SUPPORTING INFORMATION

Excited State Aromatic Character of Cibalackrot-Type Compounds in Terms of Hückel-Aromaticity: A Rationale for Singlet Fission Chromophore Design

Weixuan Zeng, [a] Ouissam El Bakouri,[b] Dariusz W. Szczepanik,[c,d]* Hugo Bronstein[a,e]* and Henrik Ottosson[b]*

[a] Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, U.K.

[b] Department of Chemistry - Ångström Laboratory, Uppsala University, 751 20 Uppsala, Sweden

[c] Department of Theoretical Chemistry Faculty of Chemistry, Jagiellonian University, Gronostajowa, 2, 30-387 Kraków, Poland.

[d] Institut de Quìmica Computacional i Catàlisi and Departament de Química, Universitat de Girona, C/ Maria Aurèlia Capmany, 69, 17003 Girona, Catalonia, Spain.

[e] Cavendish Laboratory, University of Cambridge, Cambridge, CB3 0HE, U.K.

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PARENT CIBA

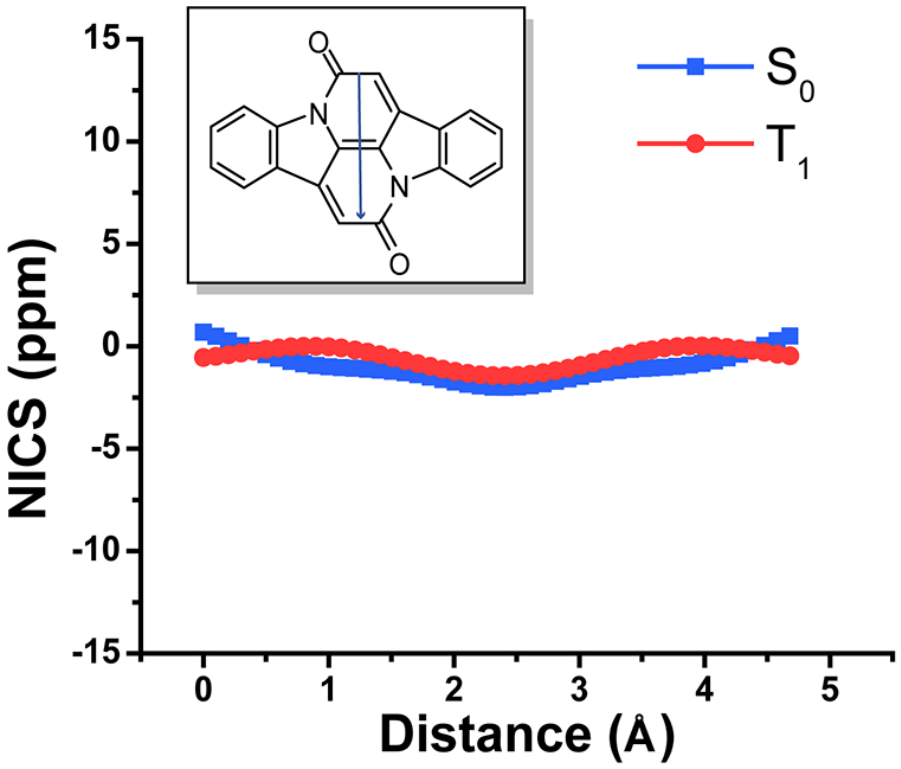


Figure S1 π-NICS-XY scan in the S_0 and T_1 states of **CIBA**, calculated at (U)B3LYP/6-311+G(d,p) level.

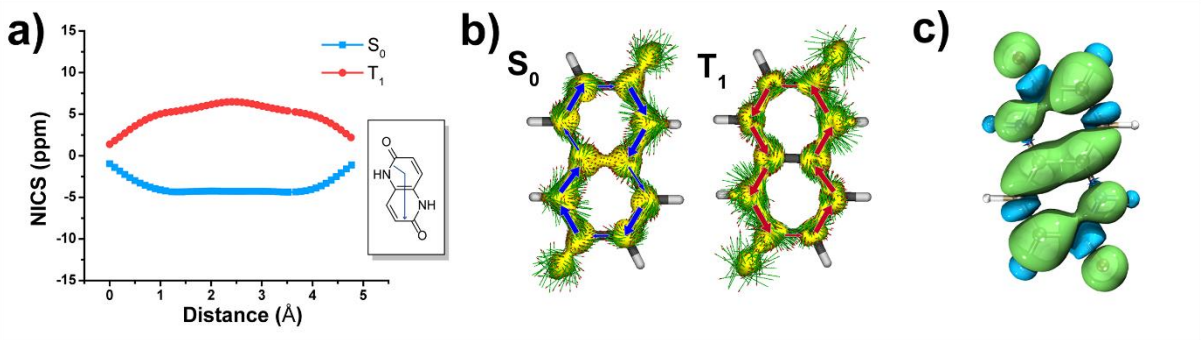


Figure S2 a) π-NICS-XY scan, b) π-Electron ring currents according to AICD in the S_0 and T_1 states and c) spin density distribution in the T1 state (ρ = 0.0008) of **NARID**, calculated at (U)B3LYP/6-311+G(d,p) level.

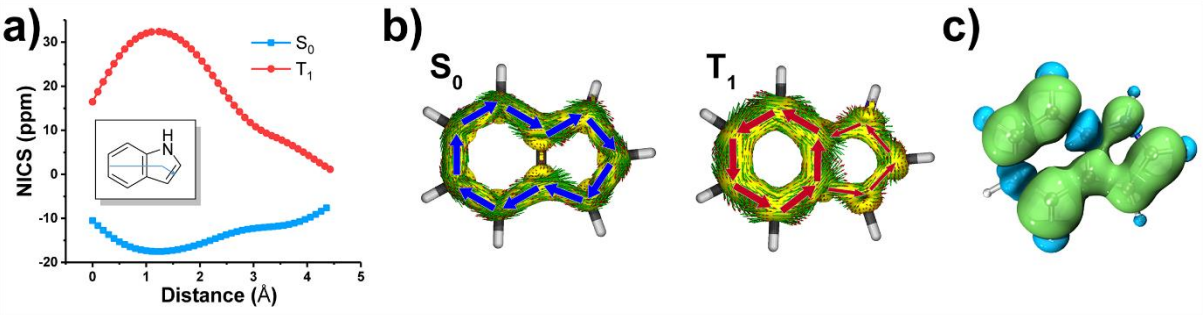


Figure S3 a) π-NICS-XY scan, b) π-Electron ring currents according to AICD in the S_0 and T_1 states and c) spin density distribution in the T1 state (ρ = 0.0008) of indole, calculated at (U)B3LYP/6-311+G(d,p) level.

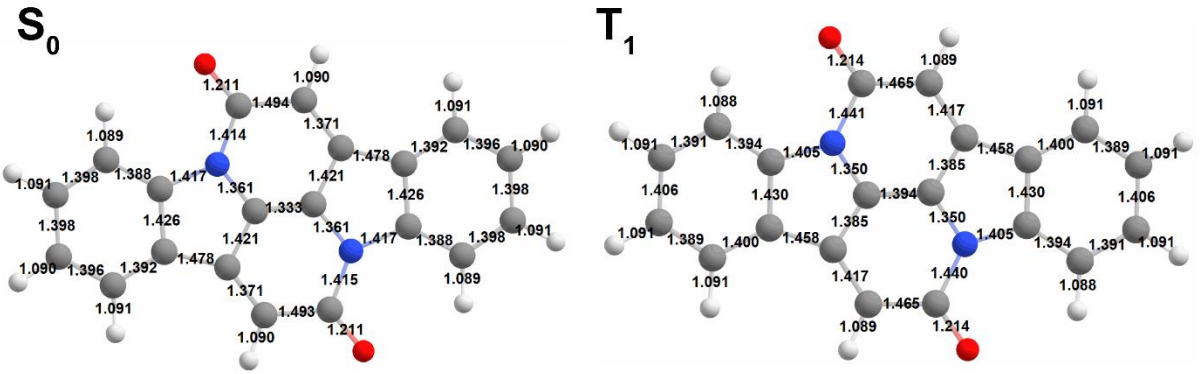


Figure S4 Bond lengths of **CIBA** in the S_0 and T_1 states.

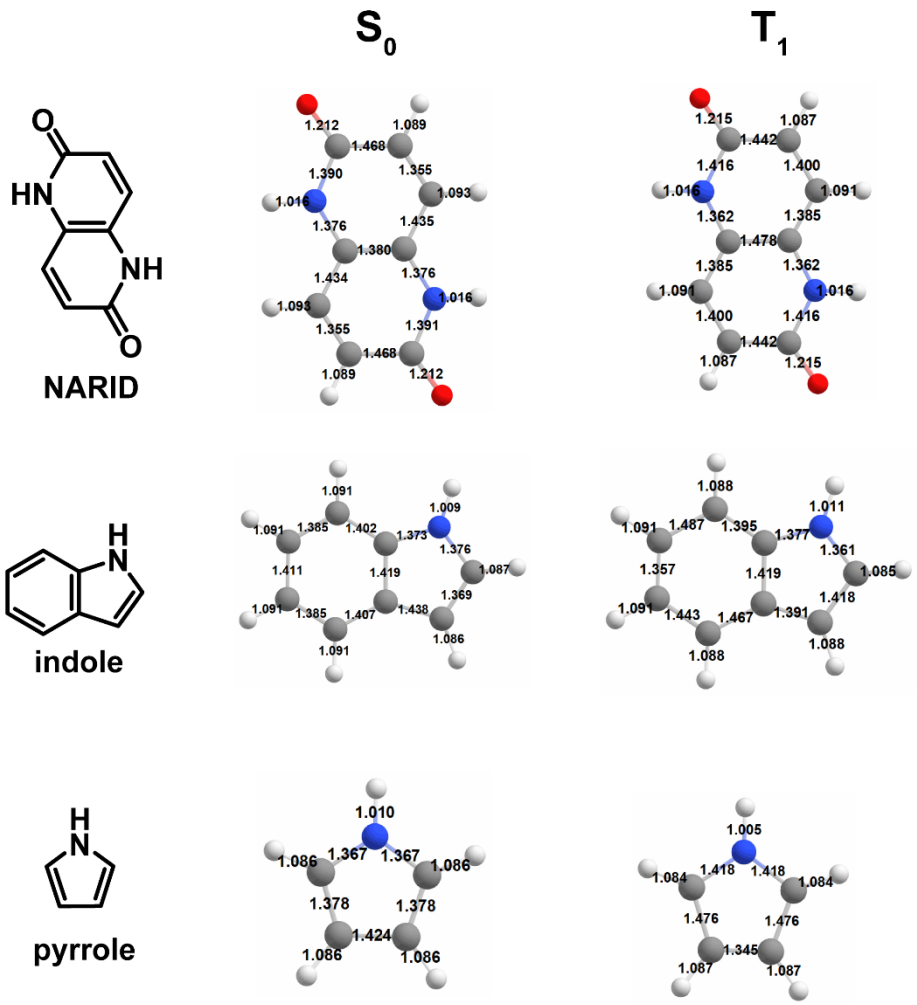


Figure S5 Chemical structures and bond lengths of **NARID**, indole and pyrrole in the S_0 and T_1 states.

Table S1 Values of key aromatic criteria for relevant rings in sub-moieties of **CIBA**.

	S_0					T_1				
	Narid		indole			Narid		indole		
	C	*CC'*	*A*	*B*	*AB*	*C*	*CC'*	*A*	*B*	*AB*
FLU	0.028	0.033	0.006	0.011	0.006	0.027	0.018	0.009	0.027	0.018
$\Delta FLU_{\alpha\beta}/FLU$	-	-	-	-	-	-1.193	-1.733	-1.806	-0.308	-0.642
MCI	0.011	-	0.045	0.022	-	0.005	-	0.017	0.007	-
HOMA	0.506	0.410	0.913	0.743	0.853	0.403	0.701	0.097	0.857	0.372

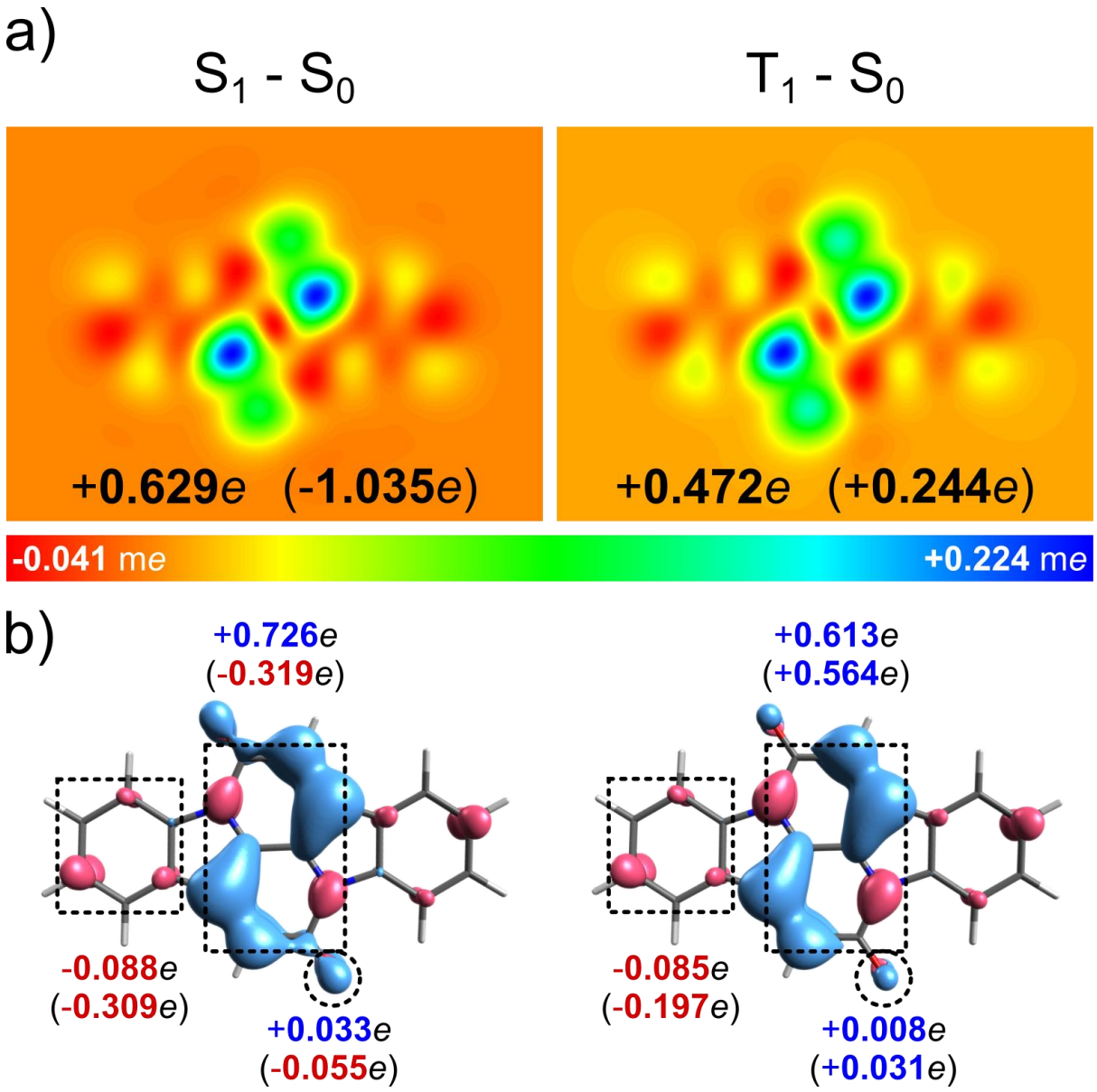


Figure S6 a) The effect of S0 to S1 and S0 to T1 vertical and adiabatic (numbers in brackets) excitations on electron delocalization in CIBA visualized and quantified by the global $EDDB_H$ function (a) calculated at 2.0A above the molecular plane and (b) the corresponding isosurface at v=0.002e. Method: (U)B3LYP/6-311+G(d,p) level.

The results of the $EDDB_H$ dissection into paired/unpaired density components in Figure S7 clearly show that the aromatic character of the pyrrolic units (5-MRs) is predominated by the closed-subshell delocalization (2.260*e*) with only a minor contribution from the unpaired electrons (0.245*e*) as the spin density is distributed mostly in the inner 6-MRs. Thus, even though the unpaired electrons enhance noticeably the total delocalization effect in the triplet state, the pyrrolic units cannot be regarded locally Baird aromatic.

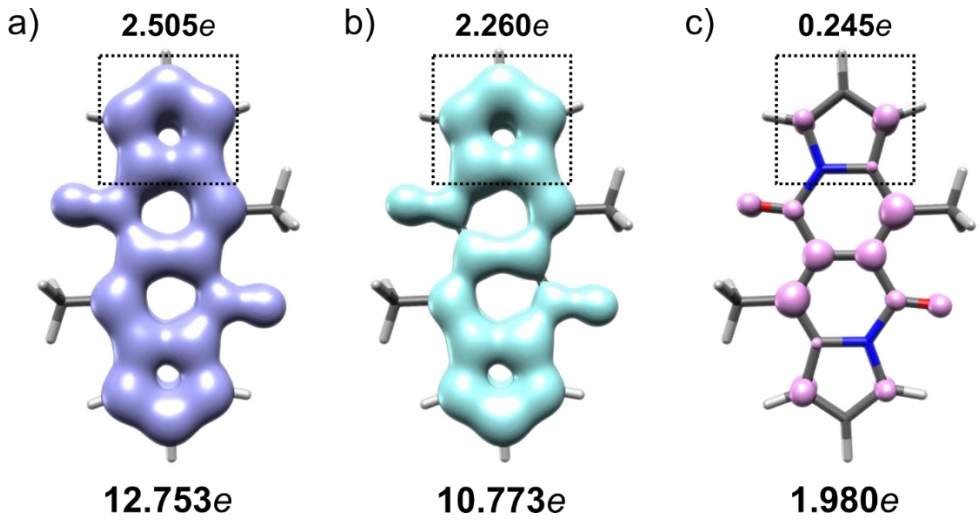
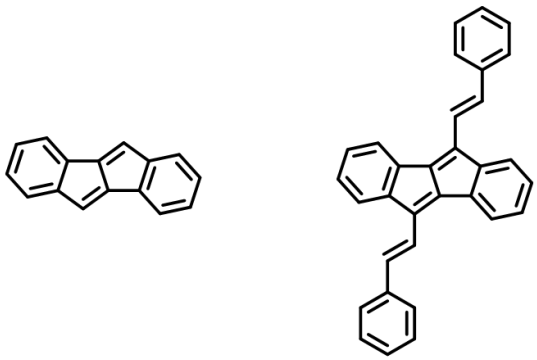


Figure S7. The electron density of delocalized bonds ($EDDB_H$), visualized at the isovalue of 0.010 e, for the compound DPND taken from Ref 10 in the maintext (*J. Am. Chem. Soc.* **2020**, *142*, 10235) at its T_1 state (a), with the corresponding density layers representing paired (b) and unpaired electrons (c). The numbers below the structures correspond to the global populations of delocalized electrons, while the numbers above the boxes refer to the population of electrons delocalized within the 5-membered rings (pyrrolic units). Method: B3LYP/6-311++G(d,p).



BENZPENT5

$E(S_1)_v = 2.68$
$E(T_1)_v = 2.04$
$E(T_1)_a = 1.70$
$\Delta E(S_1\text{-}T_1)_{v\text{-}v} = 0.64$
$\Delta E(S_1\text{-}T_1)_{v\text{-}a} = 0.98$
$\text{Ratio}_{v/v} = 1.32$
$\text{Ratio}_{v/a} = 1.58$

bis(styryl)BENZPENT5

$E(S_1)_v = 2.41$
$E(T_1)_v = 1.57$
$E(T_1)_a = 1.16$
$\Delta E(S_1\text{-}T_1)_{v\text{-}v} = 0.84$
$\Delta E(S_1\text{-}T_1)_{v\text{-}a} = 1.25$
$\text{Ratio}_{v/v} = 1.54$
$\text{Ratio}_{v/a} = 2.07$

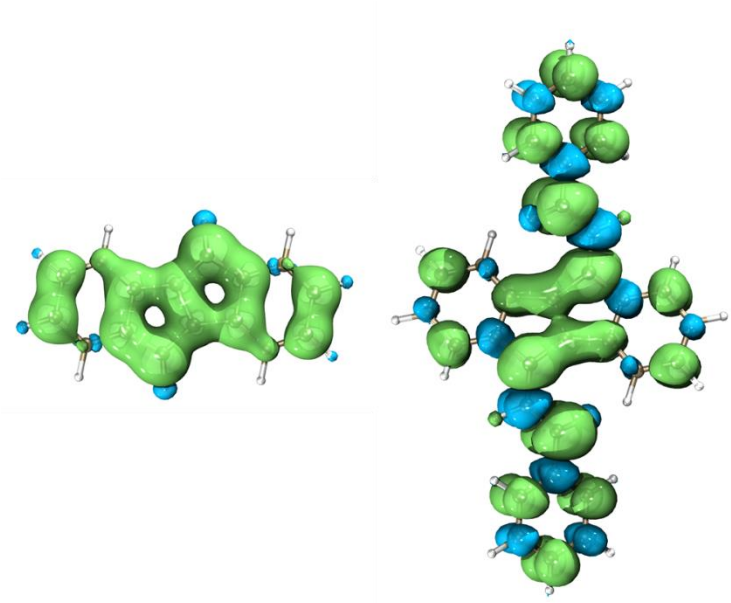


Figure S8 Chemical structures (top), relevant excited state energy levels (middle) and spin density distribution (bottom) in the T_1 state (ρ = 0.0008) of **BENZPENT5** and **bis(styryl)BENZPENT5**. The detailed discussion can be found on the Ref 8 in the maintext (*J. Am. Chem. Soc.* **2020**, *142*, 5602, Page S55-57 in the Supporting Information of that paper)

SUBSTITUTED CIBALACKROTS

Table S2 The calculated key parameters of excited states of **CIBA** and **SCIBAs**.

Emitter	Excited state	D [a)] [Å]	S_r index [b)]	t index [c)] [Å]	Electron Configurations
CIBA	S_1	0.002	0.762	-2.068	H→L: 98.4%
	T_1	0.002	0.722	-2.068	H→L: 93.3%
SCIBA1	S_1	0.079	0.770	-0.714	H→L: 98.3%
	T_1	0.079	0.727	-0.714	H→L: 93.0%
SCIBA2	S_1	0.033	0.772	-0.741	H→L: 98.4%
	T_1	0.033	0.735	-0.741	H→L: 93.7%
SCIBA3	S_1	0.000	0.763	-2.302	H→L: 98.4%
	T_1	0.000	0.728	-2.308	H→L: 93.3%
SCIBA4	S_1	0.000	0.780	-0.928	H→L: 98.1%
	T_1	0.000	0.752	-0.928	H→L: 94.5%
SCIBA5	S_1	0.001	0.783	-0.761	H→L: 98.3%
	T_1	0.001	0.770	-0.762	H→L: 92.7%; H-1→L+1: 2.3%
SCIBA6	S_1	0.000	0.772	-0.750	H→L: 97.6%
	T_1	0.000	0.745	-0.750	H→L: 94.2%
SCIBA7	S_1	0.000	0.760	-0.743	H→L: 98.0%
	T_1	0.000	0.728	-0.743	H→L: 93.8%
SCIBA8	S_1	0.032	0.774	-0.760	H→L: 97.7%
	T_1	0.004	0.781	-0.856	H→L: 90.8%; H-2→L: 2.4%
SCIBA9	S_1	0.002	0.776	-0.769	H→L: 98.5%
	T_1	0.002	0.748	-0.769	H→L: 94.9%
SCIBA10	S_1	0.025	0.756	-2.618	H→L: 97.7%
	T_1	0.022	0.744	-3.080	H→L: 91.7%; H-4→L: 2.6%
SCIBA11	S_1	0.000	0.763	-0.747	H→L: 98.2%
	T_1	0.000	0.735	-0.747	H→L: 94.6%
SCIBA12	S_1	0.005	0.773	-0.763	H→L: 98.1%
	T_1	0.000	0.709	-0.869	H→L: 93.6%

[a)] Distance between centroid of hole and electron. [b)] Overlap index of hole-electron distribution. [c)] Separate index of hole-electron distribution.

