875700	-2.11582300
C	10.18107600	-1.33458600	-1.29962200
H	10.75498300	-0.41027100	-1.16960800
H	10.48743900	-2.03072300	-0.50998200
H	10.48698400	-1.77957200	-2.25530200
C	7.90561000	-2.40687100	-1.48800500
H	6.82227000	-2.24985900	-1.52553700
H	8.20516800	-2.88173800	-2.43131300
H	8.11278300	-3.12630200	-0.68631900
C	8.94507300	1.54640100	0.38090900
H	10.00219600	1.32658200	0.59626000
C	8.40050900	2.41256900	1.52132700
H	8.51251200	1.93449800	2.49988400
H	8.92924000	3.37385400	1.56297700
H	7.33501000	2.62924600	1.37955100
C	8.88254500	2.30452000	-0.94911300
H	9.35768200	1.75320900	-1.76726500
H	7.84527200	2.50567300	-1.24382600
H	9.39173000	3.27353200	-0.86578300
C	6.27580700	0.16883800	0.03466700
C	5.07862200	0.38190400	-0.13077800
C	3.70180100	0.64270400	-0.32345300
C	3.26007200	1.97413000	-0.66623500

C	4.20017700	3.00142900	-0.91576400
H	5.25441700	2.78023300	-0.77869700
C	3.80666300	4.24724200	-1.35698900
H	4.55281900	5.01200500	-1.55288800
C	2.44607100	4.51216400	-1.59275600
H	2.13674300	5.46971700	-2.00097700
C	1.50279600	3.54169700	-1.31800900
H	0.46017700	3.73601700	-1.54234500
C	1.86648400	2.27849100	-0.80659300
C	0.88382800	1.25443600	-0.51935000
C	1.36635900	-0.05446800	-0.38806200
C	0.55252700	-1.25963400	-0.28672100
C	1.45557500	-2.31604000	0.05734800
C	1.23988100	-3.65138200	0.46288000
H	0.23582900	-4.05201900	0.53976700
C	2.32241900	-4.44449800	0.80038400
H	2.15909900	-5.46923100	1.11972500
C	3.63299000	-3.93433400	0.74385200
H	4.46807000	-4.57927500	1.00231000
C	3.87498800	-2.60801600	0.39086800
H	4.88594000	-2.21599400	0.38609900
C	2.79828500	-1.78535800	0.06823100
C	2.73624900	-0.36770900	-0.23549500
C	-0.51703500	1.37312300	-0.31418300
C	-1.41796700	2.43713600	0.01088300
C	-1.20200100	3.78223900	0.38308700
H	-0.19823300	4.18617800	0.44457500
C	-2.28370800	4.58182900	0.70792000
H	-2.11978900	5.61414800	1.00146300
C	-3.59416000	4.06909400	0.67160100
H	-4.42881900	4.71880600	0.91929400
C	-3.83526000	2.73441800	0.35216400
H	-4.84433900	2.33857700	0.36278300
C	-2.75986500	1.90587900	0.04327700
C	-2.70068600	0.48200600	-0.22724900
C	-3.66723100	-0.52972500	-0.28347900
C	-3.22674200	-1.86860900	-0.60141600
C	-4.16706900	-2.90201600	-0.82405000
H	-5.22089100	-2.67931400	-0.68701900
C	-3.77517400	-4.15671400	-1.24107400
H	-4.52218100	-4.92556200	-1.41672400
C	-2.41597800	-4.42618200	-1.47894300
H	-2.10833400	-5.39209000	-1.86829800
C	-1.47213100	-3.44918800	-1.23074400

H	-0.43060800	-3.64722200	-1.45702500
C	-1.83388700	-2.17556400	-0.74452400
C	-0.84948500	-1.14556400	-0.48606800
C	-1.33154600	0.16580800	-0.38246700
C	-5.04455500	-0.27559300	-0.08032800
C	-6.24738800	-0.09932900	0.09076900
C	-8.88684000	-0.31107100	-1.33911300
H	-8.48926900	0.48598000	-1.98680300
C	-8.46947600	-1.64557000	-1.96350600
H	-7.38068800	-1.75504100	-2.00621200
H	-8.86994400	-2.49696200	-1.40292500
H	-8.85198600	-1.72474900	-2.98946200
C	-10.41285300	-0.16996200	-1.31442500
H	-10.73983500	0.79226600	-0.90475800
H	-10.82314200	-0.25051800	-2.32935000
H	-10.87769200	-0.96143200	-0.71569000
C	-8.51074400	-1.08619400	1.80066400
H	-7.80942200	-0.76474400	2.58664700
C	-8.23702300	-2.56802100	1.52820200
H	-7.22715100	-2.73717500	1.13901500
H	-8.33925000	-3.15425300	2.45063500
H	-8.94903000	-2.97942900	0.80430500
C	-9.93178200	-0.88394100	2.33871900
H	-10.13552400	0.15882200	2.60479100
H	-10.68800000	-1.19361300	1.60876900
H	-10.08836100	-1.48839500	3.24159600
C	-8.44659000	1.87139000	0.83917600
H	-9.53338700	1.90738300	1.01279000
C	-8.12151700	2.86910400	-0.27681400
H	-8.70003200	2.67754100	-1.18657300
H	-8.34513900	3.89489500	0.04395300
H	-7.05980700	2.83667400	-0.54959600
C	-7.75267700	2.26475700	2.14745700
H	-8.04491700	1.62068500	2.98364500
H	-6.66158300	2.20659700	2.05486100
H	-8.00353900	3.29694100	2.42443400

Molecule 4 at BMK/6-31+G(d, p) level

Si	8.10114800	-0.14727000	0.25611300
Si	-8.08853900	0.10049600	0.31927700
C	8.38260700	-0.99919600	1.93123100
H	8.27459500	-2.07951700	1.73650600
C	9.82028100	-0.76180400	2.46469700