Table S2 (continued) The calculated key parameters of excited states of **CIBA** and **SCIBAs**.

Emitter	Excited state	D [a)] [Å]	S_r index [b)]	t index [c)] [Å]	Electron Configurations
SCIBA13	S_1	0.001	0.815	-0.926	H→L: 85.3%; H-1→L+1: 8.0%
	T_1	0.001	0.825	-0.897	H→L: 83.6%; H-1→L+1: 10.4%
SCIBA14	S_1	0.000	0.778	-1.300	H→L: 98.1%
	T_1	0.000	0.733	-1.300	H→L: 92.6%
SCIBA15	S_1	0.003	0.776	-0.757	H→L: 98.7%
	T_1	0.003	0.723	-0.757	H→L: 92.0%
SCIBA16	S_1	0.000	0.780	-1.007	H→L: 97.8%
	T_1	0.000	0.709	-2.611	H→L: 93.9%
SCIBA17	S_1	0.000	0.764	-1.449	H→L: 98.0%
	T_1	0.000	0.709	-1.449	H→L: 93.9%
SCIBA18	S_1	0.050	0.762	-0.746	H→L: 98.1%
	T_1	0.006	0.746	-0.826	H→L: 89.7%; H-2→L: 3.9%
SCIBA19	S_1	0.000	0.763	-0.738	H→L: 98.2%
	T_1	0.000	0.734	-0.738	H→L: 94.4%
SCIBA20	S_1	0.000	0.751	-0.764	H→L: 98.5%
	T_1	0.000	0.716	-0.764	H→L: 94.0%
SCIBA21	S_1	0.013	0.767	-0.756	H→L: 98.2%
	T_1	0.013	0.733	-0.756	H→L: 93.8%
SCIBA22	S_1	0.110	0.761	-0.688	H→L: 98.6%
	T_1	0.110	0.711	-0.688	H→L: 92.1%
SCIBA23	S_1	0.064	0.670	-0.697	H→L: 96.6%
	T_1	0.022	0.749	-0.736	H→L: 81.0%; H-2→L:11.0%
SCIBA24	S_1	0.020	0.703	-0.750	H→L: 96.7%
	T_1	0.007	0.752	-0.748	H→L: 83.1%; H-2→L:11.2%

[a)] Distance between centroid of hole and electron. [b)] Overlap index of hole-electron distribution. [c)] Separate index of hole-electron distribution.

Table S2 (continued) The calculated key parameters of excited states of **CIBA** and **SCIBAs**.

Emitter	Excited state	D [a] [Å]	S_r index [b]	t index [c] [Å]	Electron Configurations
SCIBA25	S_1	N.A.	N.A.	N.A.	H→L: 94.2%; H-1→L+1:3.0%
	T_1	N.A.	N.A.	N.A.	H→L: 70.8%; H-2→L:20.4%
SCIBA26	S_1	0.000	0.717	-0.902	H→L: 66.9%; H-1→L+1:17.1%
	T_1	0.000	0.790	-2.803	H→L: 77.0%; H-1→L+1:12.5%
SCIBA27	S_1	0.000	0.793	-4.239	H→L: 77.8%; H-1→L+1:13.3%
	T_1	0.000	0.804	-4.162	H→L: 79.0%; H-1→L+1:12.3%
SCIBA28	S_1	0.102	0.582	-0.670	H→L: 94.8%; H-1→L+1:2.4%
	T_1	0.054	0.706	-0.709	H→L: 77.6%; H-2→L:13.1%
SCIBA29	S_1	0.001	0.704	-0.865	H→L: 68.4%; H-1→L+1:16.4%
	T_1	0.001	0.771	-1.056	H→L: 68.4%; H-1→L+1:16.4%
SCIBA30	S_1	0.000	0.779	-0.789	H→L: 81.6%; H-1→L+1:10.6%
	T_1	0.000	0.785	-0.790	H→L: 79.6%; H-1→L+1:11.6%

[a] Distance between centroid of hole and electron. [b] Overlap index of hole-electron distribution. [c] Separate index of hole-electron distribution.

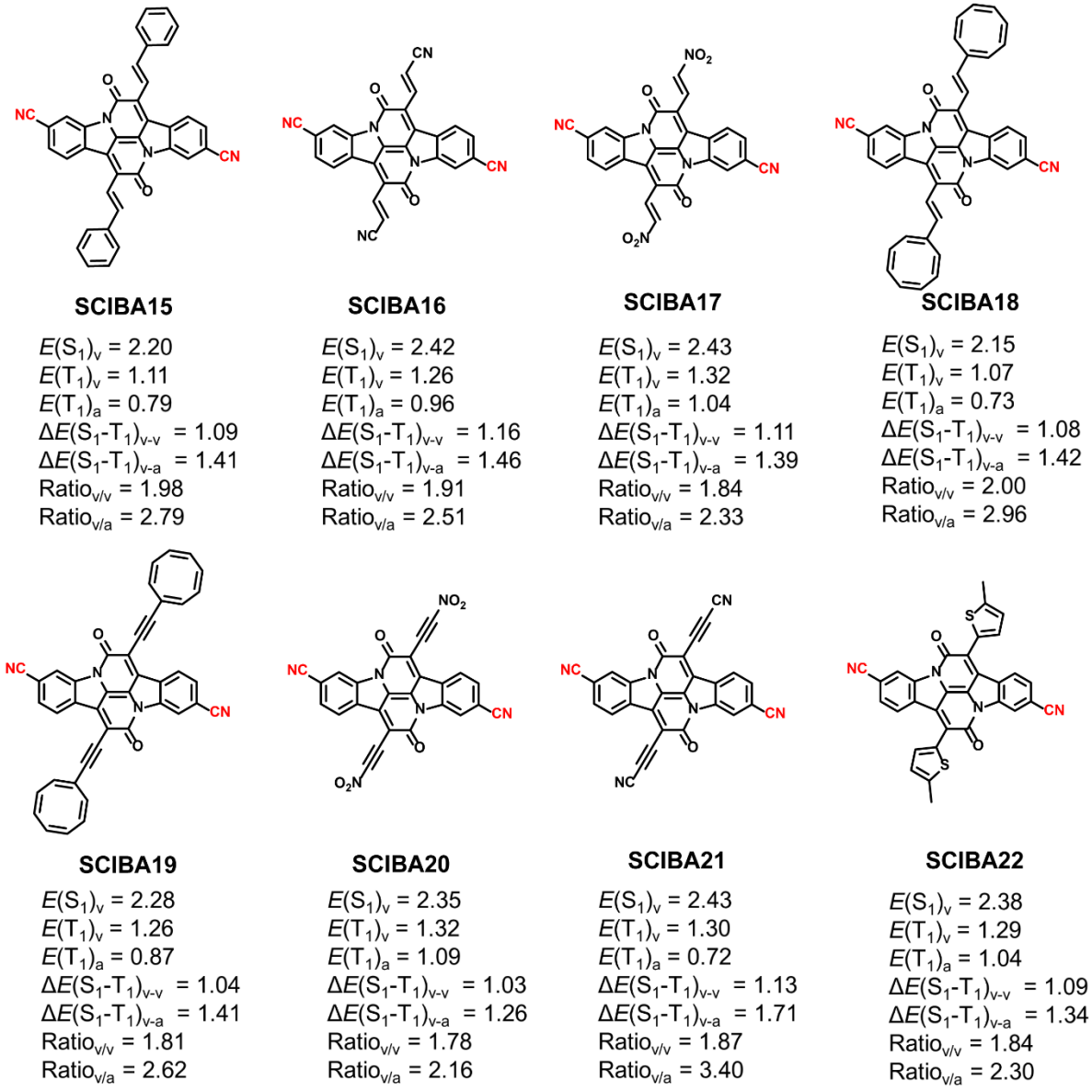


Figure S9 Chemical structures and relevant excitation energies (in eV) of **SCIBA15-22**. Calculations at TD-M06-2x/def2-SVP//M06-2X/def2-SVP level.

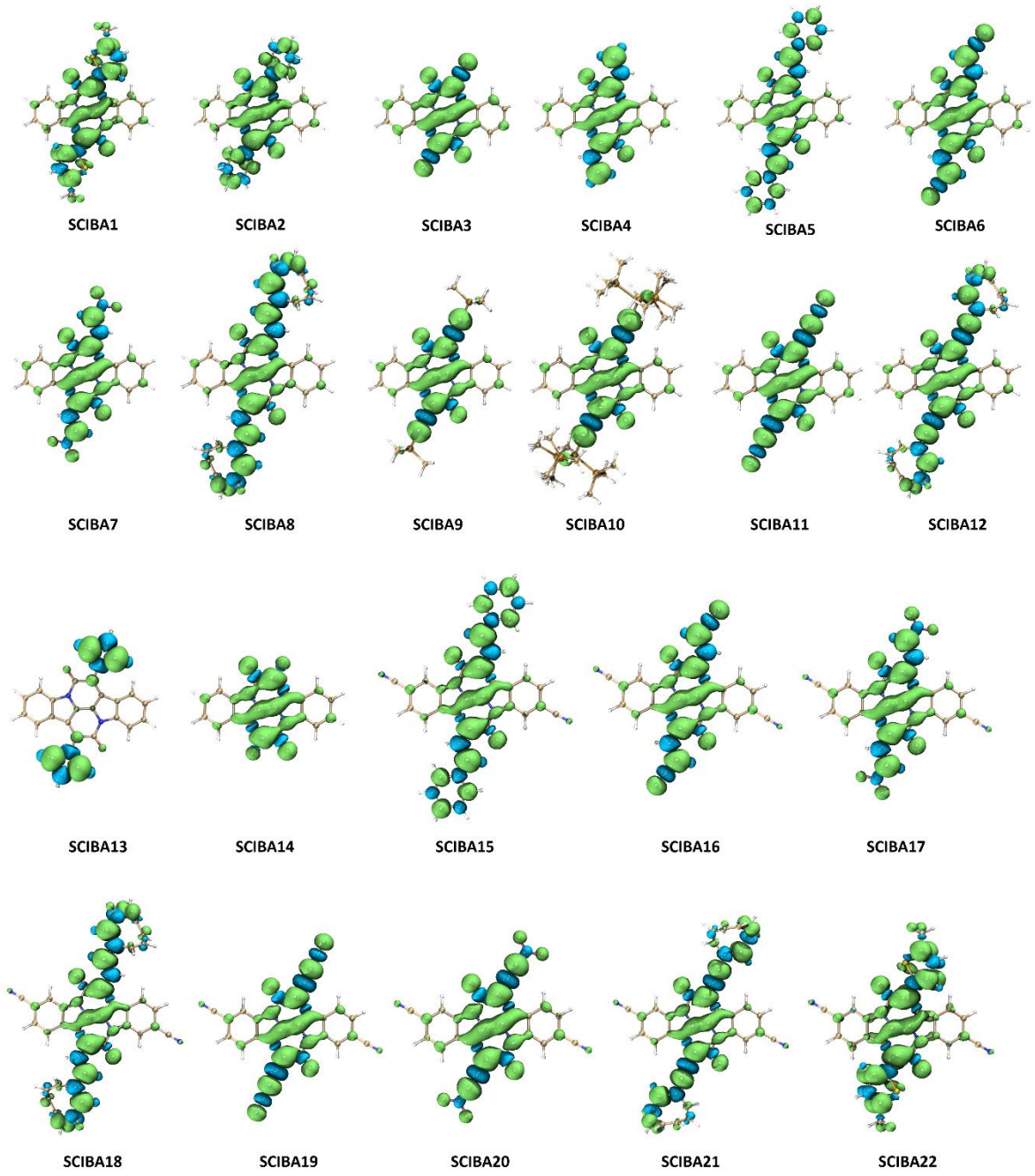


Figure S10: Spin density distribution in T_1 state of **SCIBA1-22**. Calculations at (U)M06-2X/def2-SVP level. Isosurface used: 0.0008.

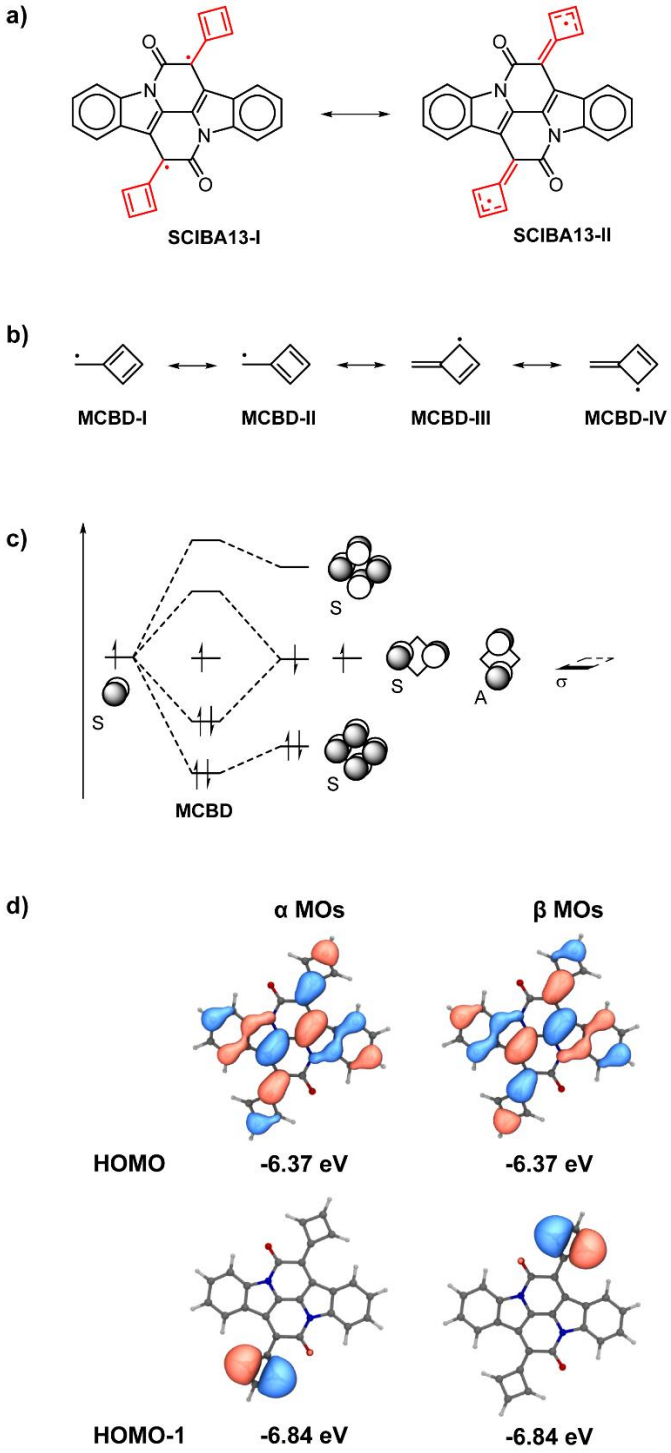


Figure S11 Open-shell singlet ground state of SCIBA13. a) Two resonance structures of **SCIBA13** described by two methyleneCBD units shown in red, b) the four possible resonance structures of methyleneCBD (**MCBD-I – MCBD-IV**), c) a qualitative MO diagram showing how the p-MOs of methyleneCBD are constructed from the π-orbitals of a methylene fragment and a CBD fragment, and d) open-shell singlet ground state with almost the same total energy comparing with opted T_1 geometry. BS state found on HOMO-1, which is mainly contributed by the radicals located on the CBD units. Calculated at UM06-2X/def2-SVP level. The unpaired electron will remain in the antisymmetric MO which is fully localized on the CBD fragment, thus revealing that resonance structures **MCBD-III** and **MCBD-IV** are the ones that fully describe methyleneCBD. From this one can conclude that resonance structure **SCIBA13-II** is the one that dominates the description of **SCIBA13**. Isosurface used: 0.023.

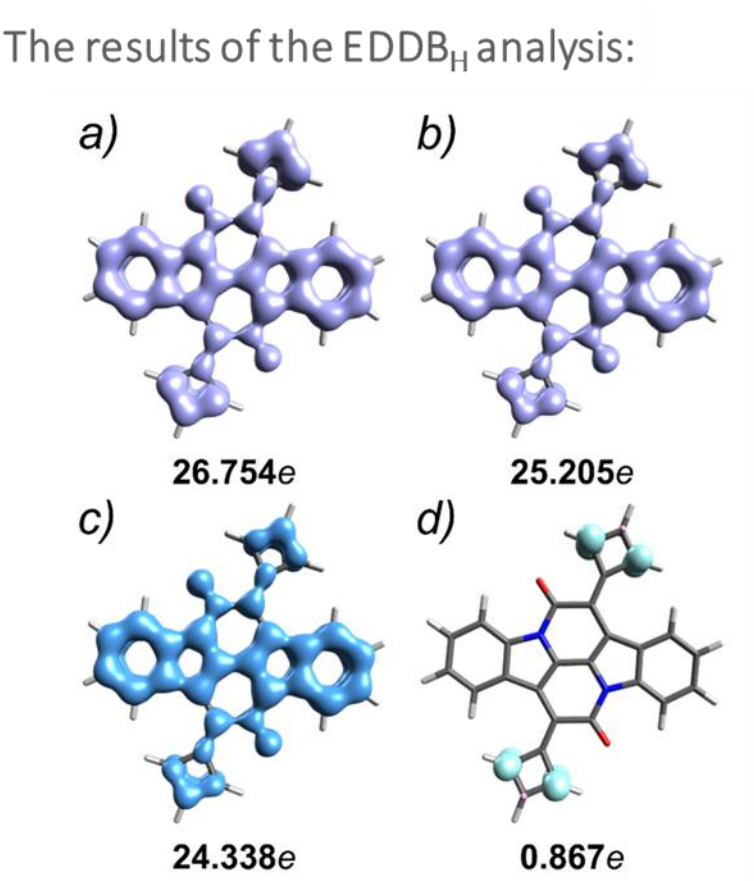
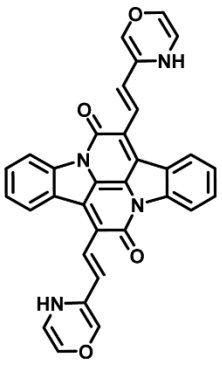
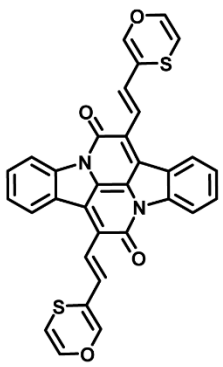


Figure S12 Isosurface contours of the electron density of delocalized bonds, $EDDB_H$ (which quantifies delocalization effects involving heavy atoms only), with the corresponding electron populations (bold numbers), for S**CIBA13** at (a) S_0 and (b) T_1 states; the $EDDB_H(r)$ function at T_1 was dissected into components representing contributions from (c) paired and (d) unpaired electrons. Isosurface used: 0.006.



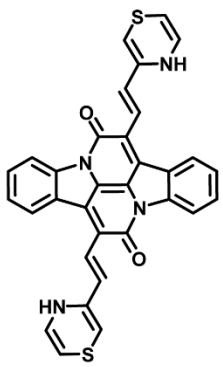
SCIBA23

$E(S_1)_v$ = 2.09
$E(T_1)_v$ = 1.10
$E(T_1)_a$ = 0.69
$\Delta E(S_1\text{-}T_1)_{v\text{-}v}$ = 0.99
$\Delta E(S_1\text{-}T_1)_{v\text{-}a}$ = 1.39
$Ratio_{v/v}$ = 1.90
$Ratio_{v/a}$ = 3.02



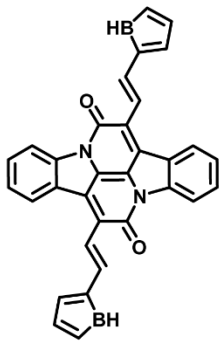
SCIBA24

$E(S_1)_v$ = 2.21
$E(T_1)_v$ = 1.19
$E(T_1)_a$ = 0.82
$\Delta E(S_1\text{-}T_1)_{v\text{-}v}$ = 1.02
$\Delta E(S_1\text{-}T_1)_{v\text{-}a}$ = 1.39
$Ratio_{v/v}$ = 1.86
$Ratio_{v/a}$ = 2.69



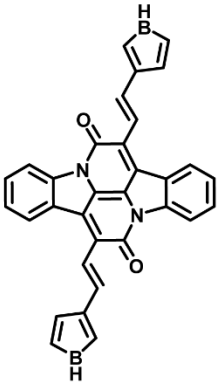
SCIBA25

$E(S_1)_v$ = 1.87
$E(T_1)_v$ = 1.07
$E(T_1)_a$ = 0.62
$\Delta E(S_1\text{-}T_1)_{v\text{-}v}$ = 0.80
$\Delta E(S_1\text{-}T_1)_{v\text{-}a}$ = 1.25
$Ratio_{v/v}$ = 1.74
$Ratio_{v/a}$ = 3.01



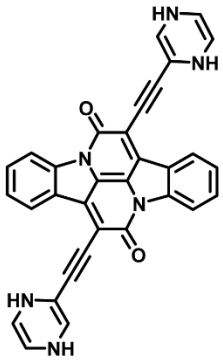
SCIBA26

$E(S_1)_v$ = N.A.
$E(T_1)_v$ = N.A.
$E(T_1)_a$ = 0.02
$\Delta E(S_1\text{-}T_1)_{v\text{-}v}$ = N.A.
$\Delta E(S_1\text{-}T_1)_{v\text{-}a}$ = N.A.
$Ratio_{v/v}$ = N.A.
$Ratio_{v/a}$ = N.A.



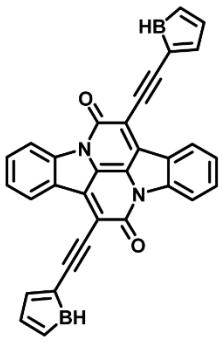
SCIBA27

$E(S_1)_v$ = 1.94
$E(T_1)_v$ = 1.01
$E(T_1)_a$ = 0.30
$\Delta E(S_1\text{-}T_1)_{v\text{-}v}$ = 0.93
$\Delta E(S_1\text{-}T_1)_{v\text{-}a}$ = 1.64
$Ratio_{v/v}$ = 1.93
$Ratio_{v/a}$ = 6.40



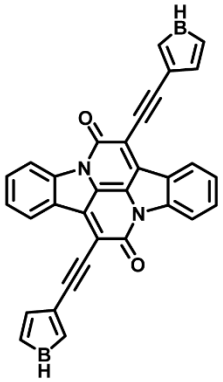
SCIBA28

$E(S_1)_v$ = 1.71
$E(T_1)_v$ = 0.93
$E(T_1)_a$ = 0.34
$\Delta E(S_1\text{-}T_1)_{v\text{-}v}$ = 0.79
$\Delta E(S_1\text{-}T_1)_{v\text{-}a}$ = 1.37
$Ratio_{v/v}$ = 1.85
$Ratio_{v/a}$ = 5.01



SCIBA29

$E(S_1)_v$ = 1.87
$E(T_1)_v$ = 1.11
$E(T_1)_a$ = 0.50
$\Delta E(S_1\text{-}T_1)_{v\text{-}v}$ = 0.76
$\Delta E(S_1\text{-}T_1)_{v\text{-}a}$ = 1.37
$Ratio_{v/v}$ = 1.68
$Ratio_{v/a}$ = 3.73



SCIBA30

$E(S_1)_v$ = 2.05
$E(T_1)_v$ = 1.17
$E(T_1)_a$ = 0.82
$\Delta E(S_1\text{-}T_1)_{v\text{-}v}$ = 0.88
$\Delta E(S_1\text{-}T_1)_{v\text{-}a}$ = 1.23
$Ratio_{v/v}$ = 1.75
$Ratio_{v/a}$ = 2.49

Figure S13 Chemical structures and relevant excitation energies (in eV) of **SCIBA23-30**. Calculations at TD-M06-2x/def2-SVP//M06-2X/def2-SVP level.