H	10.59098900	-1.03977400	1.73420300
H	9.97162600	0.29531600	2.72427000
H	9.99173200	-1.35364800	3.37531900
C	7.34508400	-0.62033400	3.01706100
H	6.32106200	-0.84520400	2.69560800
H	7.54489200	-1.17475900	3.94574000
H	7.39123900	0.45170800	3.25397400
C	8.63779600	-1.25717800	-1.18284500
H	8.38044200	-0.69485800	-2.09541900
C	10.16545800	-1.51461000	-1.19725400
H	10.74387900	-0.58059900	-1.17889700
H	10.46969900	-2.11900600	-0.33094200
H	10.45353900	-2.07008300	-2.10149100
C	7.86350500	-2.59627900	-1.22599000
H	6.77790900	-2.43518900	-1.26672600
H	8.15128800	-3.18062900	-2.11212600
H	8.08456700	-3.21032700	-0.34132000
C	8.97676200	1.52815300	0.15341000
H	10.04005500	1.33568900	0.37527600
C	8.44710400	2.53856200	1.20056100
H	8.56630200	2.17074500	2.22792200
H	8.98604500	3.49398200	1.12160400
H	7.37869700	2.74107400	1.03886100
C	8.88970000	2.13584700	-1.26819600
H	9.35667000	1.48892400	-2.02221100
H	7.84162600	2.29388400	-1.56187800
H	9.39630200	3.11139800	-1.30160700
C	6.29799500	0.16433200	0.03592000
C	5.10273100	0.37989100	-0.12671800
C	3.71414200	0.64276900	-0.31546900
C	3.26612000	1.97996300	-0.66363900
C	4.20735400	3.01718900	-0.92372900
H	5.26579600	2.80256400	-0.79371400
C	3.80197400	4.26483900	-1.36557800
H	4.54368800	5.03458700	-1.56876700
C	2.42854300	4.52535400	-1.59333600
H	2.11275200	5.48303100	-2.00131700
C	1.48707100	3.54802000	-1.31105000
H	0.44078300	3.73531100	-1.53016100
C	1.86352100	2.27850100	-0.79747200
C	0.88104800	1.24356500	-0.50315400
C	1.37285300	-0.06871700	-0.36528300
C	0.56079300	-1.28874500	-0.25810500
C	1.47749800	-2.34342200	0.09199100

C	1.27106800	-3.68639700	0.50664700
H	0.26887500	-4.09529100	0.58692700
C	2.36585600	-4.47317500	0.84956300
H	2.20934300	-5.49942500	1.17412200
C	3.68027500	-3.95134200	0.79108700
H	4.52135100	-4.58938500	1.05468000
C	3.91302600	-2.61756900	0.42856400
H	4.92266200	-2.21526400	0.42345200
C	2.82386400	-1.80285400	0.09910400
C	2.75226400	-0.37469400	-0.21503400
C	-0.52914400	1.35779000	-0.29888100
C	-1.44417400	2.42372600	0.02074800
C	-1.23851500	3.78117600	0.38665400
H	-0.23682300	4.19481800	0.44680800
C	-2.33311500	4.57782000	0.70694200
H	-2.17669900	5.61522200	0.99391700
C	-3.64734200	4.05250600	0.67310800
H	-4.48891300	4.69779400	0.91690100
C	-3.87799300	2.70645300	0.35949600
H	-4.88595100	2.30039900	0.37128300
C	-2.78943100	1.88240100	0.05468200
C	-2.72006900	0.44500100	-0.20968100
C	-3.68331700	-0.57441800	-0.26802000
C	-3.23721000	-1.92258300	-0.57619400
C	-4.17971500	-2.96803700	-0.79607300
H	-5.23731400	-2.74956800	-0.66682100
C	-3.77693800	-4.22952800	-1.19936000
H	-4.51996700	-5.00536000	-1.37245200
C	-2.40512100	-4.49755600	-1.42759200
H	-2.09180900	-5.46814500	-1.80586600
C	-1.46215100	-3.51122200	-1.18429100
H	-0.41734700	-3.70577300	-1.40424300
C	-1.83534700	-2.22545500	-0.71012700
C	-0.85067300	-1.18157400	-0.45676900
C	-1.34166100	0.13449000	-0.35971200
C	-5.07161000	-0.31159200	-0.07335400
C	-6.27135700	-0.11973700	0.08882600
C	-8.90895200	-0.30255700	-1.34165000
H	-8.62224200	0.53788100	-1.99559300
C	-8.39661100	-1.59719200	-2.01911300
H	-7.30424600	-1.59169300	-2.12410500
H	-8.67748900	-2.48819900	-1.44262200
H	-8.83491100	-1.70038200	-3.02258100
C	-10.45595300	-0.31585600	-1.24574000

H	-10.85275700	0.59523300	-0.77692500
H	-10.90223300	-0.39928900	-2.24722500
H	-10.80324500	-1.17715200	-0.65805500
C	-8.59354000	-1.01498500	1.76848300
H	-7.83257100	-0.81770900	2.54210700
C	-8.53117400	-2.52464700	1.43106700
H	-7.56590000	-2.80678600	0.98926400
H	-8.67737300	-3.12828900	2.33851600
H	-9.32308300	-2.79928200	0.72051300
C	-9.97524900	-0.65585800	2.37263600
H	-10.02552100	0.39179500	2.69638300
H	-10.78418800	-0.82337300	1.64874400
H	-10.18106100	-1.28693300	3.24950800
C	-8.39741900	1.91111400	0.78026200
H	-9.48426700	2.00760000	0.94354100
C	-8.00211600	2.89481600	-0.34786200
H	-8.58063200	2.72380800	-1.26451800
H	-8.17520500	3.93364800	-0.03137600
H	-6.93653300	2.79640800	-0.60170300
C	-7.68430800	2.29062800	2.10229900
H	-7.99548200	1.65103500	2.93877500
H	-6.59376600	2.19428900	1.99855500
H	-7.90394300	3.33282900	2.37531700

Molecule 4 at M062X/6-31+G(d, p) level

Si	8.03840500	-0.17776300	0.30156000
Si	-8.03749400	0.05065300	0.37114800
C	8.14612400	-1.19534700	1.90780900
H	8.05718300	-2.24751900	1.59745900
C	9.51444900	-1.02074600	2.58740200
H	10.35040700	-1.22828300	1.91139500
H	9.63908400	0.00211900	2.96105800
H	9.60502700	-1.69587600	3.44630600
C	7.01303800	-0.90457000	2.90176500
H	6.02873900	-1.10878800	2.47035700
H	7.12564700	-1.52041800	3.80219400
H	7.01921100	0.14520300	3.21716300
C	8.60634400	-1.21063200	-1.18266000
H	8.55493500	-0.54446700	-2.05542300
C	10.05890800	-1.67816400	-1.01246900
H	10.74555300	-0.84465100	-0.82471000
H	10.14691900	-2.38053400	-0.17459800
H	10.40700200	-2.20017800	-1.91140900

C	7.67649300	-2.40240500	-1.44506500
H	6.65009600	-2.07824200	-1.64470100
H	8.02169100	-2.97986200	-2.31093300
H	7.65252600	-3.08665900	-0.58766300
C	9.00167600	1.44959200	0.42025100
H	10.02569400	1.18970700	0.72658400
C	8.40193000	2.38283000	1.48165000
H	8.38966200	1.92810000	2.47748900
H	8.97705900	3.31401100	1.54828100
H	7.36883000	2.64674000	1.22542800
C	9.06939900	2.15701700	-0.94013400
H	9.59677900	1.55955200	-1.69048600
H	8.06259500	2.36445600	-1.32417000
H	9.59184100	3.11695300	-0.85103900
C	6.26406000	0.26344700	0.00115500
C	5.07872200	0.50216600	-0.17787900
C	3.69299900	0.75580000	-0.37672500
C	3.23040300	2.08243000	-0.70234600
C	4.15496600	3.13190700	-0.93635400
H	5.21345700	2.92928700	-0.80270900
C	3.73440900	4.37336300	-1.35754100
H	4.46207700	5.15715300	-1.54212400
C	2.36441100	4.61399200	-1.59175400
H	2.03856300	5.57026100	-1.98758800
C	1.44096000	3.62328300	-1.33514700
H	0.39469400	3.79442400	-1.56123900
C	1.83368500	2.35936700	-0.83895000
C	0.87184700	1.31180200	-0.56495400
C	1.37901200	0.01115000	-0.44200100
C	0.59227900	-1.21739200	-0.33975000
C	1.52252400	-2.25539200	-0.00181500
C	1.33715800	-3.59597300	0.40654200
H	0.34259900	-4.01651000	0.49569500
C	2.44041400	-4.36565800	0.73319300
H	2.30141600	-5.39279600	1.05340700
C	3.74022000	-3.82896300	0.66548200
H	4.59067200	-4.45596000	0.91486000
C	3.95076500	-2.49616000	0.31408300
H	4.95329600	-2.08345200	0.30237500
C	2.85229400	-1.69856200	0.00197400
C	2.75578400	-0.27334900	-0.29579000
C	-0.53137900	1.40353900	-0.36156800
C	-1.45904200	2.44829500	-0.03689400
C	-1.27646300	3.79881800	0.33992100

H	-0.28331700	4.22604900	0.41127900
C	-2.38041900	4.57124500	0.65878300
H	-2.24227600	5.60571600	0.95486900
C	-3.67954900	4.02940200	0.61348000
H	-4.53121700	4.65802300	0.85563700
C	-3.88550100	2.68873000	0.29277200
H	-4.88343900	2.26633300	0.29546500
C	-2.78687700	1.88932600	-0.00837500
C	-2.69429200	0.45906100	-0.27421400
C	-3.63322200	-0.57037700	-0.31793200
C	-3.17323700	-1.90359800	-0.62509400
C	-4.09860000	-2.95890500	-0.82877700
H	-5.15581700	-2.75627600	-0.68632800
C	-3.68144900	-4.20734900	-1.23260800
H	-4.41064300	-4.99485000	-1.39409900
C	-2.31435100	-4.45111500	-1.47913900
H	-1.99203600	-5.41407900	-1.86138300
C	-1.38949600	-3.45467000	-1.25162600
H	-0.34560400	-3.62858000	-1.48662000
C	-1.77791400	-2.18238600	-0.77383500
C	-0.81284800	-1.12997700	-0.53087200
C	-1.31889500	0.17257600	-0.43021100
C	-5.01911000	-0.32804900	-0.09962900
C	-6.21331700	-0.14399200	0.08874500
C	-8.89193500	-0.41900600	-1.25699400
H	-8.66775700	0.42069900	-1.93116300
C	-8.33605500	-1.68981200	-1.91435300
H	-7.25505600	-1.62360200	-2.07153700
H	-8.53226800	-2.57718200	-1.30353900
H	-8.80991400	-1.85284100	-2.88981200
C	-10.41734100	-0.50528500	-1.09990200
H	-10.84060200	0.38860500	-0.62769100
H	-10.90033300	-0.62542600	-2.07666600
H	-10.69915900	-1.37098600	-0.48941600
C	-8.46861900	-1.04190300	1.86294400
H	-7.68604600	-0.80803100	2.60007500
C	-8.38189100	-2.54207100	1.55261300
H	-7.43029100	-2.81058200	1.08018300
H	-8.47894100	-3.13287000	2.47107100
H	-9.19036000	-2.85090600	0.88009900
C	-9.82594100	-0.69376200	2.49239900
H	-9.88722100	0.35770200	2.79132500
H	-10.65149600	-0.89085300	1.79987000
H	-9.99881900	-1.30310200	3.38750600

C	-8.35516200	1.86898400	0.80357000
H	-9.43328800	1.95957000	1.00354500
C	-8.00564900	2.81232900	-0.35519500
H	-8.63534200	2.63649600	-1.23270700
H	-8.13822000	3.85889700	-0.05577000
H	-6.96140100	2.68878400	-0.66783900
C	-7.59842300	2.26730600	2.07926300
H	-7.88550500	1.65476700	2.94032800
H	-6.51561600	2.15582900	1.94531900
H	-7.79379700	3.31533200	2.33537500