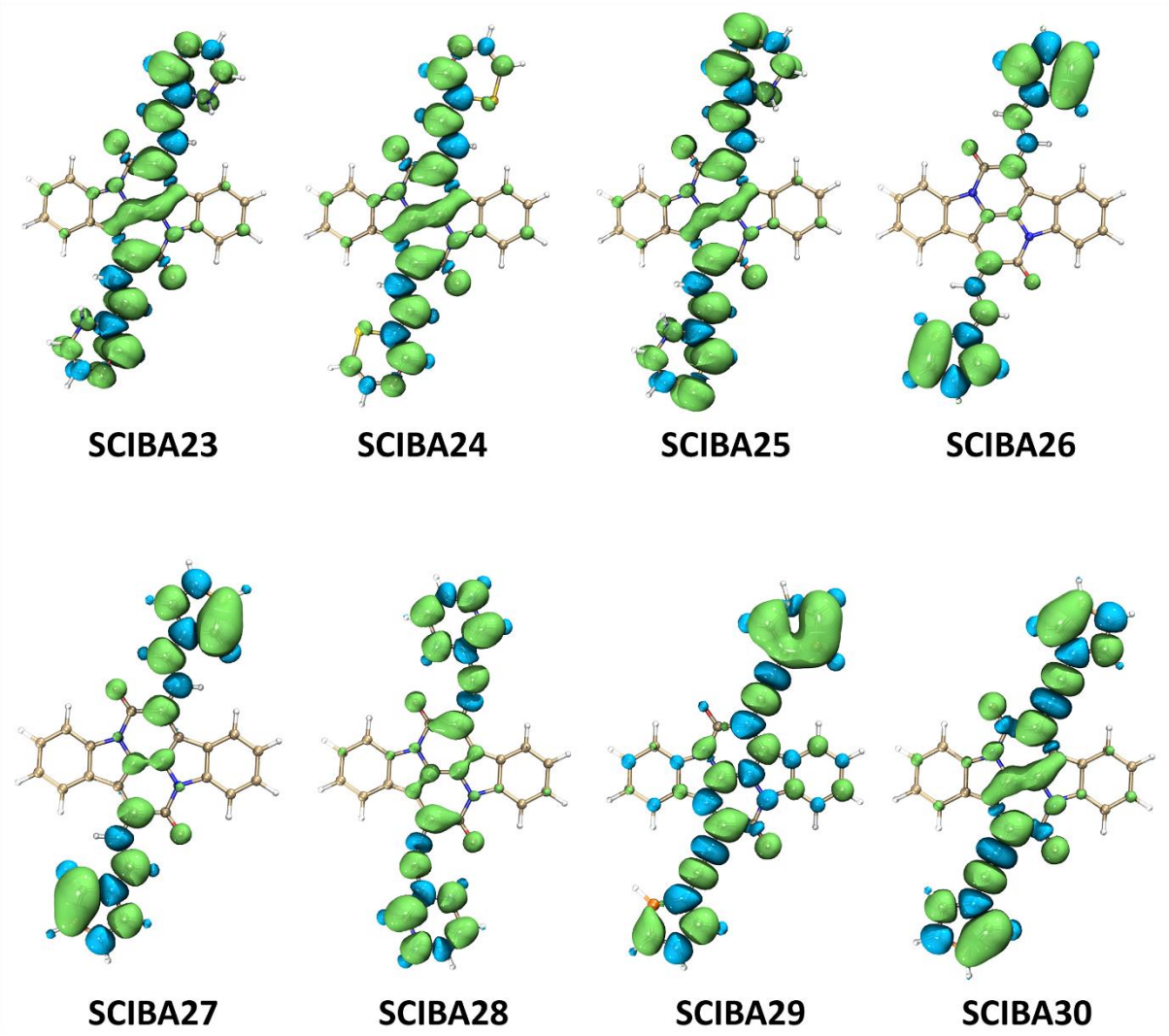


Figure S14: Spin density distribution in T_1 state of **SCIBA23-30**. Calculations at (U)M06-2X/def2-SVP level. Isosurface used: 0.0008.

Halogenated CIBAs

The $E(T_1)$ are very similar throughout the halogenated CIBA series. This finding is reflected in the $EDDB_H$ results. One sees no significant difference in the $EDDB_H$ plots (**Figure S16**) showing a similar delocalization pattern compared to the parent CIBA (**Figure 3**), and the main difference comes from the C atoms of the two pyrrolo units which apparently shows less delocalization in the halogenated compounds. In terms of quantitative delocalization (**Table S3**), the C atoms of the two pyrrolo units display some delocalization, yet very small differences through the series (σ = 0.028 e) are observed revealing a good correlation with the $E(T_1)$ (R^2 = 0.95). This indicates that the degree of delocalization of the C atoms of the two pyrrolo units might be responsible for altering the $E(T_1)$. On the other hand, the delocalization character in the other units (CCO and halogens), which experience a significant change from SCIBA-F to the other halogens (**Table S3**), does not correlate with the unaltered $E(T_1)$. In the CCO and halogen units, we have a kind of cooperativity of two effects: resonance effect and polarization. In the F case, the high resonance effect of the CCO moieties makes the number of electrons in the ring decrease but, due to the high polarization of SCIBA-F, it also withdraws electrons from the ring. $EDDB_H$ calculations (**Table S3**) show indeed a higher delocalization in the CCO units (~1.2 e) compared to SCIBA-Cl, -Br, and -I (~0.9 e). Such lower delocalization of the CCO unit in the Cl, Br, and I cases is explained by the fact that all three halogens are much less withdrawing, start donating electrons from their lone pairs, and we start to see competition in the sense that the halogen tries to donate to the ring and the oxygen tries to also donate to the ring by resonance.

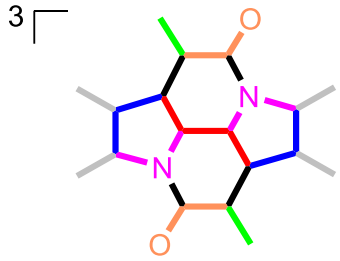


Figure S15: Color-guided CIBA structure for **Table S3**.

Table S3 Unpaired-electron contributions to $EDDB_H$ of a few SCIBAs and BCIBAs obtained at the M06-2X/def2-SVP level. The data is sorted by $E(T_1)$.

Compounds	**Total**	**2 subst.**	**2CCO**	**CCCC** (*t*-butadiene)	**2N**	**CCCCCCCC** (C atoms of pyrrolo units)	$E(T_1)$
SCIBA-Cl	0.505	-0.334	0.889	0.125	-0.136	0.116	1.33
SCIBA-Br	0.483	-0.340	0.861	0.149	-0.139	0.136	1.34
SCIBA-I	0.536	-0.333	0.867	0.195	-0.139	0.180	1.35
SCIBA-F (14)	0.997	-0.172	1.160	0.160	-0.138	0.160	1.35
BCIBA0	1.857	-	1.089	0.343	-0.060	0.827	0.99
BCIBA3	1.888	-	1.057	0.425	-0.057	0.750	1.21
BCIBA2C	1.783	-	1.080	0.482	-0.071	0.689	1.27
BCIBA2A	1.676	-	1.041	0.424	-0.107	0.613	1.39
BCIBA2	1.620	-	1.025	0.373	-0.102	0.540	1.52
SCIBA13	0.770	0.770	0.000	0.000	0.000	0.000	0.00
SCIBA8	0.284	0.025	0.401	-0.045	-0.086	-0.056	0.86
SCIBA1	0.077	-0.599	0.855	-0.054	-0.113	-0.066	0.98
SCIBA9	0.503	0.149	0.502	-0.018	-0.119	-0.029	1.12
SCIBA2	1.210	0.519	0.735	0.099	-0.139	0.095	1.24

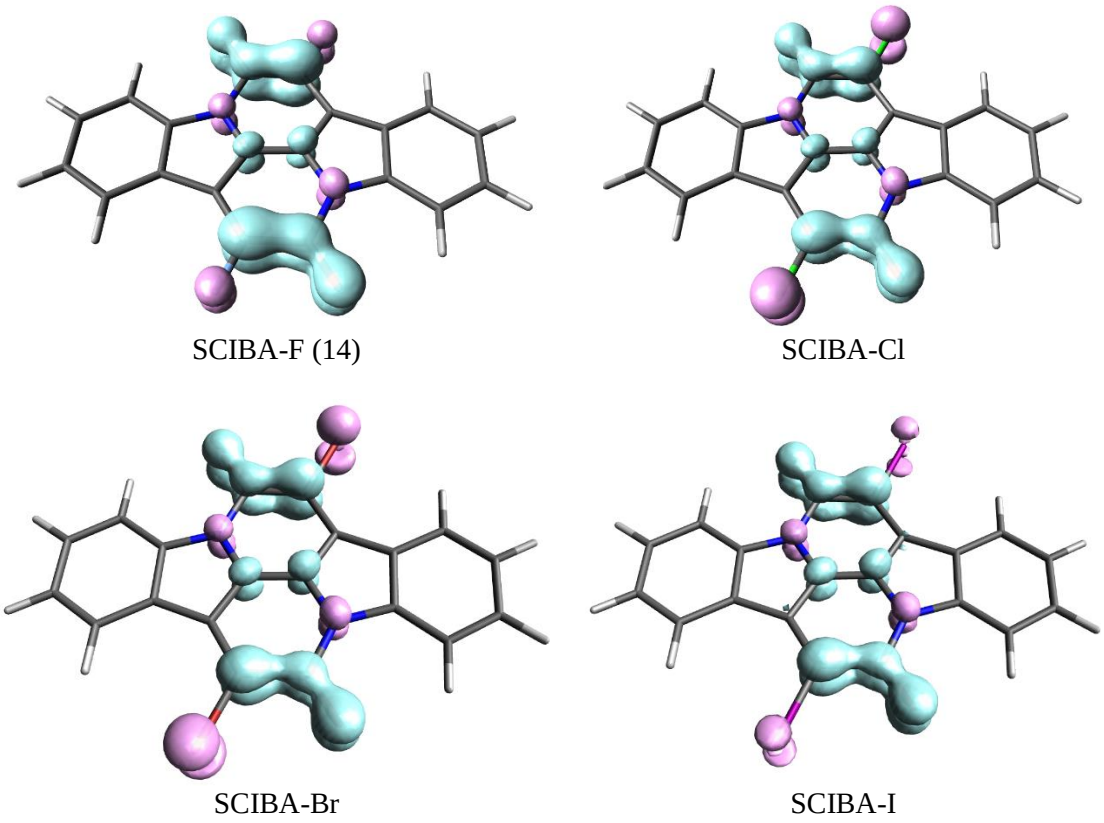
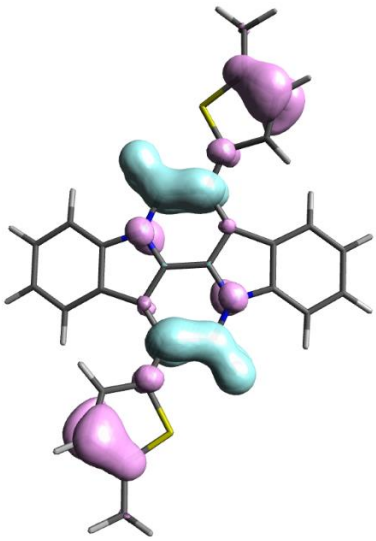


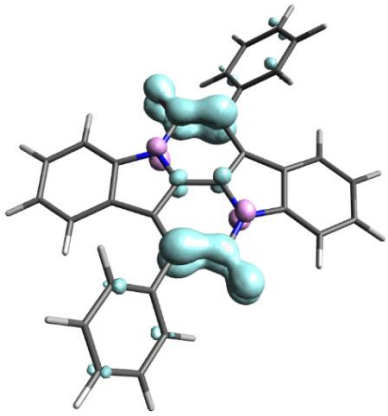
Figure S16: Plots of the unpaired-electron component of the $EDDB_H$ for **SCIBA-F(14)**, **SCIBA-Cl**, **SCIBA-Br** and **SCIBA-I** computed at the UM06-2X/def2-SVP level. Isosurface used: 0.006.

SCIBAs

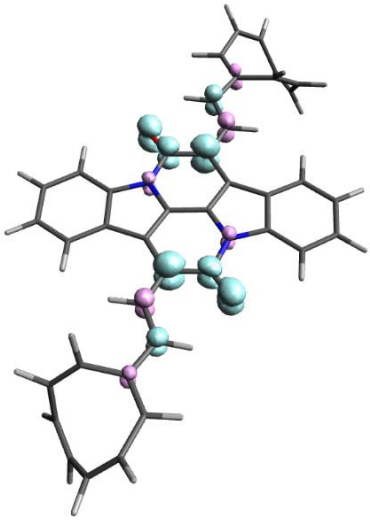
At the first glance, when ignoring the substituents, one can qualitatively see that the delocalization of the unpaired electrons varies within the series so that **SCIBA2** > **SCIBA9** > **SCIBA1** > **SCIBA8** > **SCIBA13** (**Figure S17**) and this would match with the $E(T_1)$ trend. Yet, the substituents also contain some delocalization. The exception is **SCIBA13** which for delocalization is only concentrated in the cyclobutadiene units. By analyzing the quantitative picture leaving aside SCIBA13, the other cases have a fluctuating delocalization in the various substituents as well as in the CCO units (**Table S3**) which makes the analysis difficult as we would have three variables that go in completely different directions in terms of electron delocalization, i.e. the CCO moiety, the substituents, and the C atoms of the two pyrrolo units. Actually, we have almost no delocalization in the latter unit.



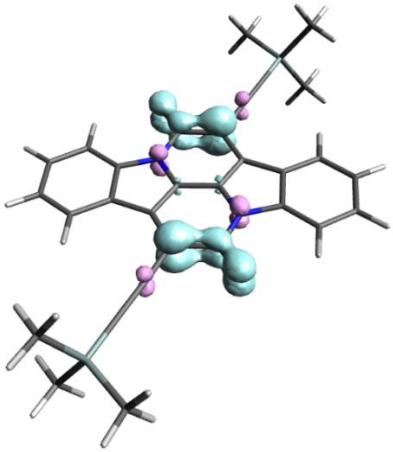
SCIBA1



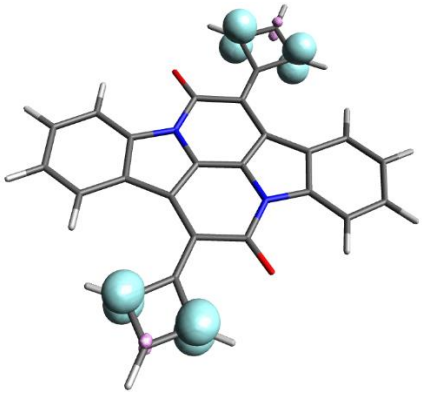
SCIBA2



SCIBA8



SCIBA9



SCIBA13

Figure S17: Plots of the unpaired-electron component of the $EDDB_H$ for **SCIBA1**, **SCIBA2**, **SCIBA8**, **SCIBA9** and **SCIBA13** computed at the UM06-2X/def2-SVP level. Isosurface used: 0.006.

One is a 'hop' spot of **SCIBA11** with the cyano ethynyl substituents, which exhibits nearly zero y_0 (and y_1) but its excited state energy levels are close to other ethynyl substituted **SCIBA**s. The other is the extreme case of **SCIBA13**, which shows an obvious divergence from the trendline of a linear fit. We find that several of our calculated compounds lie favorably on the 2D plots of the y_0 and y_1 (**Fig. S18**), which has previously been suggested as a method to identify potential singlet fission chromophores. (T. Minami and M. Nakano, *J. Phys. Chem. Lett.*, 2012, **3**, 145-150. & M. Nakano, *Chem. Rec.*, 2017, **17**, 27-62.) However, we suggest that consideration of the spin population is tentatively a more intuitive handle with which the excited state energies can be manipulated in the **CIBA** compounds.

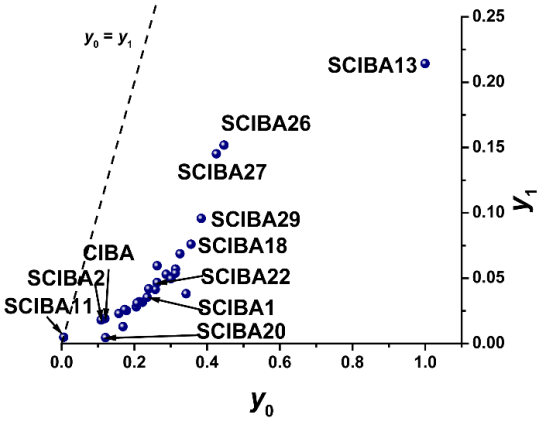


Figure S18 Diradical characters y_0 and y_1 of the parent **CIBA** and **SCIBA**s.

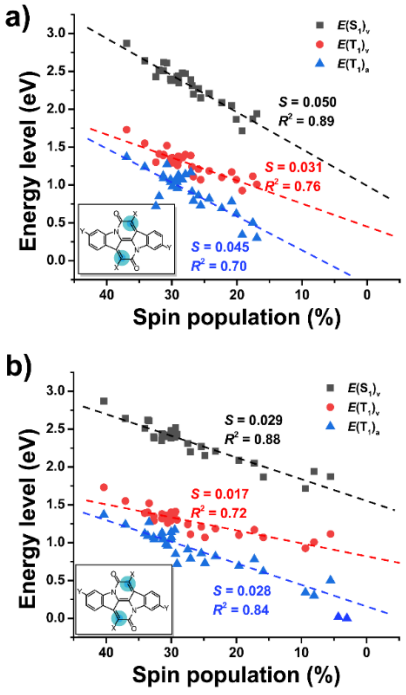


Figure S19: Plots of excited state energies versus the spin population on the C_α atoms a) on the vertical excitation of the S_0 geometries, b) on the adiabatic excitation of T_1 geometries of parent **CIBA** and **SCIBA**s. Subscripted 'v' refer to vertical excitation energies based on S_0 geometries and 'a' refer to adiabatic excitation based on optimized T_1 geometries.

STRUCTURALLY ALTERED CIBALACKROT COMPOUNDS

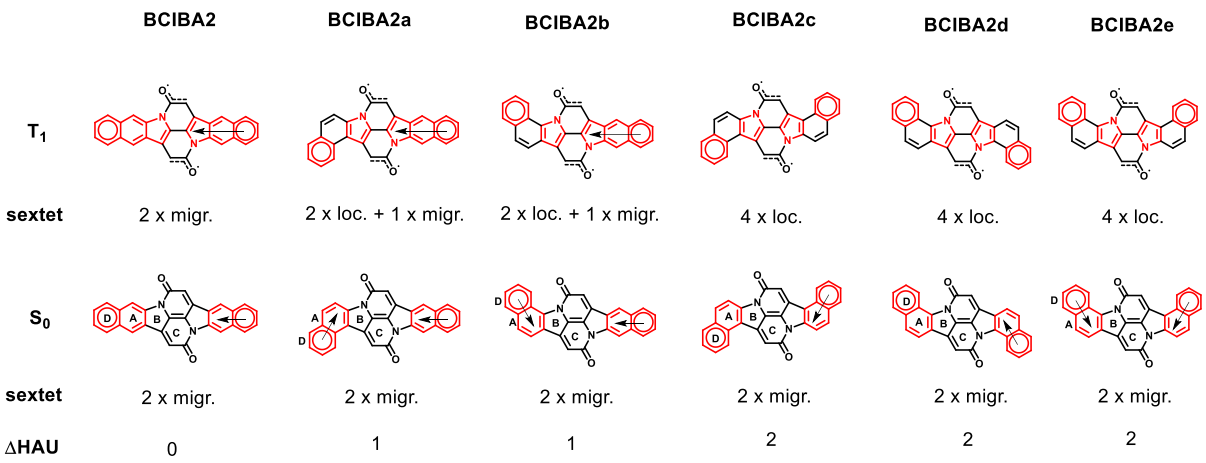


Figure S20: Chemical structure of **BCIBA2 isomers**, the relevant atoms and rings in symmetric positions are signed with apostrophe. Red units represent cycles which are Clar's sextets in the S_0 and T_1 states, respectively.

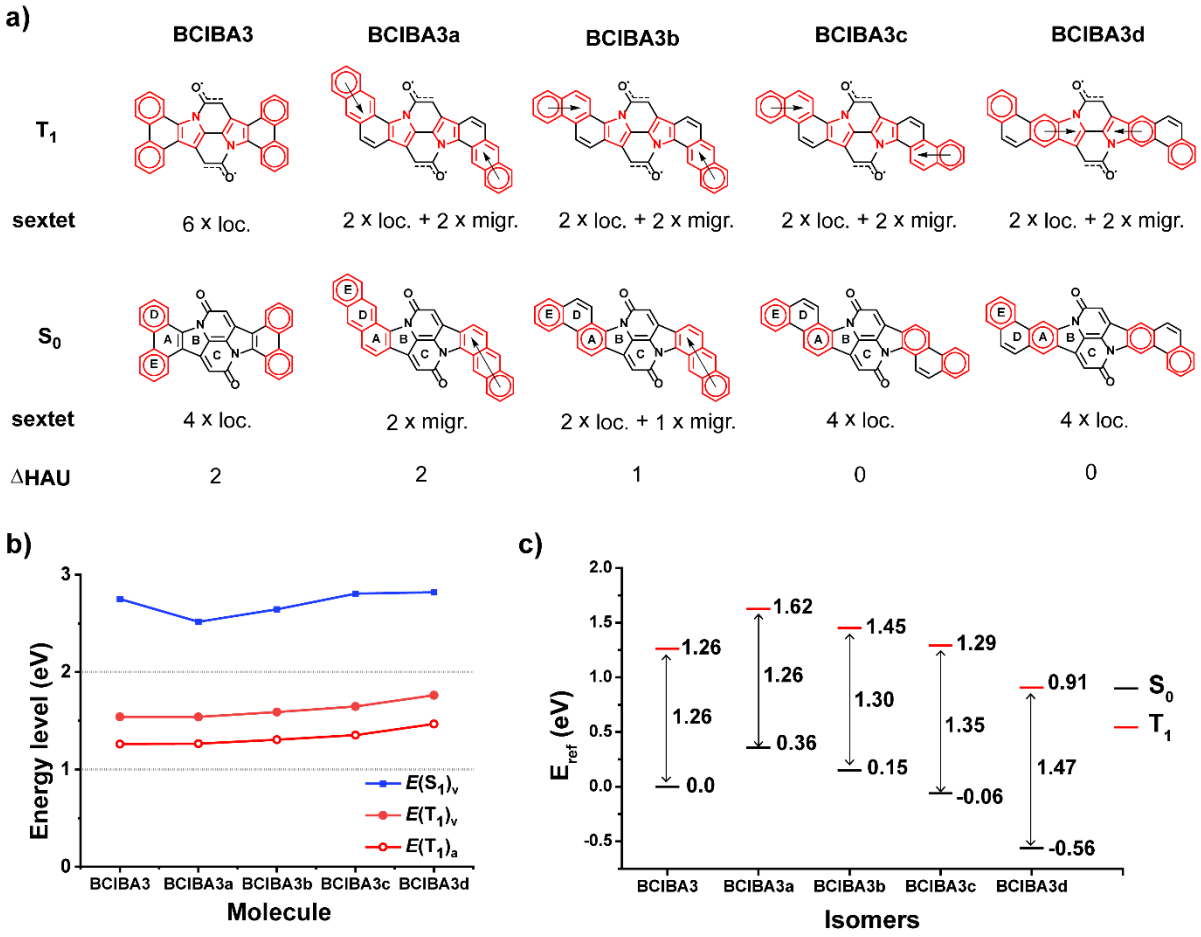


Figure S21: a) Chemical structure of **BCIBA3 isomers**, the relevant atoms and rings in symmetric positions are signed with apostrophe. Red units represent cycles which are Clar's sextets in the S_0 and T_1 states, respectively. b) Plots of excited state energies of the compounds. Subscripted 'v' refers to vertical excitation energies based on S_0 geometries and 'a' refer to adiabatic excitation based on optimized T_1 geometries. c) Relative energies E_{ref} of the **BCIBA3** isomers in the S_0 and T_1 states, with the S_0 state of **BCIBA3** as the reference.

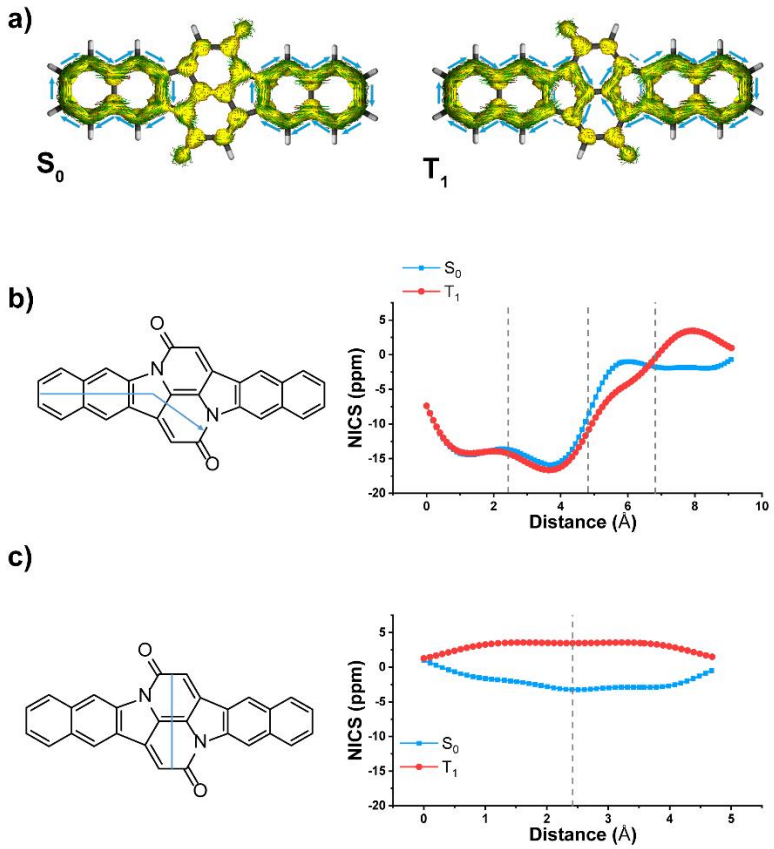


Figure S22: a) π-Electron ring currents according to AICD, b) and c) π-NICS-XY scan in the S_0 and T_1 states of **BCIBA2**, calculated at GIAO/(U)B3LYP/6-311+G(d,p)//(U)B3LYP/6-311+G(d,p) level.

Table S4 Values of key aromatic criteria for relevant rings in **BCIBA2**.

	S_0					T_1				
	A	*B*	*C*	*D*	*AB*	*A*	*B*	*C*	*D*	*AB*
π-NICS(1.7)$_{ZZ}$	-15.8	-1.1	-1.9	-14.4	-	-16.6	-4.8	3.4	-14.2	-
FLU	0.013	0.031	0.030	0.009	0.018	0.012	0.021	0.027	0.011	0.011
$\Delta FLU_{\alpha\beta}$/FLU	-	-	-	-	-	-0.066	-0.316	-1.203	0.175	-0.408
MCI	0.028	0.005	0.010	0.038	-	0.027	0.009	0.005	0.035	-
HOMA	0.611	0.185	0.234	0.774	0.506	0.656	0.415	0.537	0.716	0.663

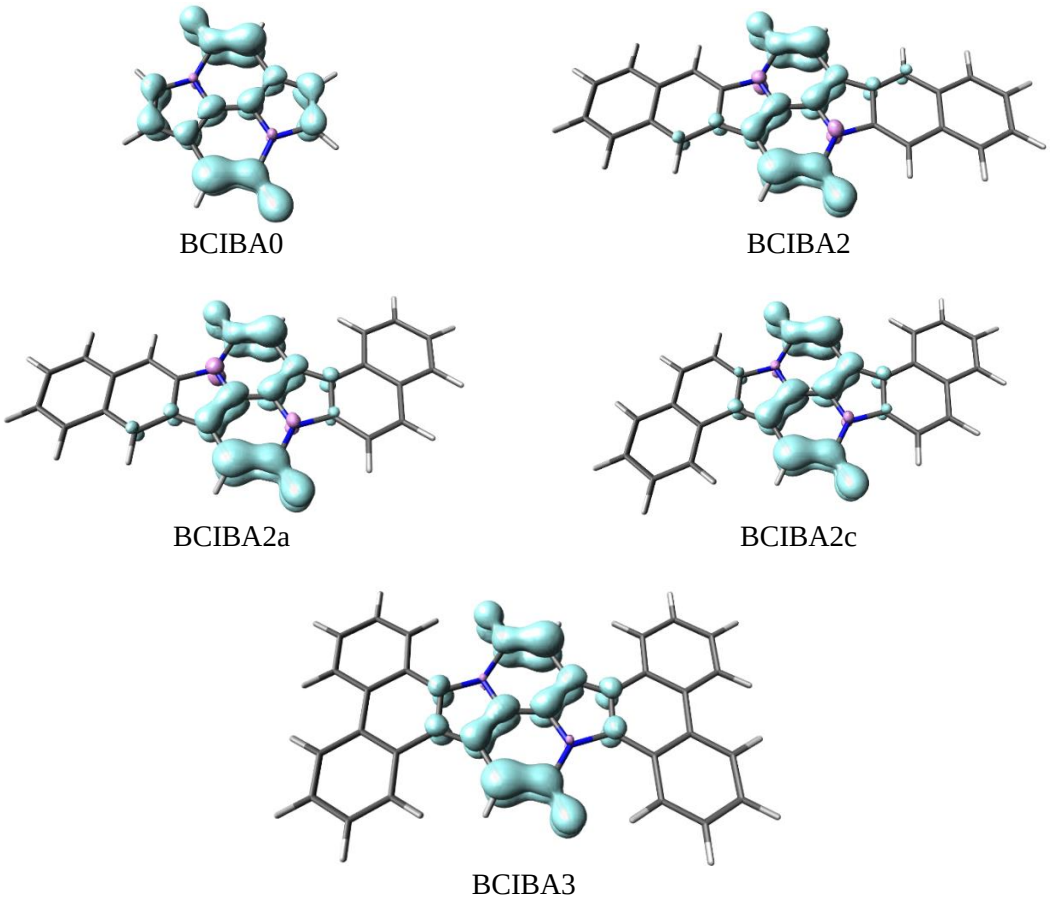


Figure S23: Plots of the unpaired-electron component of the $EDDB_H$ for **BCIBA0**, **BCIBA2**, **BCIBA2a**, **BCIBA2c** and **BCIBA3** computed at the UM06-2X/def2-SVP level. Isosurface used: 0.006.

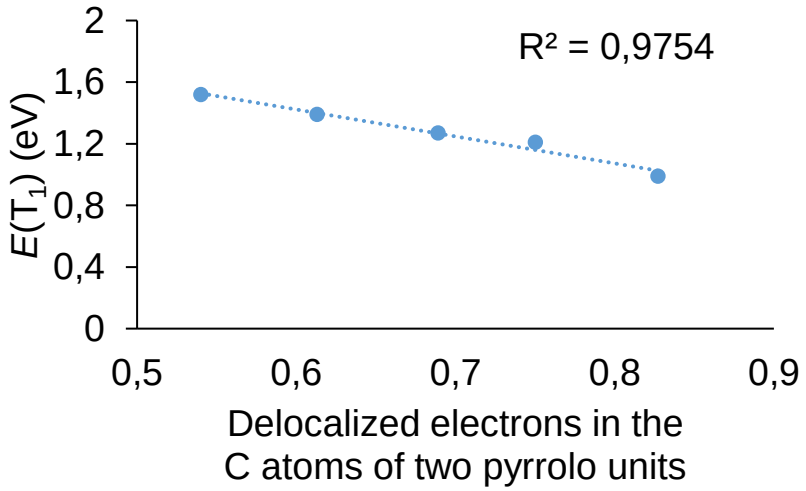


Figure S24: Plot of the $E(T_1)$ against the populations of delocalized unpaired electrons (from the $EDDB_H$ analysis) within the C atoms of two pyrrolo units for **BCIBA0**, **BCIBA2**, **BCIBA2a**, **BCIBA2c**, and **BCIBA3**.

Table S5 The calculated key parameters of excited states of **BCIBAs**.

Emitter	Excited state	D [a)] [Å]	S_r index [b)]	t index [c)] [Å]	Electron Configurations
BCIBA0	S_1	0.000	0.785	-1.943	H→L: 99.9%
	T_1	0.000	0.762	-1.943	H→L: 96.9%
BCIBA2	S_1	0.000	0.734	-0.750	H→L: 97.8%
	T_1	0.000	0.696	-0.823	H→L: 81.0%; H-1→L: 11.7%
BCIBA2a	S_1	0.546	0.742	-1.565	H→L: 96.7%
	T_1	0.267	0.692	-1.870	H→L: 87.1%; H-2→L: 4.5%
BCIBA2b	S_1	0.637	0.754	-1.406	H→L: 95.5%
	T_1	0.610	0.714	-1.630	H→L: 84.4%; H-2→L: 7.4%
BCIBA2c	S_1	0.000	0.756	-2.099	H→L: 97.0%
	T_1	0.000	0.750	-2.018	H→L: 91.3%; H→L+2: 2.8%
BCIBA2d	S_1	0.000	0.782	-0.755	H→L: 96.1%
	T_1	0.000	0.730	-1.142	H→L: 87.9%; H-2→L: 6.7%
BCIBA2e	S_1	0.775	0.760	-1.716	H→L: 96.5%
	T_1	0.179	0.721	-2.246	H→L: 88.0%; H-1→L: 2.4%
BCIBA3	S_1	0.001	0.765	-2.273	H→L: 94.9%; H-4→L: 3.6%
	T_1	0.001	0.749	-2.015	H→L: 88.0%; H-4→L: 4.9%
BCIBA3a	S_1	0.000	0.635	-2.876	H→L: 92.7%; H-5→L: 2.4%
	T_1	0.004	0.762	-2.166	H-1→L: 62.6%; H-2→L: 30.2%
BCIBA3b	S_1	3.114	0.661	-0.159	H→L: 91.1%; H-3→L: 2.4%
	T_1	0.171	0.729	-1.874	H→L: 45.2%; H-1→L: 35.8%
BCIBA3c	S_1	0.000	0.768	-1.704	H→L: 95.5%; H-4→L: 2.1%
	T_1	0.000	0.762	-1.740	H→L: 81.3%; H-2→L: 11.1%
BCIBA3d	S_1	0.000	0.738	-2.216	H→L: 95.4%; H-4→L: 2.3%
	T_1	0.000	0.746	-2.122	H→L: 79.9%; H-2→L: 12.5%

[a)] Distance between centroid of hole and electron. [b)] Overlap index of hole-electron distribution. [c)] Separate index of hole-electron distribution.

FURTHER MODIFICATIONS OF THE CIBA SCAFFOLD

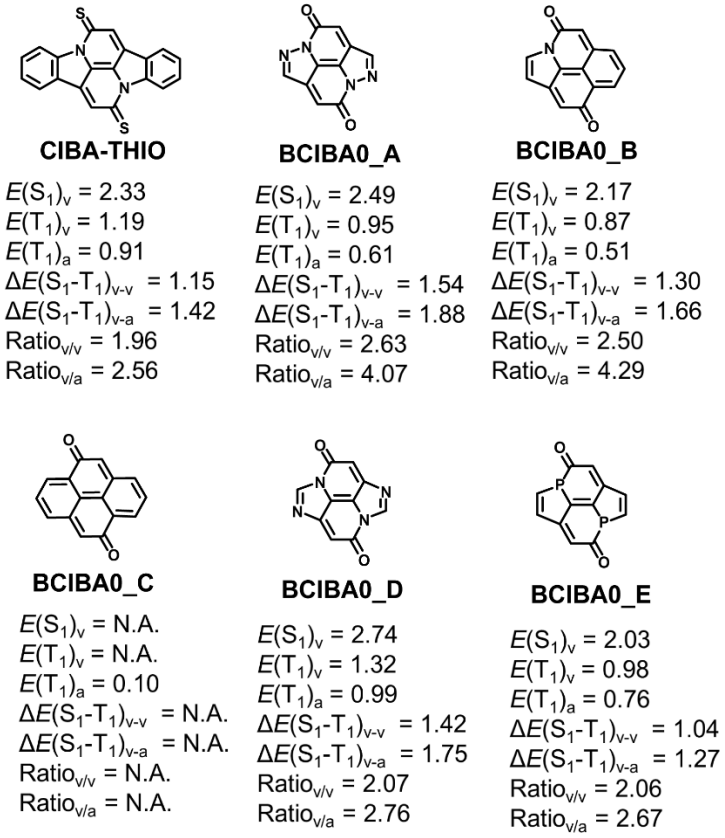


Figure S24: Chemical structures and relevant excitation energies (in eV) of **CIBA-THIO** and modified **BCIBA0**s. Calculations at TD-M06-2x/def2-SVP//M06-2X/def2-SVP level.

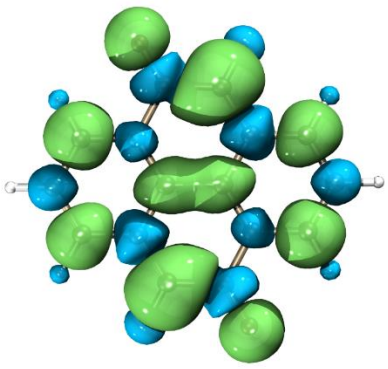


Figure S25: Spin density distribution in T1 state (ρ = 0.0008) of **BCIBA0_D** calculated at UM06-2X/def2-SVP level. The charge and spin population on carbonyl O atoms are -2.100 e and 0.510 (26%), -0.080 e and 0.876 (44%) on C_α atoms, and 0.222 e and 0.611 (31%) on B rings, respectively (QTAIM at UB3LYP/6-311+G** level).

COORDINATES AND TOTAL ELECTRONIC ENERGIES (E)

CIBA S0

E = -1026.98946483 a.u.

C	-1.015003	-2.322456	-0.000002
C	0.474039	-2.433365	0.000000
C	1.300911	-1.339853	0.000000
C	0.662812	-0.070450	-0.000001
C	-0.662820	0.070905	0.000000
C	1.015635	2.322041	-0.000008
C	-0.474096	2.433500	0.000001
C	-1.301373	1.340533	0.000000
N	-1.507486	-0.995912	-0.000001
N	1.507852	0.996476	-0.000003
C	-2.732381	0.972637	0.000000
C	-2.815368	-0.451405	0.000000
C	-3.903794	1.724142	0.000001
C	-4.030296	-1.121614	0.000000
C	-5.130856	1.059378	0.000001
H	-3.859209	2.814088	0.000001
C	-5.187756	-0.337851	0.000000
H	-4.053061	-2.209931	-0.000001
H	-6.056049	1.636237	0.000001
H	-6.159851	-0.833139	0.000000
C	2.732076	-0.972555	0.000000
C	2.815580	0.451451	-0.000001
C	3.903254	-1.724418	0.000002
C	4.030695	1.121320	-0.000001
C	5.130506	-1.060023	0.000001
H	3.858301	-2.814354	0.000003
C	5.187886	0.337207	0.000001
H	4.053771	2.209640	-0.000003
H	6.055544	-1.637129	0.000002
H	6.160168	0.832128	0.000000
H	-0.835368	3.461700	0.000006
O	1.768867	3.270593	0.000005
H	0.836668	-3.461072	0.000001
O	-1.769042	-3.270200	0.000001

CIBA T1

E = -1026.93901336 a.u.

C	-1.015003	-2.322456	-0.000002
C	0.474039	-2.433365	0.000000
C	1.300911	-1.339853	0.000000
C	0.662812	-0.070450	-0.000001
C	-0.662820	0.070905	0.000000
C	1.015635	2.322041	-0.000008
C	-0.474096	2.433500	0.000001
C	-1.301373	1.340533	0.000000
N	-1.507486	-0.995912	-0.000001
N	1.507852	0.996476	-0.000003
C	-2.732381	0.972637	0.000000
C	-2.815368	-0.451405	0.000000
C	-3.903794	1.724142	0.000001
C	-4.030296	-1.121614	0.000000
C	-5.130856	1.059378	0.000001
H	-3.859209	2.814088	0.000001
C	-5.187756	-0.337851	0.000000
H	-4.053061	-2.209931	-0.000001
H	-6.056049	1.636237	0.000001
H	-6.159851	-0.833139	0.000000
C	2.732076	-0.972555	0.000000
C	2.815580	0.451451	-0.000001
C	3.903254	-1.724418	0.000002
C	4.030695	1.121320	-0.000001
C	5.130506	-1.060023	0.000001
H	3.858301	-2.814354	0.000003
C	5.187886	0.337207	0.000001
H	4.053771	2.209640	-0.000003
H	6.055544	-1.637129	0.000002
H	6.160168	0.832128	0.000000
H	-0.835368	3.461700	0.000006
O	1.768867	3.270593	0.000005
H	0.836668	-3.461072	0.000001
O	-1.769042	-3.270200	0.000001

NARID S0

E = -567.797053713 a.u.

C	2.580950	0.132619	0.000002
C	2.171273	-1.276914	-0.000001
C	0.869092	-1.651964	0.000000
C	-0.174401	-0.667944	0.000002
C	0.174135	0.667797	0.000002
C	-2.580381	-0.133163	0.000011
C	-2.171014	1.276865	-0.000001
C	-0.869222	1.652387	0.000001
N	1.505271	1.014661	0.000001
N	-1.505690	-1.015077	0.000003
H	-2.982954	2.003147	-0.000009
O	-3.725124	-0.532242	-0.000009
H	2.982101	-2.004422	-0.000004
O	3.725182	0.533048	-0.000004
H	-0.597572	2.710771	-0.000001
H	-1.763548	-1.997404	-0.000001
H	0.598119	-2.710566	0.000000
H	1.763738	1.996837	0.000000

NARID T1

E = -567.726852622 a.u.

C	2.580950	0.132619	0.000002
C	2.171273	-1.276914	-0.000001
C	0.869092	-1.651964	0.000000
C	-0.174401	-0.667944	0.000002
C	0.174135	0.667797	0.000002
C	-2.580381	-0.133163	0.000011
C	-2.171014	1.276865	-0.000001
C	-0.869222	1.652387	0.000001
N	1.505271	1.014661	0.000001
N	-1.505690	-1.015077	0.000003
H	-2.982954	2.003147	-0.000009
O	-3.725124	-0.532242	-0.000009
H	2.982101	-2.004422	-0.000004
O	3.725182	0.533048	-0.000004
H	-0.597572	2.710771	-0.000001
H	-1.763548	-1.997404	-0.000001
H	0.598119	-2.710566	0.000000
H	1.763738	1.996837	0.000000

indole S0

E = -363.400888036 a.u.

C	-1.626162	1.166365	0.000001
C	-2.383751	0.026306	-0.000001
N	-1.562567	-1.077197	0.000000
C	-0.249898	0.749868	0.000000
C	-0.251247	-0.668820	0.000000
C	0.983230	1.427463	0.000000
C	0.933944	-1.416868	0.000000
C	2.156426	0.691419	0.000000
H	1.011230	2.518432	0.000000
C	2.131053	-0.719360	0.000000
H	0.916001	-2.507760	0.000000
H	3.117780	1.206825	0.000000
H	3.071595	-1.272300	0.000000
H	-1.873556	-2.037535	0.000000
H	-3.464433	-0.090714	-0.000002
H	-2.002224	2.185189	0.000002

indole T1

E = -363.273724107 a.u.

C	-1.626162	1.166365	0.000001
C	-2.383751	0.026306	-0.000001
N	-1.562567	-1.077197	0.000000
C	-0.249898	0.749868	0.000000
C	-0.251247	-0.668820	0.000000
C	0.983230	1.427463	0.000000
C	0.933944	-1.416868	0.000000
C	2.156426	0.691419	0.000000
H	1.011230	2.518432	0.000000
C	2.131053	-0.719360	0.000000
H	0.916001	-2.507760	0.000000
H	3.117780	1.206825	0.000000
H	3.071595	-1.272300	0.000000
H	-1.873556	-2.037535	0.000000
H	-3.464433	-0.090714	-0.000002
H	-2.002224	2.185189	0.000002

pyrrole S0

E = -209.923901747 a.u.

C	0.333255	-1.119908	-0.000034
C	-0.982448	-0.711784	-0.000127
C	-0.982438	0.711797	0.000078
C	0.333270	1.119905	0.000004
N	1.117960	-0.000008	0.000060
H	2.127792	-0.000019	0.000187
H	0.768963	-2.114856	-0.000074
H	-1.850667	-1.364986	-0.000231
H	-1.850646	1.365015	0.000136
H	0.769003	2.114841	0.000034

pyrrole T1

E = -209.771969335 a.u.

C	0.333255	-1.119908	-0.000034
C	-0.982448	-0.711784	-0.000127
C	-0.982438	0.711797	0.000078
C	0.333270	1.119905	0.000004
N	1.117960	-0.000008	0.000060
H	2.127792	-0.000019	0.000187
H	0.768963	-2.114856	-0.000074
H	-1.850667	-1.364986	-0.000231
H	-1.850646	1.365015	0.000136
H	0.769003	2.114841	0.000034

ph S0

E = -231.969001951 a.u.

C	-1.350026	-0.351153	-0.000002
C	-0.370712	-1.344348	0.000110
C	0.978965	-0.993310	-0.000081
C	1.349992	0.351262	0.000017
C	0.370824	1.344314	0.000076
C	-0.979044	0.993237	-0.000079
H	-2.405735	-0.625530	-0.000070
H	-0.660733	-2.395857	0.000043
H	1.744297	-1.770596	-0.000176
H	2.405762	0.625379	-0.000014
H	0.660605	2.395880	0.000038
H	-1.744196	1.770711	-0.000064

ph T1

E = -231.819521620 a.u.

C	-1.350026	-0.351153	-0.000002
C	-0.370712	-1.344348	0.000110

C	0.978965	-0.993310	-0.000081
C	1.349992	0.351262	0.000017
C	0.370824	1.344314	0.000076
C	-0.979044	0.993237	-0.000079
H	-2.405735	-0.625530	-0.000070
H	-0.660733	-2.395857	0.000043
H	1.744297	-1.770596	-0.000176
H	2.405762	0.625379	-0.000014
H	0.660605	2.395880	0.000038
H	-1.744196	1.770711	-0.000064

BENZPENT5 S0

E = -614.997742512 a.u.

C	1.747401	-0.532425	0.000123
C	2.002803	0.867324	0.000101
C	3.306027	1.342330	0.000053
H	3.509652	2.414537	0.000109
C	4.361126	0.417259	-0.000144
H	5.391379	0.776141	-0.000305
C	4.109396	-0.952195	-0.000049
H	4.944360	-1.654100	-0.000142
C	2.793298	-1.440291	0.000173
H	2.601815	-2.514495	0.000133
C	0.285581	-0.679124	-0.000071
C	-0.710654	-1.594312	-0.000103
C	-1.747401	0.532425	-0.000131
C	-2.002802	-0.867324	-0.000097
C	-3.306027	-1.342330	-0.000041
H	-3.509652	-2.414537	-0.000089
C	-4.361125	-0.417259	0.000154
H	-5.391379	-0.776140	0.000322
C	-4.109396	0.952195	0.000048
H	-4.944360	1.654100	0.000140
C	-2.793298	1.440291	-0.000184
H	-2.601814	2.514495	-0.000152
C	-0.285581	0.679123	0.000060
C	0.710654	1.594312	0.000103
H	-0.618968	-2.680390	-0.000006
H	0.618968	2.680390	0.000011

BENZPENT5 T1

E = -614.935427299 a.u.

C	1.747401	-0.532425	0.000123
C	2.002803	0.867324	0.000101
C	3.306027	1.342330	0.000053
H	3.509652	2.414537	0.000109
C	4.361126	0.417259	-0.000144
H	5.391379	0.776141	-0.000305
C	4.109396	-0.952195	-0.000049
H	4.944360	-1.654100	-0.000142
C	2.793298	-1.440291	0.000173
H	2.601815	-2.514495	0.000133
C	0.285581	-0.679124	-0.000071
C	-0.710654	-1.594312	-0.000103
C	-1.747401	0.532425	-0.000131
C	-2.002802	-0.867324	-0.000097
C	-3.306027	-1.342330	-0.000041
H	-3.509652	-2.414537	-0.000089
C	-4.361125	-0.417259	0.000154
H	-5.391379	-0.776140	0.000322
C	-4.109396	0.952195	0.000048
H	-4.944360	1.654100	0.000140
C	-2.793298	1.440291	-0.000184
H	-2.601814	2.514495	-0.000152
C	-0.285581	0.679123	0.000060
C	0.710654	1.594312	0.000103
H	-0.618968	-2.680390	-0.000006
H	0.618968	2.680390	0.000011

bis(styryl)BENZPENT5 S0

E = -1231.21291644 a.u.