Molecule 4 at CAM-B3LYP/6-31+G(d, p) level

Si	8.07622400	-0.14317200	0.24689700
Si	-8.06908500	0.06620400	0.32140500
C	8.31839600	-1.20705400	1.81243800
H	8.17112900	-2.24164700	1.47182700
C	9.74752000	-1.10617800	2.37072800
H	10.51069000	-1.33355200	1.62106000
H	9.95466800	-0.10282100	2.75749800
H	9.88447900	-1.80788900	3.20169800
C	7.29166700	-0.94774100	2.92420900
H	6.26520600	-1.08326800	2.57415600
H	7.45498300	-1.63562700	3.76244000
H	7.37107400	0.07010700	3.31962400
C	8.64752900	-1.06993500	-1.31525800
H	8.37578700	-0.40238900	-2.14458400
C	10.16551200	-1.29424200	-1.37528900
H	10.73229100	-0.36642200	-1.24937100
H	10.49679500	-1.99388300	-0.60054700
H	10.45239700	-1.72597400	-2.34129400
C	7.89879300	-2.39220900	-1.52970200
H	6.81381100	-2.25195800	-1.54137400
H	8.18439500	-2.84739300	-2.48534300
H	8.13433200	-3.11875300	-0.74406700
C	8.94734200	1.54255300	0.36787600
H	10.00628400	1.31715000	0.55770300
C	8.43518600	2.39826600	1.53523000
H	8.56594800	1.90542900	2.50262000
H	8.97297700	3.35282300	1.57790000
H	7.36992600	2.62649000	1.42172700
C	8.86640700	2.33054800	-0.94755000
H	9.31649200	1.79079300	-1.78572700
H	7.82701000	2.55056700	-1.21555400

H	9.38931700	3.28970800	-0.85485000
C	6.26785600	0.17800900	0.02579200
C	5.07808600	0.39219600	-0.13096500
C	3.69179400	0.65362600	-0.31428900
C	3.24745500	1.98405300	-0.65125900
C	4.18585900	3.01401700	-0.90577000
H	5.23985600	2.79529400	-0.77834300
C	3.78893100	4.25694000	-1.33689000
H	4.53104600	5.02309900	-1.53672900
C	2.42453900	4.52164600	-1.55777800
H	2.11184700	5.48059100	-1.95751300
C	1.48745700	3.55308400	-1.28063400
H	0.44507700	3.74905500	-1.49380500
C	1.85629200	2.28542000	-0.77888400
C	0.87806300	1.25810300	-0.48978100
C	1.36500600	-0.04690900	-0.36076300
C	0.55716400	-1.25998400	-0.25811200
C	1.46849000	-2.31139900	0.08384500
C	1.26254800	-3.64711800	0.48922900
H	0.26337900	-4.05390600	0.57064500
C	2.34905300	-4.43470200	0.82078700
H	2.19078000	-5.45965700	1.13890500
C	3.65476600	-3.92061300	0.75949700
H	4.49369500	-4.56018600	1.01412700
C	3.88574800	-2.59449100	0.40535000
H	4.89316100	-2.19843200	0.39568000
C	2.80502600	-1.77931200	0.08825400
C	2.73605200	-0.35447800	-0.21657000
C	-0.52277700	1.37064900	-0.28344500
C	-1.43192300	2.42900300	0.04150900
C	-1.22571800	3.77388500	0.41591900
H	-0.22682500	4.18405200	0.48217000
C	-2.31141600	4.56703700	0.73675800
H	-2.15261500	5.59903100	1.03094000
C	-3.61702800	4.05015900	0.69534700
H	-4.45548300	4.69388700	0.94093900
C	-3.84716200	2.71626600	0.37233700
H	-4.85262500	2.31618800	0.37790100
C	-2.76771700	1.89609400	0.06680100
C	-2.70160600	0.46558200	-0.20705800
C	-3.65850700	-0.54390100	-0.27448600
C	-3.21540400	-1.88151600	-0.58720800
C	-4.15397400	-2.91801700	-0.81371800
H	-5.20743400	-2.69864300	-0.68399500

C	-3.75875800	-4.16914000	-1.22227600
H	-4.50169700	-4.93969800	-1.40106500
C	-2.39591800	-4.43731100	-1.44772800
H	-2.08506900	-5.40392500	-1.83003200
C	-1.45822700	-3.46213900	-1.19730800
H	-0.41709200	-3.66105400	-1.41391600
C	-1.82495800	-2.18486600	-0.71906000
C	-0.84483500	-1.15183500	-0.45806800
C	-1.33129600	0.15544800	-0.35464100
C	-5.04540700	-0.28848300	-0.08164100
C	-6.24125500	-0.11149000	0.07892300
C	-8.87364300	-0.32180100	-1.36040200
H	-8.42562400	0.42873500	-2.02722900
C	-8.52017600	-1.69902900	-1.93773900
H	-7.44064200	-1.87587000	-1.94733700
H	-8.98662600	-2.50666600	-1.36568300
H	-8.87925200	-1.78465800	-2.97013100
C	-10.39367500	-0.10134200	-1.37719500
H	-10.67763600	0.89163000	-1.01508600
H	-10.78439800	-0.20259100	-2.39650200
H	-10.91218100	-0.84070900	-0.75839200
C	-8.52022700	-1.07243800	1.78009100
H	-7.86291000	-0.71350800	2.58494700
C	-8.18761300	-2.55406900	1.55816800
H	-7.15934800	-2.69882100	1.21361300
H	-8.30664700	-3.11732700	2.49123500
H	-8.85546400	-3.00826100	0.81986100
C	-9.96868300	-0.91089000	2.26517800
H	-10.22223000	0.12976600	2.48893400
H	-10.68445400	-1.27385400	1.52066100
H	-10.13251400	-1.49187700	3.18037700
C	-8.44294200	1.86978500	0.79605800
H	-9.53048600	1.91284800	0.95021600
C	-8.09743500	2.86299400	-0.32253600
H	-8.65075800	2.65911400	-1.24380300
H	-8.33701900	3.88795800	-0.01593000
H	-7.03018800	2.83700700	-0.56795000
C	-7.77421500	2.28205700	2.11527200
H	-8.08465600	1.65081300	2.95302700
H	-6.68259900	2.22310000	2.04669400
H	-8.03056600	3.31680100	2.37124700