C	0.713078	1.674606	-0.166199
C	-0.636698	2.088097	0.003161
C	-0.979863	3.431246	-0.038081
H	-2.017999	3.748855	0.075704
C	0.030161	4.380996	-0.246968
H	-0.223017	5.441715	-0.277754
C	1.350298	3.979547	-0.430129
H	2.123056	4.728853	-0.607874
C	1.703769	2.622482	-0.392862
H	2.740563	2.327619	-0.554958
C	0.696310	0.207498	-0.087782
C	1.509038	-0.892147	-0.146682
C	2.953447	-0.982087	-0.279800
H	3.341135	-1.875532	-0.779778
C	3.809034	-0.071419	0.223033
H	3.386646	0.751963	0.807650
C	5.272699	-0.087563	0.116884
C	6.016547	0.809409	0.899093
H	5.488676	1.495921	1.564787
C	7.407767	0.828497	0.841793
H	7.967724	1.531323	1.460451
C	8.082270	-0.048328	-0.005372
H	9.171969	-0.035416	-0.054669
C	7.355046	-0.940323	-0.797249
H	7.877354	-1.622160	-1.470131
C	5.966361	-0.958687	-0.740104
H	5.411629	-1.647539	-1.379141
C	-0.713051	-1.674795	0.166563
C	0.636724	-2.088273	-0.002869
C	0.979925	-3.431411	0.038417
H	2.018060	-3.749001	-0.075432
C	-0.030058	-4.381174	0.247435
H	0.223149	-5.441886	0.278262
C	-1.350186	-3.979744	0.430696
H	-2.122908	-4.729059	0.608562
C	-1.703693	-2.622690	0.393383

H	-2.740478	-2.327855	0.555581
C	-0.696316	-0.207683	0.088041
C	-1.509045	0.891976	0.146847
C	-2.953464	0.981972	0.279857
H	-3.341140	1.875380	0.779910
C	-3.809075	0.071456	-0.223210
H	-3.386704	-0.751831	-0.807970
C	-5.272748	0.087700	-0.117200
C	-6.016595	-0.809052	-0.899663
H	-5.488716	-1.495471	-1.565445
C	-7.407822	-0.828036	-0.842503
H	-7.967776	-1.530690	-1.461358
C	-8.082335	0.048674	0.004775
H	-9.172040	0.035844	0.053962
C	-7.355113	0.940447	0.796904
H	-7.877431	1.622192	1.469872
C	-5.966422	0.958709	0.739898
H	-5.411696	1.647385	1.379127

bis(styryl)BENZPENT5 T1

E = -1231.17017170 a.u.

C	0.713078	1.674606	-0.166199
C	-0.636698	2.088097	0.003161
C	-0.979863	3.431246	-0.038081
H	-2.017999	3.748855	0.075704
C	0.030161	4.380996	-0.246968
H	-0.223017	5.441715	-0.277754
C	1.350298	3.979547	-0.430129
H	2.123056	4.728853	-0.607874
C	1.703769	2.622482	-0.392862
H	2.740563	2.327619	-0.554958
C	0.696310	0.207498	-0.087782
C	1.509038	-0.892147	-0.146682
C	2.953447	-0.982087	-0.279800
H	3.341135	-1.875532	-0.779778
C	3.809034	-0.071419	0.223033
H	3.386646	0.751963	0.807650
C	5.272699	-0.087563	0.116884
C	6.016547	0.809409	0.899093
H	5.488676	1.495921	1.564787
C	7.407767	0.828497	0.841793
H	7.967724	1.531323	1.460451
C	8.082270	-0.048328	-0.005372
H	9.171969	-0.035416	-0.054669
C	7.355046	-0.940323	-0.797249
H	7.877354	-1.622160	-1.470131
C	5.966361	-0.958687	-0.740104
H	5.411629	-1.647539	-1.379141
C	-0.713051	-1.674795	0.166563
C	0.636724	-2.088273	-0.002869
C	0.979925	-3.431411	0.038417
H	2.018060	-3.749001	-0.075432
C	-0.030058	-4.381174	0.247435
H	0.223149	-5.441886	0.278262
C	-1.350186	-3.979744	0.430696
H	-2.122908	-4.729059	0.608562
C	-1.703693	-2.622690	0.393383
H	-2.740478	-2.327855	0.555581
C	-0.696316	-0.207683	0.088041
C	-1.509045	0.891976	0.146847
C	-2.953464	0.981972	0.279857
H	-3.341140	1.875380	0.779910
C	-3.809075	0.071456	-0.223210
H	-3.386704	-0.751831	-0.807970
C	-5.272748	0.087700	-0.117200
C	-6.016595	-0.809052	-0.899663
H	-5.488716	-1.495471	-1.565445
C	-7.407822	-0.828036	-0.842503
H	-7.967776	-1.530690	-1.461358
C	-8.082335	0.048674	0.004775
H	-9.172040	0.035844	0.053962
C	-7.355113	0.940447	0.796904
H	-7.877431	1.622192	1.469872
C	-5.966422	0.958709	0.739898
H	-5.411696	1.647385	1.379127

SCIBA1 S0

E = -2208.54762657 a.u.

C	1.889970	1.664289	0.082238
C	2.489779	0.283135	0.155596
C	1.673217	-0.840989	0.157776
C	0.278160	-0.609239	0.240244
C	-0.278157	0.609240	0.240249
C	-1.889969	-1.664289	0.082270
C	-2.489777	-0.283135	0.155628
C	-1.673214	0.840989	0.157799
N	0.491618	1.729831	0.161923
N	-0.491615	-1.729831	0.161931
C	-1.744437	2.314086	0.004411
C	-0.407117	2.811686	0.009194
C	-2.786954	3.218841	-0.206547
C	-0.101663	4.155492	-0.156176
C	-2.490271	4.570933	-0.381877
H	-3.818756	2.873036	-0.248027
C	-1.171461	5.031658	-0.347162
H	0.936392	4.482248	-0.147098
H	-3.302900	5.278681	-0.548296
C	1.744437	-2.314085	0.004386
C	0.407118	-2.811685	0.009186
C	2.786952	-3.218839	-0.206587
C	0.101662	-4.155492	-0.156180
C	2.490266	-4.570931	-0.381914
H	3.818753	-2.873035	-0.248081
C	1.171457	-5.031657	-0.347183
H	-0.936394	-4.482247	-0.147087
H	3.302894	-5.278680	-0.548345
O	-2.551605	-2.672563	-0.055716
O	2.551606	2.672564	-0.055734

C	3.941830	0.207299	0.239473
C	4.664223	-0.759605	0.908796
S	5.017702	1.351314	-0.507266
C	6.067675	-0.597366	0.785867
H	4.182998	-1.539433	1.498661
C	6.413403	0.494104	0.026578
H	6.804199	-1.252441	1.250848
C	-3.941827	-0.207298	0.239522
C	-4.664211	0.759609	0.908849
S	-5.017710	-1.351313	-0.507203
C	-6.067665	0.597368	0.785944
H	-4.182978	1.539440	1.498705
C	-6.413403	-0.494108	0.026667
H	-6.804183	1.252443	1.250936
C	7.788730	0.984109	-0.306273
H	7.951002	1.023025	-1.393265
H	7.962343	1.993882	0.093579
H	8.537507	0.309592	0.128218
C	-7.788735	-0.984120	-0.306156
H	-7.951025	-1.023047	-1.393145
H	-7.962339	-1.993888	0.093709
H	-8.537507	-0.309600	0.128341
H	-0.969613	6.095399	-0.480607
H	0.969608	-6.095398	-0.480626

SCIBA1 T1

E = -2208.51149572 a.u.

C	1.889970	1.664289	0.082238
C	2.489779	0.283135	0.155596
C	1.673217	-0.840989	0.157776
C	0.278160	-0.609239	0.240244
C	-0.278157	0.609240	0.240249
C	-1.889969	-1.664289	0.082270
C	-2.489777	-0.283135	0.155628
C	-1.673214	0.840989	0.157799
N	0.491618	1.729831	0.161923
N	-0.491615	-1.729831	0.161931
C	-1.744437	2.314086	0.004411
C	-0.407117	2.811686	0.009194
C	-2.786954	3.218841	-0.206547
C	-0.101663	4.155492	-0.156176
C	-2.490271	4.570933	-0.381877
H	-3.818756	2.873036	-0.248027
C	-1.171461	5.031658	-0.347162
H	0.936392	4.482248	-0.147098
H	-3.302900	5.278681	-0.548296
C	1.744437	-2.314085	0.004386
C	0.407118	-2.811685	0.009186
C	2.786952	-3.218839	-0.206587
C	0.101662	-4.155492	-0.156180
C	2.490266	-4.570931	-0.381914
H	3.818753	-2.873035	-0.248081
C	1.171457	-5.031657	-0.347183
H	-0.936394	-4.482247	-0.147087
H	3.302894	-5.278680	-0.548345
O	-2.551605	-2.672563	-0.055716
O	2.551606	2.672564	-0.055734
C	3.941830	0.207299	0.239473
C	4.664223	-0.759605	0.908796
S	5.017702	1.351314	-0.507266
C	6.067675	-0.597366	0.785867
H	4.182998	-1.539433	1.498661
C	6.413403	0.494104	0.026578
H	6.804199	-1.252441	1.250848
C	-3.941827	-0.207298	0.239522
C	-4.664211	0.759609	0.908849
S	-5.017710	-1.351313	-0.507203
C	-6.067665	0.597368	0.785944
H	-4.182978	1.539440	1.498705
C	-6.413403	-0.494108	0.026667
H	-6.804183	1.252443	1.250936
C	7.788730	0.984109	-0.306273
H	7.951002	1.023025	-1.393265
H	7.962343	1.993882	0.093579
H	8.537507	0.309592	0.128218
C	-7.788735	-0.984120	-0.306156
H	-7.951025	-1.023047	-1.393145
H	-7.962339	-1.993888	0.093709
H	-8.537507	-0.309600	0.128341
H	-0.969613	6.095399	-0.480607
H	0.969608	-6.095398	-0.480626

SCIBA2 S0

E = -1488.58204493 a.u.

C	-1.589836	1.964771	0.012392
C	-2.405152	0.694910	-0.027865
C	-1.789071	-0.542822	-0.041780
C	-0.372371	-0.554026	-0.091835
C	0.372375	0.554046	-0.091837
C	1.589839	-1.964749	0.012429
C	2.405154	-0.694892	-0.027876
C	1.789076	0.542842	-0.041784
N	-0.194552	1.789679	-0.040467
N	0.194556	-1.789660	-0.040451
C	2.113605	1.986791	0.053820
C	0.881178	2.706066	0.053090
C	3.305691	2.698841	0.187213
C	0.821441	4.088506	0.159863
C	3.255256	4.088981	0.300608
H	4.261480	2.175335	0.209227
C	2.034796	4.769629	0.280575
H	-0.142110	4.594519	0.155495
H	4.183799	4.650762	0.406101
H	2.025301	5.857163	0.366383
C	-2.113602	-1.986770	0.053816
C	-0.881176	-2.706046	0.053097
C	-3.305690	-2.698817	0.187196
C	-0.821442	-4.088486	0.159872

C	-3.255259	-4.088957	0.300590
H	-4.261478	-2.175309	0.209202
C	-2.034799	-4.769607	0.280571
H	0.142108	-4.594501	0.155513
H	-4.183804	-4.650736	0.406074
H	-2.025307	-5.857141	0.366379
O	2.067899	-3.076972	0.090949
O	-2.067888	3.076993	0.090969
C	-3.873914	0.851774	-0.086060
C	-4.559544	1.750394	0.744843
C	-4.607009	0.086723	-1.005637
C	-5.946229	1.851830	0.674707
H	-3.997182	2.369670	1.442067
C	-5.993156	0.195171	-1.078148
H	-4.074593	-0.588201	-1.679658
C	-6.667230	1.075820	-0.233029
H	-6.468715	2.548053	1.332316
H	-6.547189	-0.401307	-1.804611
H	-7.753295	1.164694	-0.288081
C	3.873915	-0.851772	-0.086066
C	4.559514	-1.750455	0.744793
C	4.607032	-0.086710	-1.005615
C	5.946196	-1.851926	0.674662
H	3.997127	-2.369754	1.441979
C	5.993177	-0.195190	-1.078122
H	4.074637	0.588258	-1.679608
C	6.667223	-1.075892	-0.233034
H	6.468660	-2.548196	1.332238
H	6.547230	0.401303	-1.804556
H	7.753286	-1.164790	-0.288082

SCIBA2 T1

E = -1488.53653655 a.u.

C	-1.589836	1.964771	0.012392
C	-2.405152	0.694910	-0.027865
C	-1.789071	-0.542822	-0.041780
C	-0.372371	-0.554026	-0.091835
C	0.372375	0.554046	-0.091837
C	1.589839	-1.964749	0.012429
C	2.405154	-0.694892	-0.027876
C	1.789076	0.542842	-0.041784
N	-0.194552	1.789679	-0.040467
N	0.194556	-1.789660	-0.040451
C	2.113605	1.986791	0.053820
C	0.881178	2.706066	0.053090
C	3.305691	2.698841	0.187213
C	0.821441	4.088506	0.159863
C	3.255256	4.088981	0.300608
H	4.261480	2.175335	0.209227
C	2.034796	4.769629	0.280575
H	-0.142110	4.594519	0.155495
H	4.183799	4.650762	0.406101
H	2.025301	5.857163	0.366383
C	-2.113602	-1.986770	0.053816
C	-0.881176	-2.706046	0.053097
C	-3.305690	-2.698817	0.187196
C	-0.821442	-4.088486	0.159872
C	-3.255259	-4.088957	0.300590
H	-4.261478	-2.175309	0.209202
C	-2.034799	-4.769607	0.280571
H	0.142108	-4.594501	0.155513
H	-4.183804	-4.650736	0.406074
H	-2.025307	-5.857141	0.366379
O	2.067899	-3.076972	0.090949
O	-2.067888	3.076993	0.090969
C	-3.873914	0.851774	-0.086060
C	-4.559544	1.750394	0.744843
C	-4.607009	0.086723	-1.005637
C	-5.946229	1.851830	0.674707
H	-3.997182	2.369670	1.442067
C	-5.993156	0.195171	-1.078148
H	-4.074593	-0.588201	-1.679658
C	-6.667230	1.075820	-0.233029
H	-6.468715	2.548053	1.332316
H	-6.547189	-0.401307	-1.804611
H	-7.753295	1.164694	-0.288081
C	3.873915	-0.851772	-0.086066
C	4.559514	-1.750455	0.744793
C	4.607032	-0.086710	-1.005615
C	5.946196	-1.851926	0.674662
H	3.997127	-2.369754	1.441979
C	5.993177	-0.195190	-1.078122
H	4.074637	0.588258	-1.679608
C	6.667223	-1.075892	-0.233034
H	6.468660	-2.548196	1.332238
H	6.547230	0.401303	-1.804556
H	7.753286	-1.164790	-0.288082

SCIBA3 S0

E = -1211.27478384 a.u.

C	0.509574	-2.489351	-0.000062
C	-0.983376	-2.272881	-0.000019
C	-1.560988	-1.018927	-0.000021
C	-0.663446	0.077080	-0.000044
C	0.663452	-0.077079	-0.000043
C	-0.509583	2.489342	-0.000105
C	0.983387	2.272876	-0.000023
C	1.561003	1.018932	-0.000026
N	1.263535	-1.296516	-0.000041
N	-1.263537	1.296522	-0.000058
C	2.877513	0.369632	-0.000001
C	2.660158	-1.040686	-0.000015
C	4.178185	0.870650	0.000030
C	3.707032	-1.948515	0.000000
C	5.236632	-0.037755	0.000046
H	4.353793	1.947619	0.000040
C	5.000757	-1.416980	0.000031
H	3.509381	-3.019137	-0.000012

H	6.262200	0.331527	0.000070
H	5.849942	-2.101754	0.000044
C	-2.877502	-0.369639	0.000002
C	-2.660157	1.040679	-0.000018
C	-4.178175	-0.870660	0.000038
C	-3.707033	1.948507	-0.000007
C	-5.236623	0.037742	0.000053
H	-4.353785	-1.947628	0.000054
C	-5.000756	1.416970	0.000030
H	-3.509380	3.019129	-0.000028
H	-6.262189	-0.331545	0.000080
H	-5.849945	2.101738	0.000040
O	-1.033892	3.574157	0.000037
O	1.033907	-3.574155	0.000007
C	-1.796916	-3.449982	0.000016
N	-2.509085	-4.359934	0.000044
C	1.796896	3.449998	0.000024
N	2.509036	4.359972	0.000059

SCIBA3 T1

E = -1211.22820776 a.u.

C	0.509574	-2.489351	-0.000062
C	-0.983376	-2.272881	-0.000019
C	-1.560988	-1.018927	-0.000021
C	-0.663446	0.077080	-0.000044
C	0.663452	-0.077079	-0.000043
C	-0.509583	2.489342	-0.000105
C	0.983387	2.272876	-0.000023
C	1.561003	1.018932	-0.000026
N	1.263535	-1.296516	-0.000041
N	-1.263537	1.296522	-0.000058
C	2.877513	0.369632	-0.000001
C	2.660158	-1.040686	-0.000015
C	4.178185	0.870650	0.000030
C	3.707032	-1.948515	0.000000
C	5.236632	-0.037755	0.000046
H	4.353793	1.947619	0.000040
C	5.000757	-1.416980	0.000031
H	3.509381	-3.019137	-0.000012
H	6.262200	0.331527	0.000070
H	5.849942	-2.101754	0.000044
C	-2.877502	-0.369639	0.000002
C	-2.660157	1.040679	-0.000018
C	-4.178175	-0.870660	0.000038
C	-3.707033	1.948507	-0.000007
C	-5.236623	0.037742	0.000053
H	-4.353785	-1.947628	0.000054
C	-5.000756	1.416970	0.000030
H	-3.509380	3.019129	-0.000028
H	-6.262189	-0.331545	0.000080
H	-5.849945	2.101738	0.000040
O	-1.033892	3.574157	0.000037
O	1.033907	-3.574155	0.000007
C	-1.796916	-3.449982	0.000016
N	-2.509085	-4.359934	0.000044
C	1.796896	3.449998	0.000024
N	2.509036	4.359972	0.000059

SCIBA4 S0

E = -1181.59725182 a.u.

C	-2.415907	-0.722338	-0.128291
C	-2.374382	0.784072	-0.167002
C	-1.169881	1.465654	-0.184832
C	0.003761	0.669024	-0.247416
C	-0.003761	-0.669024	-0.247416
C	2.415907	0.722338	-0.128291
C	2.374382	-0.784072	-0.167002
C	1.169881	-1.465654	-0.184832
N	-1.169881	-1.368488	-0.182025
N	1.169881	1.368488	-0.182025
C	0.618108	-2.837207	-0.065213
C	-0.804518	-2.729669	-0.066379
C	1.187990	-4.101306	0.092256
C	-1.642794	-3.828302	0.061173
C	0.354673	-5.212158	0.230304
H	2.270162	-4.219455	0.118118
C	-1.036215	-5.077236	0.207294
H	-2.722630	-3.691777	0.053785
H	0.798086	-6.200382	0.355263
H	-1.664324	-5.963215	0.310318
C	-0.618108	2.837207	-0.065213
C	0.804518	2.729669	-0.066379
C	-1.187990	4.101306	0.092256
C	1.642794	3.828302	0.061173
C	-0.354673	5.212158	0.230304
H	-2.270162	4.219455	0.118118
C	1.036215	5.077236	0.207294
H	2.722630	3.691777	0.053785
H	-0.798086	6.200382	0.355263
H	1.664324	5.963215	0.310318
O	3.447001	1.356865	-0.046937
O	-3.447001	-1.356865	-0.046937
C	3.703169	-1.401660	-0.170608
C	4.776278	-0.891535	0.443891
H	3.761267	-2.378126	-0.658625
H	5.736501	-1.409249	0.419048
H	4.715086	0.034617	1.020690
C	-3.703169	1.401660	-0.170608
C	-4.776278	0.891535	0.443891
H	-3.761267	2.378126	-0.658625
H	-5.736501	1.409249	0.419048
H	-4.715086	-0.034617	1.020690

SCIBA4 T1

E = -1181.57021765 a.u.

C	-2.415907	-0.722338	-0.128291
C	-2.374382	0.784072	-0.167002

C	-1.169881	1.465654	-0.184832
C	0.003761	0.669024	-0.247416
C	-0.003761	-0.669024	-0.247416
C	2.415907	0.722338	-0.128291
C	2.374382	-0.784072	-0.167002
C	1.169881	-1.465654	-0.184832
N	-1.169881	-1.368488	-0.182025
N	1.169881	1.368488	-0.182025
C	0.618108	-2.837207	-0.065213
C	-0.804518	-2.729669	-0.066379
C	1.187990	-4.101306	0.092256
C	-1.642794	-3.828302	0.061173
C	0.354673	-5.212158	0.230304
H	2.270162	-4.219455	0.118118
C	-1.036215	-5.077236	0.207294
H	-2.722630	-3.691777	0.053785
H	0.798086	-6.200382	0.355263
H	-1.664324	-5.963215	0.310318
C	-0.618108	2.837207	-0.065213
C	0.804518	2.729669	-0.066379
C	-1.187990	4.101306	0.092256
C	1.642794	3.828302	0.061173
C	-0.354673	5.212158	0.230304
H	-2.270162	4.219455	0.118118
C	1.036215	5.077236	0.207294
H	2.722630	3.691777	0.053785
H	-0.798086	6.200382	0.355263
H	1.664324	5.963215	0.310318
O	3.447001	1.356865	-0.046937
O	-3.447001	-1.356865	-0.046937
C	3.703169	-1.401660	-0.170608
C	4.776278	-0.891535	0.443891
H	3.761267	-2.378126	-0.658625
H	5.736501	-1.409249	0.419048
H	4.715086	0.034617	1.020690
C	-3.703169	1.401660	-0.170608
C	-4.776278	0.891535	0.443891
H	-3.761267	2.378126	-0.658625
H	-5.736501	1.409249	0.419048
H	-4.715086	-0.034617	1.020690

SCIBA5 S0

E = -1643.18884207 a.u.

C	-1.357036	2.124943	-0.231829
C	0.102701	2.500079	-0.178031
C	1.089356	1.524146	-0.162497
C	0.645506	0.179976	-0.089811
C	-0.645506	-0.179976	-0.089811
C	1.357036	-2.124943	-0.231829
C	-0.102701	-2.500079	-0.178031
C	-1.089356	-1.524146	-0.162497
N	-1.637405	0.750606	-0.167558
N	1.637405	-0.750606	-0.167558
C	-2.557043	-1.371143	-0.304576
C	-2.844528	0.026791	-0.304040
C	-3.613180	-2.265416	-0.492768
C	-4.128276	0.531618	-0.458427
C	-4.906109	-1.767723	-0.658956
H	-3.433639	-3.339391	-0.523138
C	-5.159160	-0.393621	-0.632929
H	-4.294615	1.607141	-0.451802
H	-5.730467	-2.465318	-0.809406
H	-6.181011	-0.032502	-0.757334
C	2.557043	1.371143	-0.304576
C	2.844528	-0.026791	-0.304040
C	3.613180	2.265416	-0.492768
C	4.128276	-0.531618	-0.458427
C	4.906109	1.767723	-0.658956
H	3.433639	3.339391	-0.523138
C	5.159160	0.393621	-0.632929
H	4.294615	-1.607141	-0.451802
H	5.730467	2.465318	-0.809406
H	6.181011	0.032502	-0.757334
O	2.249162	-2.941632	-0.331860
O	-2.249162	2.941632	-0.331860
C	-0.332967	-3.937074	-0.157314
C	0.483241	-4.812610	0.461302
H	-1.178229	-4.283202	-0.757517
H	1.390687	-4.424375	0.935213
C	0.332967	3.937074	-0.157314
C	-0.483241	4.812610	0.461302
H	1.178229	4.283202	-0.757517
H	-1.390687	4.424375	0.935213
C	-0.318213	6.268449	0.530479
C	-1.357036	7.040114	1.074398
C	0.838206	6.927542	0.079642
C	-1.253345	8.426338	1.156902
H	-2.259561	6.538758	1.431494
C	0.941070	8.310995	0.160828
H	1.666340	6.348841	-0.332053
C	-0.103974	9.066753	0.698563
H	-2.072832	9.009073	1.580203
H	1.845160	8.807255	-0.195078
H	-0.018040	10.152474	0.761565
C	0.318213	-6.268449	0.530479
C	1.357036	-7.040114	1.074398
C	-0.838206	-6.927542	0.079642
C	1.253345	-8.426338	1.156902
H	2.259561	-6.538758	1.431494
C	-0.941070	-8.310995	0.160828
H	-1.666340	-6.348841	-0.332053
C	0.103974	-9.066753	0.698563
H	2.072832	-9.009073	1.580203
H	-1.845160	-8.807255	-0.195078
H	0.018040	-10.152474	0.761565

SCIBA5 T1

E = -1643.17362555 a.u.