Molecule 5 at B3LYP/6-31+G(d, p) level

O	-8.10428300	0.55515900	2.02965900
O	-7.64883600	-0.91048600	-2.49233200
C	-9.50385000	0.26672800	2.00387800
H	-9.87863900	0.53166700	2.99255900
H	-9.68489300	-0.79778600	1.81686900
H	-10.01736100	0.86731700	1.24464800
C	-7.36517500	0.31354300	0.90582600
C	-5.99531100	0.61853500	1.00398400
H	-5.60927100	1.01213300	1.93813600
C	-5.15433700	0.40060200	-0.08677700
C	-5.67505900	-0.11906700	-1.28931500
H	-5.00869500	-0.28180600	-2.12669600
C	-7.03873300	-0.41074500	-1.37526600
C	-7.89358900	-0.20000500	-0.27848300
H	-8.94272200	-0.44282600	-0.38938600
C	-6.85412300	-1.15310600	-3.65572300
H	-7.54230400	-1.53990900	-4.40739400
H	-6.07519200	-1.89711700	-3.45507800
H	-6.39508300	-0.22772600	-4.02118400
C	-3.69181900	0.69283500	0.00447500
C	-3.20592200	2.04296200	0.03137200
C	-4.10713800	3.14778200	0.04104000
H	-5.16445600	2.95737100	-0.10281100
C	-3.67459000	4.43712100	0.27828100
H	-4.39039800	5.25384600	0.29687600
C	-2.31027200	4.68252900	0.54670700
H	-1.97484600	5.67870600	0.81902300
C	-1.39933800	3.64427200	0.46539200
H	-0.36276800	3.83787100	0.70578400
C	-1.78952800	2.32520700	0.12847800
C	-2.75611000	-0.33788600	0.11823000
C	-1.36121500	-0.06178300	0.05472300
C	-0.58813700	-1.29817500	0.17712100
C	-1.54135100	-2.32005200	0.51567800
C	-1.39122400	-3.63648700	1.02328800
H	-0.40874900	-4.04621300	1.21672300
C	-2.51387300	-4.39662300	1.31562500
H	-2.39452500	-5.40185600	1.70773900
C	-3.80911200	-3.87180500	1.12051300
H	-4.67603300	-4.48725900	1.34223600
C	-3.99217400	-2.55693600	0.68395300
H	-4.99332700	-2.15484400	0.58818100
C	-2.87613300	-1.76274400	0.40837400
C	0.83440500	-1.24086900	0.01940500

O	8.10428200	-0.55516000	-2.02966100
O	7.64883700	0.91048800	2.49233000
C	9.50384900	-0.26672900	-2.00388100
H	9.87863700	-0.53166800	-2.99256100
H	9.68489200	0.79778600	-1.81687200
H	10.01736100	-0.86731700	-1.24465100
C	7.36517400	-0.31354300	-0.90582800
C	5.99531100	-0.61853600	-1.00398500
H	5.60927100	-1.01213400	-1.93813600
C	5.15433700	-0.40060200	0.08677600
C	5.67506000	0.11906800	1.28931400
H	5.00869600	0.28180700	2.12669600
C	7.03873400	0.41074600	1.37526400
C	7.89358900	0.20000500	0.27848100
H	8.94272200	0.44282600	0.38938300
C	6.85412400	1.15310800	3.65572100
H	7.54230600	1.53991200	4.40739200
H	6.07519300	1.89711900	3.45507600
H	6.39508500	0.22772900	4.02118300
C	3.69181900	-0.69283500	-0.00447500
C	3.20592200	-2.04296200	-0.03137200
C	4.10713800	-3.14778200	-0.04104000
H	5.16445600	-2.95737100	0.10281100
C	3.67459000	-4.43712100	-0.27828000
H	4.39039800	-5.25384700	-0.29687500
C	2.31027200	-4.68253000	-0.54670500
H	1.97484600	-5.67870600	-0.81902100
C	1.39933800	-3.64427200	-0.46539000
H	0.36276800	-3.83787100	-0.70578200
C	1.78952800	-2.32520700	-0.12847700
C	2.75610900	0.33788600	-0.11822900
C	1.36121500	0.06178300	-0.05472200
C	0.58813700	1.29817400	-0.17711900
C	1.54135000	2.32005200	-0.51567700
C	1.39122300	3.63648700	-1.02328600
H	0.40874900	4.04621300	-1.21672100
C	2.51387200	4.39662200	-1.31562400
H	2.39452500	5.40185600	-1.70773800
C	3.80911200	3.87180400	-1.12051300
H	4.67603300	4.48725800	-1.34223600
C	3.99217400	2.55693600	-0.68395200
H	4.99332700	2.15484400	-0.58818100
C	2.87613300	1.76274400	-0.40837300
C	-0.83440500	1.24086800	-0.01940400