C	-1.357036	2.124943	-0.231829
C	0.102701	2.500079	-0.178031
C	1.089356	1.524146	-0.162497
C	0.645506	0.179976	-0.089811
C	-0.645506	-0.179976	-0.089811
C	1.357036	-2.124943	-0.231829
C	-0.102701	-2.500079	-0.178031
C	-1.089356	-1.524146	-0.162497
N	-1.637405	0.750606	-0.167558
N	1.637405	-0.750606	-0.167558
C	-2.557043	-1.371143	-0.304576
C	-2.844528	0.026791	-0.304040
C	-3.613180	-2.265416	-0.492768
C	-4.128276	0.531618	-0.458427
C	-4.906109	-1.767723	-0.658956
H	-3.433639	-3.339391	-0.523138
C	-5.159160	-0.393621	-0.632929
H	-4.294615	1.607141	-0.451802
H	-5.730467	-2.465318	-0.809406
H	-6.181011	-0.032502	-0.757334
C	2.557043	1.371143	-0.304576
C	2.844528	-0.026791	-0.304040
C	3.613180	2.265416	-0.492768
C	4.128276	-0.531618	-0.458427
C	4.906109	1.767723	-0.658956
H	3.433639	3.339391	-0.523138
C	5.159160	0.393621	-0.632929
H	4.294615	-1.607141	-0.451802
H	5.730467	2.465318	-0.809406
H	6.181011	0.032502	-0.757334
O	2.249162	-2.941632	-0.331860
O	-2.249162	2.941632	-0.331860
C	-0.332967	-3.937074	-0.157314
C	0.483241	-4.812610	0.461302
H	-1.178229	-4.283202	-0.757517
H	1.390687	-4.424375	0.935213
C	0.332967	3.937074	-0.157314
C	-0.483241	4.812610	0.461302
H	1.178229	4.283202	-0.757517
H	-1.390687	4.424375	0.935213
C	-0.318213	6.268449	0.530479
C	-1.357036	7.040114	1.074398
C	0.838206	6.927542	0.079642
C	-1.253345	8.426338	1.156902
H	-2.259561	6.538758	1.431494
C	0.941070	8.310995	0.160828
H	1.666340	6.348841	-0.332053
C	-0.103974	9.066753	0.698563
H	-2.072832	9.009073	1.580203
H	1.845160	8.807255	-0.195078
H	-0.018040	10.152474	0.761565
C	0.318213	-6.268449	0.530479
C	1.357036	-7.040114	1.074398
C	-0.838206	-6.927542	0.079642
C	1.253345	-8.426338	1.156902
H	2.259561	-6.538758	1.431494
C	-0.941070	-8.310995	0.160828
H	-1.666340	-6.348841	-0.332053
C	0.103974	-9.066753	0.698563
H	2.072832	-9.009073	1.580203
H	-1.845160	-8.807255	-0.195078
H	0.018040	-10.152474	0.761565

SCIBA6 S0

E = -1365.88837072 a.u.

C	1.513459	2.018146	-0.177298
C	2.371823	0.778672	-0.220934
C	1.811056	-0.489386	-0.229234
C	0.393196	-0.542677	-0.288902
C	-0.393196	0.542677	-0.288902
C	-1.513459	-2.018146	-0.177298
C	-2.371823	-0.778672	-0.220934
C	-1.811056	0.489386	-0.229234
N	0.127526	1.797514	-0.227785
N	-0.127526	-1.797514	-0.227785
C	-2.182639	1.917678	-0.104669
C	-0.974862	2.677116	-0.111015
C	-3.391970	2.595094	0.068149
C	-0.952850	4.058502	0.015950
C	-3.380963	3.982727	0.206413
H	-4.335871	2.053804	0.111288
C	-2.182639	4.701243	0.170513
H	-0.004796	4.592862	0.002510
H	-4.323758	4.512787	0.342579
H	-2.203682	5.787091	0.272335
C	2.182639	-1.917678	-0.104669
C	0.974862	-2.677116	-0.111015
C	3.391970	-2.595094	0.068149
C	0.952850	-4.058502	0.015950
C	3.380963	-3.982727	0.206413
H	4.335871	-2.053804	0.111288
C	2.182639	-4.701243	0.170513
H	0.004796	-4.592862	0.002510
H	4.323758	-4.512787	0.342579
H	2.203682	-5.787091	0.272335
O	-1.969888	-3.137468	-0.101343
O	1.969888	3.137468	-0.101343
C	-3.798765	-1.076410	-0.242838
C	-4.357048	-2.115984	0.404429
H	-4.433057	-0.355958	-0.765917
H	-3.757434	-2.788040	1.023408
C	3.798765	1.076410	-0.242838
C	4.357048	2.115984	0.404429
H	4.433057	0.355958	-0.765917
H	3.757434	2.788040	1.023408
C	-5.765654	-2.377403	0.360315
N	-6.897322	-2.609003	0.330539
C	5.765654	2.377403	0.360315
N	6.897322	2.609003	0.330539

SCIBA6 T1

E = -1365.86498539 a.u.

C	1.513459	2.018146	-0.177298
C	2.371823	0.778672	-0.220934
C	1.811056	-0.489386	-0.229234
C	0.393196	-0.542677	-0.288902
C	-0.393196	0.542677	-0.288902
C	-1.513459	-2.018146	-0.177298
C	-2.371823	-0.778672	-0.220934
C	-1.811056	0.489386	-0.229234
N	0.127526	1.797514	-0.227785
N	-0.127526	-1.797514	-0.227785
C	-2.182639	1.917678	-0.104669
C	-0.974862	2.677116	-0.111015
C	-3.391970	2.595094	0.068149
C	-0.952850	4.058502	0.015950
C	-3.380963	3.982727	0.206413
H	-4.335871	2.053804	0.111288
C	-2.182639	4.701243	0.170513
H	-0.004796	4.592862	0.002510
H	-4.323758	4.512787	0.342579
H	-2.203682	5.787091	0.272335
C	2.182639	-1.917678	-0.104669
C	0.974862	-2.677116	-0.111015
C	3.391970	-2.595094	0.068149
C	0.952850	-4.058502	0.015950
C	3.380963	-3.982727	0.206413
H	4.335871	-2.053804	0.111288
C	2.182639	-4.701243	0.170513
H	0.004796	-4.592862	0.002510
H	4.323758	-4.512787	0.342579
H	2.203682	-5.787091	0.272335
O	-1.969888	-3.137468	-0.101343
O	1.969888	3.137468	-0.101343
C	-3.798765	-1.076410	-0.242838
C	-4.357048	-2.115984	0.404429
H	-4.433057	-0.355958	-0.765917
H	-3.757434	-2.788040	1.023408
C	3.798765	1.076410	-0.242838
C	4.357048	2.115984	0.404429
H	4.433057	0.355958	-0.765917
H	3.757434	2.788040	1.023408
C	-5.765654	-2.377403	0.360315
N	-6.897322	-2.609003	0.330539
C	5.765654	2.377403	0.360315
N	6.897322	2.609003	0.330539

SCIBA7 S0

E = -1590.13948626 a.u.

C	2.522371	0.030991	-0.214677
C	2.060910	-1.404095	-0.251379
C	0.715146	-1.736057	-0.268664
C	-0.191089	-0.642319	-0.325521
C	0.191089	0.642319	-0.325521
C	-2.522371	-0.030991	-0.214677
C	-2.060910	1.404095	-0.251379
C	-0.715146	1.736057	-0.268664
N	1.502381	0.994814	-0.265243
N	-1.502381	-0.994814	-0.265243
C	0.191089	2.902639	-0.154434
C	1.528576	2.405252	-0.155758
C	-0.003562	4.278653	-0.003254
C	2.640104	3.225450	-0.031287
C	1.106540	5.111805	0.130729
H	-1.003280	4.708973	0.019996
C	2.404831	4.594436	0.109689
H	3.639809	2.794866	-0.036904
H	0.955259	6.184810	0.250011
H	3.254422	5.271339	0.209023
C	-0.191089	-2.902639	-0.154434
C	-1.528576	-2.405252	-0.155758
C	0.003562	-4.278653	-0.003254
C	-2.640104	-3.225450	-0.031287
C	-1.106540	-5.111805	0.130729
H	1.003280	-4.708973	0.019996
C	-2.404831	-4.594436	0.109689
H	-3.639809	-2.794866	-0.036904
H	-0.955259	-6.184810	0.250011
H	-3.254422	-5.271339	0.209023
O	-3.687998	-0.348653	-0.142217
O	3.687998	0.348653	-0.142217
C	-3.164333	2.355152	-0.229977
C	-4.299148	2.153524	0.442515
H	-3.028878	3.306266	-0.752987
H	-4.543874	1.313579	1.088664
C	3.164333	-2.355152	-0.229977
C	4.299148	-2.153524	0.442515
H	3.028878	-3.306266	-0.752987
H	4.543874	-1.313579	1.088664
N	5.388874	-3.122939	0.362777
O	6.421345	-2.783499	0.896014
O	5.205068	-4.161205	-0.222350
N	-5.388874	3.122939	0.362777
O	-6.421345	2.783499	0.896014
O	-5.205068	4.161205	-0.222350

SCIBA7 T1

E = -1590.11595384 a.u.

C	2.522371	0.030991	-0.214677
C	2.060910	-1.404095	-0.251379
C	0.715146	-1.736057	-0.268664
C	-0.191089	-0.642319	-0.325521
C	0.191089	0.642319	-0.325521
C	-2.522371	-0.030991	-0.214677
C	-2.060910	1.404095	-0.251379
C	-0.715146	1.736057	-0.268664

N	1.502381	0.994814	-0.265243
N	-1.502381	-0.994814	-0.265243
C	0.191089	2.902639	-0.154434
C	1.528576	2.405252	-0.155758
C	-0.003562	4.278653	-0.003254
C	2.640104	3.225450	-0.031287
C	1.106540	5.111805	0.130729
H	-1.003280	4.708973	0.019996
C	2.404831	4.594436	0.109689
H	3.639809	2.794866	-0.036904
H	0.955259	6.184810	0.250011
H	3.254422	5.271339	0.209023
C	-0.191089	-2.902639	-0.154434
C	-1.528576	-2.405252	-0.155758
C	0.003562	-4.278653	-0.003254
C	-2.640104	-3.225450	-0.031287
C	-1.106540	-5.111805	0.130729
H	1.003280	-4.708973	0.019996
C	-2.404831	-4.594436	0.109689
H	-3.639809	-2.794866	-0.036904
H	-0.955259	-6.184810	0.250011
H	-3.254422	-5.271339	0.209023
O	-3.687998	-0.348653	-0.142217
O	3.687998	0.348653	-0.142217
C	-3.164333	2.355152	-0.229977
C	-4.299148	2.153524	0.442515
H	-3.028878	3.306266	-0.752987
H	-4.543874	1.313579	1.088664
C	3.164333	-2.355152	-0.229977
C	4.299148	-2.153524	0.442515
H	3.028878	-3.306266	-0.752987
H	4.543874	-1.313579	1.088664
N	5.388874	-3.122939	0.362777
O	6.421345	-2.783499	0.896014
O	5.205068	-4.161205	-0.222350
N	-5.388874	3.122939	0.362777
O	-6.421345	2.783499	0.896014
O	-5.205068	4.161205	-0.222350

SCIBA8 S0

E = -1797.70556810 a.u.

C	0.841276	2.385802	-0.230411
C	-0.669536	2.422004	-0.239305
C	-1.398051	1.234660	-0.233507
C	-0.668443	0.028457	-0.234801
C	0.668443	-0.028457	-0.234801
C	-0.841276	-2.385802	-0.230411
C	0.669536	-2.422004	-0.239305
C	1.398051	-1.234660	-0.233507
N	1.421539	1.103556	-0.232939
N	-1.421539	-1.103556	-0.232939
C	2.799051	-0.760029	-0.223238
C	2.768722	0.669097	-0.225730
C	4.040342	-1.398742	-0.202450
C	3.919800	1.443973	-0.217092
C	5.203270	-0.627214	-0.193902
H	4.114960	-2.485775	-0.185706
C	5.142427	0.768737	-0.202967
H	3.845096	2.529515	-0.219454
H	6.173804	-1.123761	-0.177524
H	6.067541	1.346705	-0.195721
C	-2.799051	0.760029	-0.223238
C	-2.768722	-0.669097	-0.225730
C	-4.040342	1.398742	-0.202450
C	-3.919800	-1.443973	-0.217092
C	-5.203270	0.627214	-0.193902
H	-4.114960	2.485775	-0.185706
C	-5.142427	-0.768737	-0.202967
H	-3.845096	-2.529515	-0.219454
H	-6.173804	1.123761	-0.177524
H	-6.067541	-1.346705	-0.195721
O	-1.551968	-3.370320	-0.223030
O	1.551968	3.370320	-0.223030
C	1.358099	-3.696300	-0.267549
C	0.845779	-4.948378	-0.205948
H	2.443306	-3.607088	-0.335696
H	-0.229544	-5.091895	-0.108968
C	-1.358099	3.696300	-0.267549
C	-0.845779	4.948378	-0.205948
H	-2.443306	3.607088	-0.335696
H	0.229544	5.091895	-0.108968
C	-1.679259	6.149791	-0.242749
C	-1.088623	7.353876	-0.066993
C	-3.116690	5.988088	-0.585011
H	0.000926	7.357179	0.054386
C	-1.724303	8.676172	-0.076138
C	-4.166892	6.377537	0.145635
H	-3.311007	5.442911	-1.515720
C	-2.768722	9.074367	0.668489
H	-1.218444	9.438349	-0.678995
C	-4.119928	7.093923	1.433625
H	-5.167938	6.121868	-0.220470
H	-3.049339	10.131803	0.614402
C	-3.519584	8.272499	1.649923
H	-4.705136	6.659148	2.250820
H	-3.648449	8.735862	2.634173
C	1.679259	-6.149791	-0.242749
C	1.088623	-7.353876	-0.066993
C	3.116690	-5.988088	-0.585011
H	-0.000926	-7.357179	0.054386
C	1.724303	-8.676172	-0.076138
C	4.166892	-6.377537	0.145635
H	3.311007	-5.442911	-1.515720
C	2.768722	-9.074367	0.668489
H	1.218444	-9.438349	-0.678995
C	4.119928	-7.093923	1.433625
H	5.167938	-6.121868	-0.220470
H	3.049339	-10.131803	0.614402
C	3.519584	-8.272499	1.649923

H	4.705136	-6.659148	2.250820
H	3.648449	-8.735862	2.634173

SCIBA8 T1

E = -1797.67394429 a.u.

C	0.841276	2.385802	-0.230411
C	-0.669536	2.422004	-0.239305
C	-1.398051	1.234660	-0.233507
C	-0.668443	0.028457	-0.234801
C	0.668443	-0.028457	-0.234801
C	-0.841276	-2.385802	-0.230411
C	0.669536	-2.422004	-0.239305
C	1.398051	-1.234660	-0.233507
N	1.421539	1.103556	-0.232939
N	-1.421539	-1.103556	-0.232939
C	2.799051	-0.760029	-0.223238
C	2.768722	0.669097	-0.225730
C	4.040342	-1.398742	-0.202450
C	3.919800	1.443973	-0.217092
C	5.203270	-0.627214	-0.193902
H	4.114960	-2.485775	-0.185706
C	5.142427	0.768737	-0.202967
H	3.845096	2.529515	-0.219454
H	6.173804	-1.123761	-0.177524
H	6.067541	1.346705	-0.195721
C	-2.799051	0.760029	-0.223238
C	-2.768722	-0.669097	-0.225730
C	-4.040342	1.398742	-0.202450
C	-3.919800	-1.443973	-0.217092
C	-5.203270	0.627214	-0.193902
H	-4.114960	2.485775	-0.185706
C	-5.142427	-0.768737	-0.202967
H	-3.845096	-2.529515	-0.219454
H	-6.173804	1.123761	-0.177524
H	-6.067541	-1.346705	-0.195721
O	-1.551968	-3.370320	-0.223030
O	1.551968	3.370320	-0.223030
C	1.358099	-3.696300	-0.267549
C	0.845779	-4.948378	-0.205948
H	2.443306	-3.607088	-0.335696
H	-0.229544	-5.091895	-0.108968
C	-1.358099	3.696300	-0.267549
C	-0.845779	4.948378	-0.205948
H	-2.443306	3.607088	-0.335696
H	0.229544	5.091895	-0.108968
C	-1.679259	6.149791	-0.242749
C	-1.088623	7.353876	-0.066993
C	-3.116690	5.988088	-0.585011
H	0.000926	7.357179	0.054386
C	-1.724303	8.676172	-0.076138
C	-4.166892	6.377537	0.145635
H	-3.311007	5.442911	-1.515720
C	-2.768722	9.074367	0.668489
H	-1.218444	9.438349	-0.678995
C	-4.119928	7.093923	1.433625
H	-5.167938	6.121868	-0.220470
H	-3.049339	10.131803	0.614402
C	-3.519584	8.272499	1.649923
H	-4.705136	6.659148	2.250820
H	-3.648449	8.735862	2.634173
C	1.679259	-6.149791	-0.242749
C	1.088623	-7.353876	-0.066993
C	3.116690	-5.988088	-0.585011
H	-0.000926	-7.357179	0.054386
C	1.724303	-8.676172	-0.076138
C	4.166892	-6.377537	0.145635
H	3.311007	-5.442911	-1.515720
C	2.768722	-9.074367	0.668489
H	1.218444	-9.438349	-0.678995
C	4.119928	-7.093923	1.433625
H	5.167938	-6.121868	-0.220470
H	3.049339	-10.131803	0.614402
C	3.519584	-8.272499	1.649923
H	4.705136	-6.659148	2.250820
H	3.648449	-8.735862	2.634173

SCIBA9 S0

E = -1995.98241922 a.u.

C	1.736108	1.852250	-0.010526
C	2.439251	0.511711	-0.009710
C	1.734613	-0.679922	-0.010933
C	0.325392	-0.584151	-0.014168
C	-0.325359	0.582545	-0.014175
C	-1.736108	-1.853848	-0.010478
C	-2.439221	-0.513319	-0.009656
C	-1.734571	0.678307	-0.010922
N	0.327017	1.776808	-0.012507
N	-0.327002	-1.778406	-0.012479
C	-1.964146	2.130075	-0.007346
C	-0.687370	2.767888	-0.008439
C	-3.121239	2.906259	-0.002442
C	-0.551010	4.147878	-0.005151
C	-2.991281	4.295786	0.000806
H	-4.099920	2.424147	-0.000839
C	-1.729807	4.900084	-0.000602
H	0.439024	4.600720	-0.006035
H	-3.885225	4.920115	0.004520
H	-1.659779	5.988823	0.002040
C	1.964159	-2.131697	-0.007335
C	0.687376	-2.769494	-0.008418
C	3.121238	-2.907896	-0.002402
C	0.551000	-4.149484	-0.005118
C	2.991268	-4.297421	0.000858
H	4.099920	-2.425788	-0.000776
C	1.729787	-4.901704	-0.000560
H	-0.439040	-4.602313	-0.006002
H	3.885205	-4.921760	0.004586
H	1.659746	-5.990442	0.002082

O	-2.308160	-2.917147	-0.008715
O	2.308158	2.915550	-0.008771
C	-3.860210	-0.542612	-0.005336
C	-5.080703	-0.527882	-0.000892
C	3.860232	0.541286	-0.005434
C	5.080735	0.527415	-0.001024
Si	6.936090	0.547557	0.011404
Si	-6.936074	-0.545071	0.011349
C	7.524008	1.344117	-1.581671
H	7.180396	0.773504	-2.456440
H	7.136160	2.369228	-1.668102
H	8.623459	1.386742	-1.607312
C	7.524539	-1.233021	0.127360
H	7.146797	-1.710139	1.043614
H	7.177159	-1.818625	-0.736663
H	8.624011	-1.275764	0.148381
C	7.498265	1.536026	1.502918
H	7.118250	2.566325	1.448860
H	7.128846	1.084691	2.434912
H	8.597203	1.573963	1.548419
C	-7.521329	1.236926	0.121743
H	-7.172028	1.819492	-0.743566
H	-8.620739	1.281794	0.141643
H	-7.143539	1.715857	1.037037
C	-7.525119	-1.345443	-1.579359
H	-7.139028	-2.371470	-1.662746
H	-8.624633	-1.386227	-1.605110
H	-7.180327	-0.777996	-2.455719
C	-7.500453	-1.527429	1.506039
H	-7.122495	-2.558670	1.455903
H	-7.130537	-1.073404	2.436524
H	-8.599484	-1.563037	1.551302

SCIBA9 T1

E = -1995.94112340 a.u.

C	1.736108	1.852250	-0.010526
C	2.439251	0.511711	-0.009710
C	1.734613	-0.679922	-0.010933
C	0.325392	-0.584151	-0.014168
C	-0.325359	0.582545	-0.014175
C	-1.736108	-1.853848	-0.010478
C	-2.439221	-0.513319	-0.009656
C	-1.734571	0.678307	-0.010922
N	0.327017	1.776808	-0.012507
N	-0.327002	-1.778406	-0.012479
C	-1.964146	2.130075	-0.007346
C	-0.687370	2.767888	-0.008439
C	-3.121239	2.906259	-0.002442
C	-0.551010	4.147878	-0.005151
C	-2.991281	4.295786	0.000806
H	-4.099920	2.424147	-0.000839
C	-1.729807	4.900084	-0.000602
H	0.439024	4.600720	-0.006035
H	-3.885225	4.920115	0.004520
H	-1.659779	5.988823	0.002040
C	1.964159	-2.131697	-0.007335
C	0.687376	-2.769494	-0.008418
C	3.121238	-2.907896	-0.002402
C	0.551000	-4.149484	-0.005118
C	2.991268	-4.297421	0.000858
H	4.099920	-2.425788	-0.000776
C	1.729787	-4.901704	-0.000560
H	-0.439040	-4.602313	-0.006002
H	3.885205	-4.921760	0.004586
H	1.659746	-5.990442	0.002082
O	-2.308160	-2.917147	-0.008715
O	2.308158	2.915550	-0.008771
C	-3.860210	-0.542612	-0.005336
C	-5.080703	-0.527882	-0.000892
C	3.860232	0.541286	-0.005434
C	5.080735	0.527415	-0.001024
Si	6.936090	0.547557	0.011404
Si	-6.936074	-0.545071	0.011349
C	7.524008	1.344117	-1.581671
H	7.180396	0.773504	-2.456440
H	7.136160	2.369228	-1.668102
H	8.623459	1.386742	-1.607312
C	7.524539	-1.233021	0.127360
H	7.146797	-1.710139	1.043614
H	7.177159	-1.818625	-0.736663
H	8.624011	-1.275764	0.148381
C	7.498265	1.536026	1.502918
H	7.118250	2.566325	1.448860
H	7.128846	1.084691	2.434912
H	8.597203	1.573963	1.548419
C	-7.521329	1.236926	0.121743
H	-7.172028	1.819492	-0.743566
H	-8.620739	1.281794	0.141643
H	-7.143539	1.715857	1.037037
C	-7.525119	-1.345443	-1.579359
H	-7.139028	-2.371470	-1.662746
H	-8.624633	-1.386227	-1.605110
H	-7.180327	-0.777996	-2.455719
C	-7.500453	-1.527429	1.506039
H	-7.122495	-2.558670	1.455903
H	-7.130537	-1.073404	2.436524
H	-8.599484	-1.563037	1.551302

SCIBA10 S0

E = -4210.81579111 a.u.