Molecule 5 at PBE0/6-31+G(d, p) level

O	5.16400600	-3.57568400	5.49473700
O	6.97907900	0.53616400	3.95415100
C	6.16194000	-3.64917100	6.49825400
H	5.96846400	-4.57162200	7.04582500
H	6.09749100	-2.79789900	7.18584200
H	7.16523500	-3.69095300	6.05873700
C	5.17264200	-2.50669800	4.66031800
C	4.15830900	-2.48572100	3.69085700
H	3.43650400	-3.29579500	3.66387700
C	4.08068200	-1.42554500	2.79463000
C	5.01648500	-0.37832200	2.85033100
H	4.93761300	0.43898100	2.14333100
C	6.02232600	-0.41577500	3.81400800
C	6.10586700	-1.47717000	4.72754400
H	6.90314600	-1.46188400	5.46105100
C	6.95791800	1.64046900	3.06551800
H	7.80139900	2.26935300	3.35073100
H	6.02818300	2.21250300	3.16376300
H	7.08118700	1.31621200	2.02584600
C	2.99266800	-1.36397800	1.78417600
C	2.94581700	-2.27769800	0.68494400
C	3.90888900	-3.31474200	0.55601000
H	4.75608700	-3.32372200	1.23399200
C	3.76477600	-4.32465100	-0.36858400
H	4.50983700	-5.11283800	-0.43047000
C	2.62542600	-4.36083600	-1.19631600
H	2.45995500	-5.19973400	-1.86595900
C	1.71495500	-3.32557800	-1.14983500
H	0.82467600	-3.37878600	-1.76446800
C	1.88028400	-2.22246400	-0.28320600
C	1.95300600	-0.44693100	1.91033700
C	0.99454200	-0.29462800	0.87624600
C	0.01873600	0.72737300	1.23251000
C	0.28877500	1.06153300	2.59927200
C	-0.46309800	1.76006500	3.57314100
H	-1.43631500	2.17044500	3.33236200
C	0.02775600	1.88395400	4.86043800
H	-0.55311700	2.41635000	5.60756300
C	1.26447000	1.31437000	5.21557600

H	1.63760300	1.43312800	6.22891100
C	1.99812300	0.56459300	4.29782500
H	2.92429900	0.08937400	4.60189800
C	1.51168900	0.40711800	3.00168700
C	-0.96396900	1.10462400	0.26850000
O	-5.16400600	3.57568400	-5.49473700
O	-6.97907900	-0.53616400	-3.95415100
C	-6.16194000	3.64917100	-6.49825400
H	-5.96846400	4.57162200	-7.04582500
H	-6.09749100	2.79789900	-7.18584200
H	-7.16523500	3.69095300	-6.05873700
C	-5.17264200	2.50669800	-4.66031800
C	-4.15830900	2.48572100	-3.69085700
H	-3.43650400	3.29579500	-3.66387700
C	-4.08068200	1.42554500	-2.79463000
C	-5.01648500	0.37832200	-2.85033100
H	-4.93761300	-0.43898100	-2.14333100
C	-6.02232600	0.41577500	-3.81400800
C	-6.10586700	1.47717000	-4.72754400
H	-6.90314600	1.46188400	-5.46105100
C	-6.95791800	-1.64046900	-3.06551800
H	-7.80139900	-2.26935300	-3.35073100
H	-6.02818300	-2.21250300	-3.16376300
H	-7.08118700	-1.31621200	-2.02584600
C	-2.99266800	1.36397800	-1.78417600
C	-2.94581700	2.27769800	-0.68494400
C	-3.90888900	3.31474200	-0.55601000
H	-4.75608700	3.32372200	-1.23399200
C	-3.76477600	4.32465100	0.36858400
H	-4.50983700	5.11283800	0.43047000
C	-2.62542600	4.36083600	1.19631600
H	-2.45995500	5.19973400	1.86595900
C	-1.71495500	3.32557800	1.14983500
H	-0.82467600	3.37878600	1.76446800
C	-1.88028400	2.22246400	0.28320600
C	-1.95300600	0.44693100	-1.91033700
C	-0.99454200	0.29462800	-0.87624600
C	-0.01873600	-0.72737300	-1.23251000
C	-0.28877500	-1.06153300	-2.59927200
C	0.46309800	-1.76006500	-3.57314100
H	1.43631500	-2.17044500	-3.33236200
C	-0.02775600	-1.88395400	-4.86043800
H	0.55311700	-2.41635000	-5.60756300
C	-1.26447000	-1.31437000	-5.21557600

H	-1.63760300	-1.43312800	-6.22891100
C	-1.99812300	-0.56459300	-4.29782500
H	-2.92429900	-0.08937400	-4.60189800
C	-1.51168900	-0.40711800	-3.00168700
C	0.96396900	-1.10462400	-0.26850000

Molecule 5 at BMK/6-31+G(d, p) level

O	-8.09245600	-0.63038200	-2.00769300
O	-7.63600000	0.98853000	2.44110300
C	-9.47215900	-0.31553100	-2.00301100
H	-9.85227200	-0.60522000	-2.98518500
H	-9.62980100	0.76098400	-1.85053500
H	-10.00201400	-0.87900700	-1.22286900
C	-7.36175500	-0.36312700	-0.90370200
C	-5.99072400	-0.69395100	-0.98130600
H	-5.60274200	-1.12826500	-1.89958500
C	-5.15577800	-0.44258600	0.10858000
C	-5.67137800	0.13073000	1.29311400
H	-5.00146300	0.32005100	2.12518700
C	-7.03553300	0.44519300	1.35924800
C	-7.88939600	0.20525200	0.26068100
H	-8.93684500	0.46991500	0.35877400
C	-6.85234600	1.26051300	3.58821200
H	-7.53641300	1.68199600	4.32819500
H	-6.06149200	1.98855000	3.36213300
H	-6.40265600	0.34029100	3.98518600
C	-3.68853500	-0.73454300	0.02823800
C	-3.18863500	-2.08450600	0.00811600
C	-4.08544800	-3.19966900	0.00628300
H	-5.14654400	-3.01457600	0.14919000
C	-3.63775000	-4.48793900	-0.21674400
H	-4.34537500	-5.31452500	-0.22807200
C	-2.26383900	-4.72290700	-0.48324700
H	-1.91926600	-5.72063300	-0.74683300
C	-1.36128200	-3.67540000	-0.41526300
H	-0.32120000	-3.85681100	-0.66095100
C	-1.76942400	-2.35148100	-0.09050700
C	-2.76511100	0.30491000	-0.09330800
C	-1.36418500	0.04572600	-0.03982400
C	-0.60597800	1.29650800	-0.17878900
C	-1.57808900	2.30572500	-0.51782100
C	-1.44728200	3.62300700	-1.04177600
H	-0.46923100	4.04295300	-1.25051300

C	-2.58614000	4.36600600	-1.33283400
H	-2.48274700	5.37069500	-1.73688100
C	-3.87656400	3.82493400	-1.12298400
H	-4.75488100	4.42774200	-1.34543500
C	-4.03941700	2.50773500	-0.67173000
H	-5.03606700	2.08904100	-0.56444900
C	-2.90625800	1.73391100	-0.39438600
C	0.82370400	1.25389100	-0.03755900
O	8.09245700	0.63038700	2.00769100
O	7.63599600	-0.98854200	-2.44109800
C	9.47216000	0.31553500	2.00300900
H	9.85227400	0.60522700	2.98518300
H	9.62980100	-0.76098100	1.85053800
H	10.00201500	0.87900700	1.22286600
C	7.36175500	0.36312900	0.90370200
C	5.99072500	0.69395500	0.98130500
H	5.60274300	1.12827300	1.89958200
C	5.15577800	0.44258700	-0.10858000
C	5.67137700	-0.13073500	-1.29311100
H	5.00146100	-0.32005900	-2.12518300
C	7.03553200	-0.44519900	-1.35924500
C	7.88939500	-0.20525500	-0.26068000
H	8.93684400	-0.46992000	-0.35877200
C	6.85234000	-1.26052800	-3.58820500
H	7.53640400	-1.68201600	-4.32818700
H	6.06148500	-1.98856300	-3.36212100
H	6.40265200	-0.34030600	-3.98518200
C	3.68853600	0.73454500	-0.02823900
C	3.18863500	2.08450800	-0.00811700
C	4.08544900	3.19967000	-0.00628300
H	5.14654500	3.01457800	-0.14919000
C	3.63775100	4.48794100	0.21674400
H	4.34537600	5.31452600	0.22807200
C	2.26384000	4.72290900	0.48324600
H	1.91926700	5.72063500	0.74683300
C	1.36128200	3.67540200	0.41526300
H	0.32120100	3.85681300	0.66095100
C	1.76942500	2.35148300	0.09050600
C	2.76511100	-0.30490800	0.09330700
C	1.36418500	-0.04572400	0.03982300
C	0.60597900	-1.29650600	0.17878800
C	1.57808900	-2.30572300	0.51782000
C	1.44728300	-3.62300500	1.04177400
H	0.46923300	-4.04295200	1.25051200

C	2.58614100	-4.36600400	1.33283100
H	2.48274900	-5.37069400	1.73687800
C	3.87656600	-3.82493200	1.12298000
H	4.75488300	-4.42773900	1.34543100
C	4.03941800	-2.50773300	0.67172600
H	5.03606800	-2.08903800	0.56444500
C	2.90625900	-1.73390900	0.39438400
C	-0.82370300	-1.25388900	0.03755800

Molecule 5 at M062X/6-31+G(d, p) level

O	-8.04929500	-0.75514500	-1.96593400
O	-7.57411900	1.11572500	2.37815400
C	-9.42972700	-0.42501300	-1.95518500
H	-9.82729900	-0.76660500	-2.90936200
H	-9.57279900	0.65680800	-1.86344500
H	-9.94801600	-0.93599300	-1.13697900
C	-7.31095400	-0.42818100	-0.87446800
C	-5.94988100	-0.76872300	-0.93661000
H	-5.56524700	-1.25162700	-1.82925800
C	-5.11717300	-0.46487100	0.13182600
C	-5.62447000	0.17088700	1.27817400
H	-4.95123000	0.40303600	2.09434300
C	-6.97711800	0.49912900	1.32498900
C	-7.83015700	0.20590800	0.24909500
H	-8.87301600	0.48497100	0.33286400
C	-6.75982100	1.46291900	3.48815400
H	-7.42159800	1.94497900	4.20576800
H	-5.96929000	2.15994300	3.19044900
H	-6.31362100	0.57136300	3.94082800
C	-3.65886100	-0.75231100	0.06064900
C	-3.15414800	-2.09229300	0.05656200
C	-4.03962100	-3.20733300	0.07628500
H	-5.09883200	-3.02869000	0.22808300
C	-3.58543500	-4.48772300	-0.13352700
H	-4.28390900	-5.31845400	-0.12787500
C	-2.21832700	-4.71445300	-0.40959000
H	-1.87097700	-5.70996100	-0.66641700
C	-1.32793400	-3.66581200	-0.36152800
H	-0.28932800	-3.83780800	-0.61526200
C	-1.74432400	-2.34909400	-0.04705700
C	-2.75085000	0.28733000	-0.07511100
C	-1.35569600	0.03804200	-0.02553700
C	-0.61170100	1.28511000	-0.18681800

C	-1.58572500	2.27900400	-0.53300500
C	-1.46120500	3.57943000	-1.08056200
H	-0.48694400	3.99756300	-1.30160600
C	-2.59915100	4.30688700	-1.38088900
H	-2.50280000	5.30142700	-1.80370800
C	-3.87959200	3.76577000	-1.16075700
H	-4.75845200	4.35839000	-1.39436400
C	-4.03576500	2.46274200	-0.68823800
H	-5.02945800	2.04261900	-0.57639800
C	-2.90278500	1.70604900	-0.39682100
C	0.81136900	1.25115600	-0.05953000
O	8.04929400	0.75514300	1.96593500
O	7.57412000	-1.11572200	-2.37815500
C	9.42972600	0.42501200	1.95518600
H	9.82729700	0.76660300	2.90936400
H	9.57279800	-0.65680900	1.86344500
H	9.94801500	0.93599300	1.13698200
C	7.31095300	0.42818000	0.87446800
C	5.94988100	0.76872100	0.93661000
H	5.56524500	1.25162400	1.82925800
C	5.11717300	0.46487100	-0.13182600
C	5.62447000	-0.17088600	-1.27817500
H	4.95123100	-0.40303500	-2.09434500
C	6.97711900	-0.49912800	-1.32499000
C	7.83015700	-0.20590700	-0.24909500
H	8.87301600	-0.48497000	-0.33286300
C	6.75982400	-1.46291500	-3.48815600
H	7.42160100	-1.94497400	-4.20577000
H	5.96929200	-2.15994000	-3.19045200
H	6.31362300	-0.57135900	-3.94082900
C	3.65886100	0.75231100	-0.06065000
C	3.15414800	2.09229200	-0.05656400
C	4.03962100	3.20733200	-0.07628500
H	5.09883200	3.02868900	-0.22808400
C	3.58543500	4.48772300	0.13352600
H	4.28390900	5.31845300	0.12787500
C	2.21832700	4.71445200	0.40958900
H	1.87097700	5.70996000	0.66641600
C	1.32793400	3.66581100	0.36152700
H	0.28932800	3.83780700	0.61526100
C	1.74432400	2.34909400	0.04705600
C	2.75085000	-0.28733000	0.07510900
C	1.35569600	-0.03804300	0.02553600
C	0.61170100	-1.28511100	0.18681600