C	1.898094	1.738425	0.010786
C	2.482075	0.342196	0.002960
C	1.674486	-0.782544	-0.002941
C	0.281074	-0.566206	-0.006438
C	-0.265290	0.653687	-0.006085
C	-1.881313	-1.651187	-0.016289
C	-2.465919	-0.255008	-0.014671
C	-1.658789	0.870239	-0.011678

N	0.489196	1.787919	0.001856
N	-0.472910	-1.700720	-0.012921
C	-1.763512	2.335732	-0.009390
C	-0.436988	2.863160	0.000876
C	-2.851193	3.205875	-0.017853
C	-0.185919	4.227014	0.007028
C	-2.605185	4.579918	-0.012628
H	-3.866707	2.806943	-0.030482
C	-1.297450	5.075905	0.000654
H	0.838256	4.595795	0.016078
H	-3.443948	5.276593	-0.019528
H	-1.135920	6.154852	0.005103
C	1.779784	-2.247846	-0.007665
C	0.453604	-2.775874	-0.013624
C	2.868034	-3.117248	-0.005106
C	0.203378	-4.139888	-0.018737
C	2.622986	-4.491514	-0.009095
H	3.883339	-2.717909	0.001630
C	1.315483	-4.988213	-0.016523
H	-0.820577	-4.509365	-0.023855
H	3.462596	-5.187258	-0.005912
H	1.154449	-6.067238	-0.020055
O	-2.545146	-2.662574	-0.020279
O	2.562188	2.749283	0.024152
C	3.897087	0.251745	-0.001070
C	5.116231	0.154026	-0.007132
C	-3.881232	-0.171324	-0.010896
C	-5.101736	-0.093170	-0.002965
Si	6.970034	0.135030	0.000760
Si	-6.953419	-0.152201	0.002924
Si	-7.650683	0.569780	-2.123932
Si	-7.725439	1.273919	1.704043
Si	-7.426230	-2.419199	0.419604
Si	7.640425	-1.057184	-1.912592
Si	7.589380	-0.952083	1.991075
Si	7.548474	2.415298	-0.053493
C	6.605102	-0.495096	-3.384083
H	5.534774	-0.643046	-3.176984
H	6.764080	0.572683	-3.594111
H	6.866857	-1.067870	-4.287503
C	7.392497	-2.911099	-1.641205
H	7.674480	-3.474303	-2.544722
H	8.009479	-3.277902	-0.806816
H	6.339108	-3.137830	-1.415817
C	9.472709	-0.714449	-2.231376
H	9.830744	-1.295864	-3.095449
H	9.645202	0.350981	-2.447957
H	10.087155	-0.987765	-1.359939
C	6.534320	-2.504353	2.186037
H	6.673782	-3.192933	1.339320
H	6.791559	-3.042018	3.111913
H	5.469259	-2.230340	2.233528
C	7.284473	0.195200	3.458084
H	6.233513	0.521771	3.477716
H	7.502398	-0.318337	4.407628
H	7.919259	1.092609	3.403460
C	9.421970	-1.406100	1.899864
H	10.039547	-0.514524	1.711172
H	9.759521	-1.859199	2.845036
H	9.613585	-2.129256	1.092377
C	7.380989	3.050076	-1.823553
H	7.579526	4.132408	-1.866554
H	8.086800	2.547574	-2.502551
H	6.359279	2.876215	-2.194074
C	6.356905	3.346094	1.067171
H	6.427567	2.991326	2.106163
H	6.577827	4.424972	1.056933
H	5.320028	3.198918	0.726024
C	9.335002	2.624375	0.530390
H	9.640615	3.680861	0.472972
H	9.454227	2.296723	1.574463
H	10.027275	2.037255	-0.092420
C	-6.662884	2.110049	-2.587651
H	-6.953007	2.479852	-3.583426
H	-6.826710	2.917855	-1.859050
H	-5.586659	1.880391	-2.604634
C	-9.496934	0.974517	-2.064433
H	-9.856660	1.283568	-3.058352
H	-10.085851	0.099854	-1.748473
H	-9.704165	1.796384	-1.361873
C	-7.337059	-0.789624	-3.395474
H	-6.274834	-1.077643	-3.397398
H	-7.933550	-1.687847	-3.173802
H	-7.602145	-0.446329	-4.407724
C	-9.226858	-2.769703	-0.037788
H	-9.406924	-2.583806	-1.107706
H	-9.484462	-3.819887	0.170302
H	-9.912643	-2.130538	0.539227
C	-6.244682	-3.460355	-0.610930
H	-6.401847	-4.532888	-0.416006
H	-6.393846	-3.282095	-1.686216
H	-5.200054	-3.209846	-0.365661
C	-7.148885	-2.771411	2.253780
H	-7.296711	-3.840469	2.472616
H	-6.118950	-2.503914	2.535527
H	-7.841560	-2.194854	2.885688
C	-9.527445	0.833116	2.068472
H	-9.609901	-0.188222	2.470971
H	-9.953953	1.524289	2.812154
H	-10.144385	0.889400	1.158598
C	-7.620796	3.077464	1.146192
H	-8.244545	3.262293	0.258354
H	-7.964617	3.750246	1.947527
H	-6.583421	3.349657	0.897732
C	-6.669678	1.041305	3.247948
H	-7.014019	1.698828	4.061356
H	-6.711144	0.001346	3.603140
H	-5.617521	1.280306	3.031594

SCIBA10 T1

E = -4210.77655802 a.u.

C	1.898094	1.738425	0.010786
C	2.482075	0.342196	0.002960
C	1.674486	-0.782544	-0.002941
C	0.281074	-0.566206	-0.006438
C	-0.265290	0.653687	-0.006085
C	-1.881313	-1.651187	-0.016289
C	-2.465919	-0.255008	-0.014671
C	-1.658789	0.870239	-0.011678
N	0.489196	1.787919	0.001856
N	-0.472910	-1.700720	-0.012921
C	-1.763512	2.335732	-0.009390
C	-0.436988	2.863160	0.000876
C	-2.851193	3.205875	-0.017853
C	-0.185919	4.227014	0.007028
C	-2.605185	4.579918	-0.012628
H	-3.866707	2.806943	-0.030482
C	-1.297450	5.075905	0.000654
H	0.838256	4.595795	0.016078
H	-3.443948	5.276593	-0.019528
H	-1.135920	6.154852	0.005103
C	1.779784	-2.247846	-0.007665
C	0.453604	-2.775874	-0.013624
C	2.868034	-3.117248	-0.005106
C	0.203378	-4.139888	-0.018737
C	2.622986	-4.491514	-0.009095
H	3.883339	-2.717909	0.001630
C	1.315483	-4.988213	-0.016523
H	-0.820577	-4.509365	-0.023855
H	3.462596	-5.187258	-0.005912
H	1.154449	-6.067238	-0.020055
O	-2.545146	-2.662574	-0.020279
O	2.562188	2.749283	0.024152
C	3.897087	0.251745	-0.001070
C	5.116231	0.154026	-0.007132
C	-3.881232	-0.171324	-0.010896
C	-5.101736	-0.093170	-0.002965
Si	6.970034	0.135030	0.000760
Si	-6.953419	-0.152201	0.002924
Si	-7.650683	0.569780	-2.123932
Si	-7.725439	1.273919	1.704043
Si	-7.426230	-2.419199	0.419604
Si	7.640425	-1.057184	-1.912592
Si	7.589380	-0.952083	1.991075
Si	7.548474	2.415298	-0.053493
C	6.605102	-0.495096	-3.384083
H	5.534774	-0.643046	-3.176984
H	6.764080	0.572683	-3.594111
H	6.866857	-1.067870	-4.287503
C	7.392497	-2.911099	-1.641205
H	7.674480	-3.474303	-2.544722
H	8.009479	-3.277902	-0.806816
H	6.339108	-3.137830	-1.415817
C	9.472709	-0.714449	-2.231376
H	9.830744	-1.295864	-3.095449
H	9.645202	0.350981	-2.447957
H	10.087155	-0.987765	-1.359939
C	6.534320	-2.504353	2.186037
H	6.673782	-3.192933	1.339320
H	6.791559	-3.042018	3.111913
H	5.469259	-2.230340	2.233528
C	7.284473	0.195200	3.458084
H	6.233513	0.521771	3.477716
H	7.502398	-0.318337	4.407628
H	7.919259	1.092609	3.403460
C	9.421970	-1.406100	1.899864
H	10.039547	-0.514524	1.711172
H	9.759521	-1.859199	2.845036
H	9.613585	-2.129256	1.092377
C	7.380989	3.050076	-1.823553
H	7.579526	4.132408	-1.866554
H	8.086800	2.547574	-2.502551
H	6.359279	2.876215	-2.194074
C	6.356905	3.346094	1.067171
H	6.427567	2.991326	2.106163
H	6.577827	4.424972	1.056933
H	5.320028	3.198918	0.726024
C	9.335002	2.624375	0.530390
H	9.640615	3.680861	0.472972
H	9.454227	2.296723	1.574463
H	10.027275	2.037255	-0.092420
C	-6.662884	2.110049	-2.587651
H	-6.953007	2.479852	-3.583426
H	-6.826710	2.917855	-1.859050
H	-5.586659	1.880391	-2.604634
C	-9.496934	0.974517	-2.064433
H	-9.856660	1.283568	-3.058352
H	-10.085851	0.099854	-1.748473
H	-9.704165	1.796384	-1.361873
C	-7.337059	-0.789624	-3.395474
H	-6.274834	-1.077643	-3.397398
H	-7.933550	-1.687847	-3.173802
H	-7.602145	-0.446329	-4.407724
C	-9.226858	-2.769703	-0.037788
H	-9.406924	-2.583806	-1.107706
H	-9.484462	-3.819887	0.170302
H	-9.912643	-2.130538	0.539227
C	-6.244682	-3.460355	-0.610930
H	-6.401847	-4.532888	-0.416006
H	-6.393846	-3.282095	-1.686216
H	-5.200054	-3.209846	-0.365661
C	-7.148885	-2.771411	2.253780
H	-7.296711	-3.840469	2.472616
H	-6.118950	-2.503914	2.535527
H	-7.841560	-2.194854	2.885688
C	-9.527445	0.833116	2.068472
H	-9.609901	-0.188222	2.470971
H	-9.953953	1.524289	2.812154
H	-10.144385	0.889400	1.158598

C	-7.620796	3.077464	1.146192
H	-8.244545	3.262293	0.258354
H	-7.964617	3.750246	1.947527
H	-6.583421	3.349657	0.897732
C	-6.669678	1.041305	3.247948
H	-7.014019	1.698828	4.061356
H	-6.711144	0.001346	3.603140
H	-5.617521	1.280306	3.031594

SCIBA11 S0

E = -1363.40890385 a.u.

C	-1.328157	-2.164144	-0.001603
C	-2.281132	-0.987248	-0.001446
C	-1.837510	0.325367	-0.002260
C	-0.434228	0.508755	-0.003679
C	0.434227	-0.508755	-0.003632
C	1.328156	2.164145	-0.001792
C	2.281132	0.987248	-0.001527
C	1.837510	-0.325367	-0.002223
N	0.036018	-1.808433	-0.002790
N	-0.036019	1.808433	-0.002952
C	2.351481	-1.700428	-0.000785
C	1.227028	-2.578945	-0.001044
C	3.639997	-2.233314	0.000904
C	1.364833	-3.958034	0.000420
C	3.787020	-3.620164	0.002383
H	4.508946	-1.574331	0.001086
C	2.669222	-4.461766	0.002164
H	0.485507	-4.599878	0.000257
H	4.786886	-4.054323	0.003774
H	2.815935	-5.542719	0.003369
C	-2.351482	1.700429	-0.000949
C	-1.227028	2.578945	-0.001279
C	-3.639998	2.233314	0.000681
C	-1.364834	3.958034	0.000062
C	-3.787021	3.620165	0.002035
H	-4.508947	1.574332	0.000911
C	-2.669223	4.461767	0.001750
H	-0.485507	4.599878	-0.000152
H	-4.786887	4.054324	0.003375
H	-2.815935	5.542720	0.002856
O	1.683407	3.315715	-0.000852
O	-1.683409	-3.315714	-0.000572
C	3.661286	1.313502	0.000011
C	4.848722	1.574474	0.001255
C	-3.661288	-1.313495	0.000123
C	-4.848724	-1.574468	0.001393
C	6.201544	1.867964	0.002732
N	7.334664	2.103881	0.004007
C	-6.201542	-1.867958	0.002850
N	-7.334656	-2.103903	0.004114

SCIBA11 T1

E = -1363.36732413 a.u.

C	-1.328157	-2.164144	-0.001603
C	-2.281132	-0.987248	-0.001446
C	-1.837510	0.325367	-0.002260
C	-0.434228	0.508755	-0.003679
C	0.434227	-0.508755	-0.003632
C	1.328156	2.164145	-0.001792
C	2.281132	0.987248	-0.001527
C	1.837510	-0.325367	-0.002223
N	0.036018	-1.808433	-0.002790
N	-0.036019	1.808433	-0.002952
C	2.351481	-1.700428	-0.000785
C	1.227028	-2.578945	-0.001044
C	3.639997	-2.233314	0.000904
C	1.364833	-3.958034	0.000420
C	3.787020	-3.620164	0.002383
H	4.508946	-1.574331	0.001086
C	2.669222	-4.461766	0.002164
H	0.485507	-4.599878	0.000257
H	4.786886	-4.054323	0.003774
H	2.815935	-5.542719	0.003369
C	-2.351482	1.700429	-0.000949
C	-1.227028	2.578945	-0.001279
C	-3.639998	2.233314	0.000681
C	-1.364834	3.958034	0.000062
C	-3.787021	3.620165	0.002035
H	-4.508947	1.574332	0.000911
C	-2.669223	4.461767	0.001750
H	-0.485507	4.599878	-0.000152
H	-4.786887	4.054324	0.003375
H	-2.815935	5.542720	0.002856
O	1.683407	3.315715	-0.000852
O	-1.683409	-3.315714	-0.000572
C	3.661286	1.313502	0.000011
C	4.848722	1.574474	0.001255
C	-3.661288	-1.313495	0.000123
C	-4.848724	-1.574468	0.001393
C	6.201544	1.867964	0.002732
N	7.334664	2.103881	0.004007
C	-6.201542	-1.867958	0.002850
N	-7.334656	-2.103903	0.004114

SCIBA12 S0

E = -1795.20895321 a.u.

C	-1.952865	1.621831	-0.110531
C	-2.485618	0.203806	-0.107898
C	-1.637657	-0.889909	-0.111251
C	-0.250614	-0.618985	-0.113867
C	0.250616	0.619066	-0.113866
C	1.952866	-1.621751	-0.110383
C	2.485619	-0.203728	-0.107834
C	1.637659	0.889989	-0.111223
N	-0.545771	1.722704	-0.112825
N	0.545773	-1.722623	-0.112757

C	1.682726	2.360554	-0.110263
C	0.335709	2.832735	-0.110923
C	2.731358	3.277557	-0.110239
C	0.025824	4.184538	-0.110194
C	2.427073	4.639905	-0.109708
H	3.763770	2.925620	-0.111779
C	1.099482	5.079960	-0.109343
H	-1.013550	4.508503	-0.110554
H	3.235550	5.371439	-0.109838
H	0.892495	6.151160	-0.108819
C	-1.682723	-2.360474	-0.110288
C	-0.335707	-2.832654	-0.110899
C	-2.731355	-3.277477	-0.110316
C	-0.025821	-4.184457	-0.110167
C	-2.427070	-4.639825	-0.109787
H	-3.763766	-2.925540	-0.111908
C	-1.099479	-5.079880	-0.109372
H	1.013553	-4.508422	-0.110496
H	-3.235547	-5.371359	-0.109968
H	-0.892492	-6.151080	-0.108855
O	2.652221	-2.605999	-0.109869
O	-2.652222	2.606077	-0.109982
C	3.901079	-0.065468	-0.095944
C	5.109983	0.070973	-0.092354
C	-3.901077	0.065543	-0.096006
C	-5.109977	-0.070937	-0.092415
C	6.538235	0.233715	-0.028125
C	7.255038	0.329820	-1.167104
C	7.086785	0.370259	1.348047
H	6.699556	0.297288	-2.110196
C	8.703831	0.557478	-1.277142
C	8.052772	-0.376342	1.894152
H	6.573398	1.102383	1.979335
C	9.676698	-0.185615	-0.729918
H	9.001358	1.365382	-1.954392
C	8.799955	-1.469555	1.245978
H	8.282185	-0.207527	2.952074
H	10.710633	0.066605	-0.990056
C	9.507896	-1.383645	0.111793
H	8.833254	-2.413815	1.799605
H	10.082951	-2.262989	-0.197896
C	-6.538220	-0.233742	-0.028158
C	-7.255051	-0.329879	-1.167112
C	-7.086722	-0.370329	1.348032
H	-6.699607	-0.297306	-2.110224
C	-8.703833	-0.557629	-1.277099
C	-8.052732	0.376221	1.894175
H	-6.573275	-1.102436	1.979291
C	-9.676725	0.185406	-0.729842
H	-9.001344	-1.365547	-1.954340
C	-8.799990	1.469395	1.246020
H	-8.282107	0.207389	2.952103
H	-10.710653	-0.066866	-0.989955
C	-9.507966	1.383446	0.111860
H	-8.833317	2.413657	1.799645
H	-10.083078	2.262756	-0.197816

SCIBA12 T1

E = -1795.17899820 a.u.

C	-1.952865	1.621831	-0.110531
C	-2.485618	0.203806	-0.107898
C	-1.637657	-0.889909	-0.111251
C	-0.250614	-0.618985	-0.113867
C	0.250616	0.619066	-0.113866
C	1.952866	-1.621751	-0.110383
C	2.485619	-0.203728	-0.107834
C	1.637659	0.889989	-0.111223
N	-0.545771	1.722704	-0.112825
N	0.545773	-1.722623	-0.112757
C	1.682726	2.360554	-0.110263
C	0.335709	2.832735	-0.110923
C	2.731358	3.277557	-0.110239
C	0.025824	4.184538	-0.110194
C	2.427073	4.639905	-0.109708
H	3.763770	2.925620	-0.111779
C	1.099482	5.079960	-0.109343
H	-1.013550	4.508503	-0.110554
H	3.235550	5.371439	-0.109838
H	0.892495	6.151160	-0.108819
C	-1.682723	-2.360474	-0.110288
C	-0.335707	-2.832654	-0.110899
C	-2.731355	-3.277477	-0.110316
C	-0.025821	-4.184457	-0.110167
C	-2.427070	-4.639825	-0.109787
H	-3.763766	-2.925540	-0.111908
C	-1.099479	-5.079880	-0.109372
H	1.013553	-4.508422	-0.110496
H	-3.235547	-5.371359	-0.109968
H	-0.892492	-6.151080	-0.108855
O	2.652221	-2.605999	-0.109869
O	-2.652222	2.606077	-0.109982
C	3.901079	-0.065468	-0.095944
C	5.109983	0.070973	-0.092354
C	-3.901077	0.065543	-0.096006
C	-5.109977	-0.070937	-0.092415
C	6.538235	0.233715	-0.028125
C	7.255038	0.329820	-1.167104
C	7.086785	0.370259	1.348047
H	6.699556	0.297288	-2.110196
C	8.703831	0.557478	-1.277142
C	8.052772	-0.376342	1.894152
H	6.573398	1.102383	1.979335
C	9.676698	-0.185615	-0.729918
H	9.001358	1.365382	-1.954392
C	8.799955	-1.469555	1.245978
H	8.282185	-0.207527	2.952074
H	10.710633	0.066605	-0.990056
C	9.507896	-1.383645	0.111793
H	8.833254	-2.413815	1.799605

H	10.082951	-2.262989	-0.197896
C	-6.538220	-0.233742	-0.028158
C	-7.255051	-0.329879	-1.167112
C	-7.086722	-0.370329	1.348032
H	-6.699607	-0.297306	-2.110224
C	-8.703833	-0.557629	-1.277099
C	-8.052732	0.376221	1.894175
H	-6.573275	-1.102436	1.979291
C	-9.676725	0.185406	-0.729842
H	-9.001344	-1.365547	-1.954340
C	-8.799990	1.469395	1.246020
H	-8.282107	0.207389	2.952103
H	-10.710653	-0.066866	-0.989955
C	-9.507966	1.383446	0.111860
H	-8.833317	2.413657	1.799645
H	-10.083078	2.262756	-0.197816

SCIBA13 BS-S0

E = -1333.68300099 a.u.

C	1.109794	-2.277548	-0.002162
C	2.224366	-1.233209	-0.001034
C	1.857410	0.191967	-0.000995
C	0.518937	0.467071	-0.000251
C	-0.518893	-0.467023	-0.000216
C	-1.109764	2.277595	0.001250
C	-2.224336	1.233246	0.001225
C	-1.857363	-0.191917	0.000503
N	-0.211996	-1.799450	-0.001236
N	0.212028	1.799496	0.000376
C	-2.483978	-1.518359	0.000014
C	-1.432042	-2.486283	-0.001181
C	-3.800918	-1.998948	0.000510
C	-1.659509	-3.861293	-0.001996
C	-4.037748	-3.368322	-0.000258
H	-4.643916	-1.317681	0.001597
C	-2.981911	-4.290002	-0.001529
H	-0.820623	-4.552955	-0.002933
H	-5.066609	-3.730076	0.000151
H	-3.197928	-5.359020	-0.002136
C	2.484013	1.518422	-0.001306
C	1.432066	2.486337	-0.000171
C	3.800942	1.999043	-0.002875
C	1.659508	3.861350	-0.000017
C	4.037750	3.368421	-0.002800
H	4.643953	1.317801	-0.004521
C	2.981900	4.290084	-0.001266
H	0.820609	4.552997	0.000938
H	5.066603	3.730192	-0.004052
H	3.197899	5.359106	-0.001225
O	-1.306334	3.468316	0.002210
O	1.306385	-3.468266	-0.003371
C	-3.477191	1.761143	0.001368
C	-4.887546	1.293566	0.000901
C	-4.020290	3.145559	0.001991
C	-5.325480	2.630235	0.001365
H	-5.402073	0.341045	0.000142
H	-3.565038	4.128515	0.002593
H	-6.313544	3.089658	0.001308
C	3.477178	-1.761202	0.000928
C	4.020111	-3.145680	0.001143
C	4.887586	-1.293794	0.004270
C	5.325360	-2.630515	0.004403
H	3.564738	-4.128580	-0.000494
H	5.402231	-0.341343	0.006665
H	6.313365	-3.090058	0.006402

SCIBA13 T1

E = -1333.68290553 a.u.