C	1.58572500	-2.27900400	0.53300600
C	1.46120500	-3.57942900	1.08056500
H	0.48694400	-3.99756200	1.30160900
C	2.59915000	-4.30688600	1.38089400
H	2.50279900	-5.30142500	1.80371500
C	3.87959200	-3.76576900	1.16076100
H	4.75845100	-4.35838800	1.39437100
C	4.03576500	-2.46274200	0.68824000
H	5.02945800	-2.04261900	0.57639900
C	2.90278500	-1.70605000	0.39682100
C	-0.81136900	-1.25115700	0.05952700

Molecule 5 at CAM-B3LYP/6-31+G(d, p) level

O	-8.02179900	0.44781800	2.08537200
O	-7.65472300	-0.78653000	-2.48971800
C	-9.41238500	0.15574500	2.06936300
H	-9.77453700	0.36930400	3.07387800
H	-9.59152800	-0.89818600	1.83349300
H	-9.94020000	0.78892500	1.34903100
C	-7.30713900	0.26594500	0.94298000
C	-5.94151500	0.56993400	1.02687500
H	-5.53699400	0.91937700	1.97015400
C	-5.13013200	0.40987800	-0.08621200
C	-5.67021300	-0.04825300	-1.29790800
H	-5.02064000	-0.16783600	-2.15474800
C	-7.02796200	-0.34074800	-1.36745500
C	-7.85645600	-0.18936000	-0.24785100
H	-8.90589900	-0.43168300	-0.34962000
C	-6.88442100	-0.96574500	-3.67075300
H	-7.58043700	-1.31875800	-4.43024600
H	-6.09886800	-1.71307200	-3.52044700
H	-6.43660200	-0.02168800	-3.99693500
C	-3.66911400	0.69681800	-0.00794000
C	-3.18382400	2.04229000	0.03500600
C	-4.08738500	3.14017000	0.06202900
H	-5.14382100	2.94680400	-0.08019600
C	-3.65866000	4.42004100	0.30823100
H	-4.37370200	5.23586400	0.33869500
C	-2.29567500	4.66275700	0.57354100
H	-1.96226300	5.65627800	0.85507800
C	-1.38892900	3.63403300	0.48410100
H	-0.35398000	3.82395700	0.72991200
C	-1.77934900	2.31909100	0.13661600

C	-2.74475800	-0.32904500	0.09068400
C	-1.35466800	-0.05647600	0.04225200
C	-0.59098500	-1.29687400	0.15335800
C	-1.54829400	-2.31647800	0.46613300
C	-1.40894400	-3.63672700	0.95318100
H	-0.43191800	-4.05228600	1.15732900
C	-2.53399200	-4.39518700	1.21438000
H	-2.42197000	-5.40644100	1.59109700
C	-3.81934200	-3.86795400	1.01017200
H	-4.69032100	-4.48446800	1.20790800
C	-3.99018400	-2.54948000	0.59715500
H	-4.98743000	-2.14061500	0.49400900
C	-2.87123300	-1.76118600	0.35281500
C	0.82954000	-1.24002600	0.01049000
O	8.02179900	-0.44781700	-2.08537200
O	7.65472300	0.78653200	2.48971700
C	9.41238400	-0.15574300	-2.06936400
H	9.77453700	-0.36930200	-3.07387800
H	9.59152700	0.89818800	-1.83349400
H	9.94020000	-0.78892300	-1.34903200
C	7.30713800	-0.26594400	-0.94298100
C	5.94151500	-0.56993300	-1.02687600
H	5.53699400	-0.91937700	-1.97015400
C	5.13013200	-0.40987700	0.08621100
C	5.67021300	0.04825400	1.29790700
H	5.02064000	0.16783600	2.15474800
C	7.02796200	0.34075000	1.36745400
C	7.85645600	0.18936200	0.24785000
H	8.90589900	0.43168500	0.34961900
C	6.88442100	0.96574600	3.67075200
H	7.58043700	1.31876000	4.43024500
H	6.09886700	1.71307300	3.52044600
H	6.43660300	0.02168900	3.99693400
C	3.66911400	-0.69681800	0.00794000
C	3.18382400	-2.04229000	-0.03500500
C	4.08738600	-3.14017000	-0.06202700
H	5.14382200	-2.94680300	0.08019800
C	3.65866200	-4.42004200	-0.30822700
H	4.37370400	-5.23586400	-0.33869000
C	2.29567700	-4.66275800	-0.57353600
H	1.96226500	-5.65628000	-0.85507100
C	1.38893100	-3.63403500	-0.48409800
H	0.35398100	-3.82396000	-0.72990800
C	1.77934900	-2.31909200	-0.13661500

C	2.74475800	0.32904500	-0.09068400
C	1.35466800	0.05647500	-0.04225300
C	0.59098400	1.29687300	-0.15335900
C	1.54829400	2.31647600	-0.46613400
C	1.40894300	3.63672500	-0.95318400
H	0.43191700	4.05228300	-1.15733300
C	2.53399000	4.39518500	-1.21438300
H	2.42196800	5.40643900	-1.59110200
C	3.81934100	3.86795300	-1.01017400
H	4.69031900	4.48446700	-1.20791000
C	3.99018300	2.54948000	-0.59715500
H	4.98742900	2.14061500	-0.49400700
C	2.87123200	1.76118500	-0.35281500
C	-0.82954000	1.24002500	-0.01049000