C	1.109794	-2.277548	-0.002162
C	2.224366	-1.233209	-0.001034
C	1.857410	0.191967	-0.000995
C	0.518937	0.467071	-0.000251
C	-0.518893	-0.467023	-0.000216
C	-1.109764	2.277595	0.001250
C	-2.224336	1.233246	0.001225
C	-1.857363	-0.191917	0.000503
N	-0.211996	-1.799450	-0.001236
N	0.212028	1.799496	0.000376
C	-2.483978	-1.518359	0.000014
C	-1.432042	-2.486283	-0.001181
C	-3.800918	-1.998948	0.000510
C	-1.659509	-3.861293	-0.001996
C	-4.037748	-3.368322	-0.000258
H	-4.643916	-1.317681	0.001597
C	-2.981911	-4.290002	-0.001529
H	-0.820623	-4.552955	-0.002933
H	-5.066609	-3.730076	0.000151
H	-3.197928	-5.359020	-0.002136
C	2.484013	1.518422	-0.001306
C	1.432066	2.486337	-0.000171
C	3.800942	1.999043	-0.002875
C	1.659508	3.861350	-0.000017
C	4.037750	3.368421	-0.002800
H	4.643953	1.317801	-0.004521
C	2.981900	4.290084	-0.001266
H	0.820609	4.552997	0.000938
H	5.066603	3.730192	-0.004052
H	3.197899	5.359106	-0.001225
O	-1.306334	3.468316	0.002210
O	1.306385	-3.468266	-0.003371
C	-3.477191	1.761143	0.001368
C	-4.887546	1.293566	0.000901
C	-4.020290	3.145559	0.001991
C	-5.325480	2.630235	0.001365
H	-5.402073	0.341045	0.000142
H	-3.565038	4.128515	0.002593
H	-6.313544	3.089658	0.001308
C	3.477178	-1.761202	0.000928

C	4.020111	-3.145680	0.001143
C	4.887586	-1.293794	0.004270
C	5.325360	-2.630515	0.004403
H	3.564738	-4.128580	-0.000494
H	5.402231	-0.341343	0.006665
H	6.313365	-3.090058	0.006402

SCIBA14 S0

E = -1225.24019213 a.u.

C	2.421954	-0.744716	0.000000
C	2.339693	0.757227	-0.000000
C	1.168211	1.461990	-0.000000
C	-0.006037	0.666289	-0.000000
C	0.006037	-0.666289	-0.000000
C	-2.421954	0.744716	0.000000
C	-2.339693	-0.757227	-0.000000
C	-1.168211	-1.461990	-0.000000
N	1.168211	-1.380715	0.000000
N	-1.168211	1.380715	0.000000
C	-0.637189	-2.836484	0.000000
C	0.785875	-2.747303	0.000000
C	-1.247469	-4.086680	0.000000
C	1.596836	-3.872142	0.000000
C	-0.437979	-5.224407	0.000000
H	-2.334960	-4.164882	0.000000
C	0.955859	-5.114880	0.000000
H	2.680536	-3.766733	0.000000
H	-0.899282	-6.212246	0.000000
H	1.562886	-6.021203	0.000000
C	0.637189	2.836484	0.000000
C	-0.785875	2.747303	0.000000
C	1.247469	4.086680	0.000000
C	-1.596836	3.872142	0.000000
C	0.437979	5.224407	0.000000
H	2.334960	4.164882	0.000000
C	-0.955859	5.114880	0.000000
H	-2.680536	3.766733	0.000000
H	0.899282	6.212246	0.000000
H	-1.562886	6.021203	0.000000
O	-3.464897	1.353491	-0.000000
O	3.464897	-1.353491	-0.000000
F	3.518185	1.350592	-0.000000
F	-3.518185	-1.350592	-0.000000

SCIBA14 T1

E = -1225.19043729 a.u.

C	2.421954	-0.744716	0.000000
C	2.339693	0.757227	-0.000000
C	1.168211	1.461990	-0.000000
C	-0.006037	0.666289	-0.000000
C	0.006037	-0.666289	-0.000000
C	-2.421954	0.744716	0.000000
C	-2.339693	-0.757227	-0.000000
C	-1.168211	-1.461990	-0.000000
N	1.168211	-1.380715	0.000000
N	-1.168211	1.380715	0.000000
C	-0.637189	-2.836484	0.000000
C	0.785875	-2.747303	0.000000
C	-1.247469	-4.086680	0.000000
C	1.596836	-3.872142	0.000000
C	-0.437979	-5.224407	0.000000
H	-2.334960	-4.164882	0.000000
C	0.955859	-5.114880	0.000000
H	2.680536	-3.766733	0.000000
H	-0.899282	-6.212246	0.000000
H	1.562886	-6.021203	0.000000
C	0.637189	2.836484	0.000000
C	-0.785875	2.747303	0.000000
C	1.247469	4.086680	0.000000
C	-1.596836	3.872142	0.000000
C	0.437979	5.224407	0.000000
H	2.334960	4.164882	0.000000
C	-0.955859	5.114880	0.000000
H	-2.680536	3.766733	0.000000
H	0.899282	6.212246	0.000000
H	-1.562886	6.021203	0.000000
O	-3.464897	1.353491	-0.000000
O	3.464897	-1.353491	-0.000000
F	3.518185	1.350592	-0.000000
F	-3.518185	-1.350592	-0.000000

SCIBA15 S0

E = -1827.48928761 a.u.

C	-2.121986	1.379235	-0.001722
C	-2.518173	-0.081642	-0.004677
C	-1.531366	-1.066886	-0.003398
C	-0.187501	-0.641930	-0.005510
C	0.187501	0.641930	-0.005510
C	2.121986	-1.379235	-0.001722
C	2.518173	0.081642	-0.004677
C	1.531366	1.066886	-0.003398
N	-0.737325	1.638538	-0.003860
N	0.737325	-1.638538	-0.003860
C	1.395693	2.540011	0.001604
C	-0.002514	2.843666	0.000373
C	2.305154	3.599007	0.010502
C	-0.491440	4.139735	0.004747
C	1.833841	4.909176	0.014939
H	3.379070	3.421315	0.015963
C	0.455465	5.174886	0.011547
H	-1.562949	4.329882	0.003577
H	2.535187	5.742972	0.021996
C	-1.395693	-2.540011	0.001604
C	0.002514	-2.843666	0.000373
C	-2.305154	-3.599007	0.010502
C	0.491440	-4.139735	0.004747
C	-1.833841	-4.909176	0.014939

H	-3.379070	-3.421315	0.015963
C	-0.455465	-5.174886	0.011547
H	1.562949	-4.329882	0.003577
H	-2.535187	-5.742972	0.021996
O	2.903485	-2.306558	0.002241
O	-2.903485	2.306558	0.002241
C	3.920016	0.445537	-0.012805
C	5.004696	-0.363585	0.004990
H	4.088431	1.522696	-0.033030
H	4.857608	-1.442137	0.037791
C	-3.920016	-0.445537	-0.012805
C	-5.004696	0.363585	0.004990
H	-4.088431	-1.522696	-0.033030
H	-4.857608	1.442137	0.037791
C	-6.397021	-0.095332	-0.007690
C	-7.412963	0.867920	0.106673
C	-6.773892	-1.445013	-0.129104
C	-8.755961	0.500837	0.109290
H	-7.134427	1.919780	0.197156
C	-8.113656	-1.812471	-0.127792
H	-6.013543	-2.220304	-0.234257
C	-9.111297	-0.841603	-0.006946
H	-9.527745	1.266183	0.201428
H	-8.386127	-2.864391	-0.224754
H	-10.162217	-1.134034	-0.006825
C	6.397021	0.095332	-0.007690
C	7.412963	-0.867920	0.106673
C	6.773892	1.445013	-0.129104
C	8.755961	-0.500837	0.109290
H	7.134427	-1.919780	0.197156
C	8.113656	1.812471	-0.127792
H	6.013543	2.220304	-0.234257
C	9.111297	0.841603	-0.006946
H	9.527745	-1.266183	0.201428
H	8.386127	2.864391	-0.224754
H	10.162217	1.134034	-0.006825
C	0.002514	6.543970	0.016514
N	-0.352756	7.642381	0.020120
C	-0.002514	-6.543970	0.016514
N	0.352756	-7.642381	0.020120

SCIBA15 T1

E = -1827.46034978 a.u.

C	-2.121986	1.379235	-0.001722
C	-2.518173	-0.081642	-0.004677
C	-1.531366	-1.066886	-0.003398
C	-0.187501	-0.641930	-0.005510
C	0.187501	0.641930	-0.005510
C	2.121986	-1.379235	-0.001722
C	2.518173	0.081642	-0.004677
C	1.531366	1.066886	-0.003398
N	-0.737325	1.638538	-0.003860
N	0.737325	-1.638538	-0.003860
C	1.395693	2.540011	0.001604
C	-0.002514	2.843666	0.000373
C	2.305154	3.599007	0.010502
C	-0.491440	4.139735	0.004747
C	1.833841	4.909176	0.014939
H	3.379070	3.421315	0.015963
C	0.455465	5.174886	0.011547
H	-1.562949	4.329882	0.003577
H	2.535187	5.742972	0.021996
C	-1.395693	-2.540011	0.001604
C	0.002514	-2.843666	0.000373
C	-2.305154	-3.599007	0.010502
C	0.491440	-4.139735	0.004747
C	-1.833841	-4.909176	0.014939
H	-3.379070	-3.421315	0.015963
C	-0.455465	-5.174886	0.011547
H	1.562949	-4.329882	0.003577
H	-2.535187	-5.742972	0.021996
O	2.903485	-2.306558	0.002241
O	-2.903485	2.306558	0.002241
C	3.920016	0.445537	-0.012805
C	5.004696	-0.363585	0.004990
H	4.088431	1.522696	-0.033030
H	4.857608	-1.442137	0.037791
C	-3.920016	-0.445537	-0.012805
C	-5.004696	0.363585	0.004990
H	-4.088431	-1.522696	-0.033030
H	-4.857608	1.442137	0.037791
C	-6.397021	-0.095332	-0.007690
C	-7.412963	0.867920	0.106673
C	-6.773892	-1.445013	-0.129104
C	-8.755961	0.500837	0.109290
H	-7.134427	1.919780	0.197156
C	-8.113656	-1.812471	-0.127792
H	-6.013543	-2.220304	-0.234257
C	-9.111297	-0.841603	-0.006946
H	-9.527745	1.266183	0.201428
H	-8.386127	-2.864391	-0.224754
H	-10.162217	-1.134034	-0.006825
C	6.397021	0.095332	-0.007690
C	7.412963	-0.867920	0.106673
C	6.773892	1.445013	-0.129104
C	8.755961	-0.500837	0.109290
H	7.134427	-1.919780	0.197156
C	8.113656	1.812471	-0.127792
H	6.013543	2.220304	-0.234257
C	9.111297	0.841603	-0.006946
H	9.527745	-1.266183	0.201428
H	8.386127	2.864391	-0.224754
H	10.162217	1.134034	-0.006825
C	0.002514	6.543970	0.016514
N	-0.352756	7.642381	0.020120
C	-0.002514	-6.543970	0.016514
N	0.352756	-7.642381	0.020120

SCIBA16 S0

E = -1550.18102691 a.u.

C	2.438849	0.670664	0.000035
C	2.364972	-0.838768	0.000021
C	1.133612	-1.485311	0.000034
C	-0.019815	-0.668814	0.000060
C	0.019815	0.668814	0.000060
C	-2.438849	-0.670664	0.000035
C	-2.364972	0.838768	0.000021
C	-1.133612	1.485311	0.000034
N	1.199907	1.339929	0.000055
N	-1.199907	-1.339929	0.000055
C	-0.558477	2.848474	0.000017
C	0.864316	2.713180	0.000035
C	-1.107279	4.131929	0.000002
C	1.723744	3.798786	0.000038
C	-0.260482	5.237193	0.000008
H	-2.184443	4.290473	-0.000007
C	1.133612	5.071754	0.000027
H	2.802975	3.657973	0.000052
H	-0.676515	6.244147	-0.000000
C	0.558477	-2.848474	0.000017
C	-0.864316	-2.713180	0.000035
C	1.107279	-4.131929	0.000002
C	-1.723744	-3.798786	0.000038
C	0.260482	-5.237193	0.000008
H	2.184443	-4.290473	-0.000007
C	-1.133612	-5.071754	0.000027
H	-2.802975	-3.657973	0.000052
H	0.676515	-6.244147	-0.000000
O	-3.469891	-1.305836	0.000035
O	3.469891	1.305836	0.000035
C	-3.596413	1.606980	-0.000031
C	-4.867758	1.150275	-0.000050
H	-3.458484	2.689084	-0.000062
H	-5.103448	0.087337	-0.000026
C	3.596413	-1.606980	-0.000031
C	4.867758	-1.150275	-0.000050
H	3.458484	-2.689084	-0.000062
H	5.103448	-0.087337	-0.000026
C	-5.958245	2.080802	-0.000114
N	-6.839548	2.828544	-0.000220
C	5.958245	-2.080802	-0.000114
N	6.839548	-2.828544	-0.000220
C	-1.981256	-6.238492	0.000032
N	-2.655238	-7.175404	0.000034
C	1.981256	6.238492	0.000032
N	2.655238	7.175404	0.000034

SCIBA16 T1

E = -1550.14565723 a.u.

C	2.438849	0.670664	0.000035
C	2.364972	-0.838768	0.000021
C	1.133612	-1.485311	0.000034
C	-0.019815	-0.668814	0.000060
C	0.019815	0.668814	0.000060
C	-2.438849	-0.670664	0.000035
C	-2.364972	0.838768	0.000021
C	-1.133612	1.485311	0.000034
N	1.199907	1.339929	0.000055
N	-1.199907	-1.339929	0.000055
C	-0.558477	2.848474	0.000017
C	0.864316	2.713180	0.000035
C	-1.107279	4.131929	0.000002
C	1.723744	3.798786	0.000038
C	-0.260482	5.237193	0.000008
H	-2.184443	4.290473	-0.000007
C	1.133612	5.071754	0.000027
H	2.802975	3.657973	0.000052
H	-0.676515	6.244147	-0.000000
C	0.558477	-2.848474	0.000017
C	-0.864316	-2.713180	0.000035
C	1.107279	-4.131929	0.000002
C	-1.723744	-3.798786	0.000038
C	0.260482	-5.237193	0.000008
H	2.184443	-4.290473	-0.000007
C	-1.133612	-5.071754	0.000027
H	-2.802975	-3.657973	0.000052
H	0.676515	-6.244147	-0.000000
O	-3.469891	-1.305836	0.000035
O	3.469891	1.305836	0.000035
C	-3.596413	1.606980	-0.000031
C	-4.867758	1.150275	-0.000050
H	-3.458484	2.689084	-0.000062
H	-5.103448	0.087337	-0.000026
C	3.596413	-1.606980	-0.000031
C	4.867758	-1.150275	-0.000050
H	3.458484	-2.689084	-0.000062
H	5.103448	-0.087337	-0.000026
C	-5.958245	2.080802	-0.000114
N	-6.839548	2.828544	-0.000220
C	5.958245	-2.080802	-0.000114
N	6.839548	-2.828544	-0.000220
C	-1.981256	-6.238492	0.000032
N	-2.655238	-7.175404	0.000034
C	1.981256	6.238492	0.000032
N	2.655238	7.175404	0.000034

SCIBA17 S0

E = -1774.43353212 a.u.

C	2.256825	-1.143293	-0.000050
C	1.183789	-2.205190	-0.000048
C	-0.161366	-1.860731	-0.000054
C	-0.466265	-0.480035	-0.000055
C	0.466265	0.480035	-0.000055
C	-2.256825	1.143293	-0.000050
C	-1.183789	2.205190	-0.000048
C	0.161366	1.860731	-0.000054

N	1.791528	0.186098	-0.000040
N	-1.791528	-0.186098	-0.000040
C	1.500511	2.485597	-0.000041
C	2.464323	1.430650	-0.000016
C	1.949022	3.807247	-0.000048
C	3.829362	1.660458	0.000004
C	3.318522	4.059183	-0.000019
H	1.254005	4.646148	-0.000080
C	4.242448	3.001749	0.000009
H	4.537096	0.833304	0.000011
H	3.685004	5.085194	-0.000021
C	-1.500511	-2.485597	-0.000041
C	-2.464323	-1.430650	-0.000016
C	-1.949022	-3.807247	-0.000048
C	-3.829362	-1.660458	0.000004
C	-3.318522	-4.059183	-0.000019
H	-1.254005	-4.646148	-0.000080
C	-4.242448	-3.001749	0.000009
H	-4.537096	-0.833304	0.000011
H	-3.685004	-5.085194	-0.000021
O	-3.443698	1.377721	-0.000084
O	3.443698	-1.377721	-0.000084
C	-1.580919	3.598914	-0.000015
C	-2.816390	4.115078	0.000029
H	-0.775473	4.334149	0.000004
H	-3.769845	3.597636	0.000068
C	1.580919	-3.598914	-0.000015
C	2.816390	-4.115078	0.000029
H	0.775473	-4.334149	0.000004
H	3.769845	-3.597636	0.000068
N	2.948834	-5.576638	0.000081
O	4.081072	-5.993994	0.000203
O	1.949022	-6.258345	0.000008
N	-2.948834	5.576638	0.000081
O	-4.081072	5.993994	0.000203
O	-1.949022	6.258345	0.000008
C	5.653337	3.300686	0.000031
N	6.781247	3.545176	0.000050
C	-5.653337	-3.300686	0.000031
N	-6.781247	-3.545176	0.000050

SCIBA17 T1

E = -1774.39524054 a.u.

C	2.256825	-1.143293	-0.000050
C	1.183789	-2.205190	-0.000048
C	-0.161366	-1.860731	-0.000054
C	-0.466265	-0.480035	-0.000055
C	0.466265	0.480035	-0.000055
C	-2.256825	1.143293	-0.000050
C	-1.183789	2.205190	-0.000048
C	0.161366	1.860731	-0.000054
N	1.791528	0.186098	-0.000040
N	-1.791528	-0.186098	-0.000040
C	1.500511	2.485597	-0.000041
C	2.464323	1.430650	-0.000016
C	1.949022	3.807247	-0.000048
C	3.829362	1.660458	0.000004
C	3.318522	4.059183	-0.000019
H	1.254005	4.646148	-0.000080
C	4.242448	3.001749	0.000009
H	4.537096	0.833304	0.000011
H	3.685004	5.085194	-0.000021
C	-1.500511	-2.485597	-0.000041
C	-2.464323	-1.430650	-0.000016
C	-1.949022	-3.807247	-0.000048
C	-3.829362	-1.660458	0.000004
C	-3.318522	-4.059183	-0.000019
H	-1.254005	-4.646148	-0.000080
C	-4.242448	-3.001749	0.000009
H	-4.537096	-0.833304	0.000011
H	-3.685004	-5.085194	-0.000021
O	-3.443698	1.377721	-0.000084
O	3.443698	-1.377721	-0.000084
C	-1.580919	3.598914	-0.000015
C	-2.816390	4.115078	0.000029
H	-0.775473	4.334149	0.000004
H	-3.769845	3.597636	0.000068
C	1.580919	-3.598914	-0.000015
C	2.816390	-4.115078	0.000029
H	0.775473	-4.334149	0.000004
H	3.769845	-3.597636	0.000068
N	2.948834	-5.576638	0.000081
O	4.081072	-5.993994	0.000203
O	1.949022	-6.258345	0.000008
N	-2.948834	5.576638	0.000081
O	-4.081072	5.993994	0.000203
O	-1.949022	6.258345	0.000008
C	5.653337	3.300686	0.000031
N	6.781247	3.545176	0.000050
C	-5.653337	-3.300686	0.000031
N	-6.781247	-3.545176	0.000050

SCIBA18 S0

E = -1981.98836553 a.u.

C	1.193191	2.232891	-0.224296
C	-0.295661	2.500032	-0.233107
C	-1.193191	1.433169	-0.228459
C	-0.655920	0.131081	-0.232345
C	0.655920	-0.131081	-0.232345
C	-1.193191	-2.232891	-0.224296
C	0.295661	-2.500032	-0.233107
C	1.193191	-1.433169	-0.228459
N	1.570780	0.875103	-0.228539
N	-1.570780	-0.875103	-0.228539
C	2.648824	-1.175114	-0.214804
C	2.833615	0.243947	-0.217790
C	3.778559	-1.995087	-0.190220
C	4.084325	0.839036	-0.206176

C	5.044535	-1.414971	-0.178442
H	3.689189	-3.080548	-0.173260
C	5.194390	-0.019127	-0.188260
H	4.185018	1.922676	-0.209026
H	5.934207	-2.043730	-0.159257
C	-2.648824	1.175114	-0.214804
C	-2.833615	-0.243947	-0.217790
C	-3.778559	1.995087	-0.190220
C	-4.084325	-0.839036	-0.206176
C	-5.044535	1.414971	-0.178442
H	-3.689189	3.080548	-0.173260
C	-5.194390	0.019127	-0.188260
H	-4.185018	-1.922676	-0.209026
H	-5.934207	2.043730	-0.159257
O	-2.047768	-3.093311	-0.215391
O	2.047768	3.093311	-0.215391
C	0.780549	-3.862493	-0.259242
C	0.079125	-5.020521	-0.193921
H	1.866165	-3.944252	-0.328144
H	-1.005370	-4.995114	-0.095492
C	-0.780549	3.862493	-0.259242
C	-0.079125	5.020521	-0.193921
H	-1.866165	3.944252	-0.328144
H	1.005370	4.995114	-0.095492
C	-0.714104	6.336007	-0.228992
C	0.062230	7.430324	-0.053767
C	-2.159961	6.404276	-0.567564
H	1.138939	7.260463	0.063450
C	-0.356344	8.835939	-0.055798
C	-3.132696	6.950478	0.170019
H	-2.440061	5.905197	-1.502327
C	-1.321695	9.388563	0.697006
H	0.262410	9.511515	-0.656213
C	-2.966948	7.643575	1.460840
H	-4.162837	6.860896	-0.193593
H	-1.431490	10.477356	0.650828
C	-2.185170	8.710190	1.678817
H	-3.612035	7.305327	2.278479
H	-2.235127	9.184194	2.665040
C	0.714104	-6.336007	-0.228992
C	-0.062230	-7.430324	-0.053767
C	2.159961	-6.404276	-0.567564
H	-1.138939	-7.260463	0.063450
C	0.356344	-8.835939	-0.055798
C	3.132696	-6.950478	0.170019
H	2.440061	-5.905197	-1.502327
C	1.321695	-9.388563	0.697006
H	-0.262410	-9.511515	-0.656213
C	2.966948	-7.643575	1.460840
H	4.162837	-6.860896	-0.193593
H	1.431490	-10.477356	0.650828
C	2.185170	-8.710190	1.678817
H	3.612035	-7.305327	2.278479
H	2.235127	-9.184194	2.665040
C	6.521182	0.545759	-0.175927
N	7.586376	0.990859	-0.166143
C	-6.521182	-0.545759	-0.175927
N	-7.586376	-0.990859	-0.166143

SCIBA18 T1

E = -1981.96166205 a.u.

C	1.193191	2.232891	-0.224296
C	-0.295661	2.500032	-0.233107
C	-1.193191	1.433169	-0.228459
C	-0.655920	0.131081	-0.232345
C	0.655920	-0.131081	-0.232345
C	-1.193191	-2.232891	-0.224296
C	0.295661	-2.500032	-0.233107
C	1.193191	-1.433169	-0.228459
N	1.570780	0.875103	-0.228539
N	-1.570780	-0.875103	-0.228539
C	2.648824	-1.175114	-0.214804
C	2.833615	0.243947	-0.217790
C	3.778559	-1.995087	-0.190220
C	4.084325	0.839036	-0.206176
C	5.044535	-1.414971	-0.178442
H	3.689189	-3.080548	-0.173260
C	5.194390	-0.019127	-0.188260
H	4.185018	1.922676	-0.209026
H	5.934207	-2.043730	-0.159257
C	-2.648824	1.175114	-0.214804
C	-2.833615	-0.243947	-0.217790
C	-3.778559	1.995087	-0.190220
C	-4.084325	-0.839036	-0.206176
C	-5.044535	1.414971	-0.178442
H	-3.689189	3.080548	-0.173260
C	-5.194390	0.019127	-0.188260
H	-4.185018	-1.922676	-0.209026
H	-5.934207	2.043730	-0.159257
O	-2.047768	-3.093311	-0.215391
O	2.047768	3.093311	-0.215391
C	0.780549	-3.862493	-0.259242
C	0.079125	-5.020521	-0.193921
H	1.866165	-3.944252	-0.328144
H	-1.005370	-4.995114	-0.095492
C	-0.780549	3.862493	-0.259242
C	-0.079125	5.020521	-0.193921
H	-1.866165	3.944252	-0.328144
H	1.005370	4.995114	-0.095492
C	-0.714104	6.336007	-0.228992
C	0.062230	7.430324	-0.053767
C	-2.159961	6.404276	-0.567564
H	1.138939	7.260463	0.063450
C	-0.356344	8.835939	-0.055798
C	-3.132696	6.950478	0.170019
H	-2.440061	5.905197	-1.502327
C	-1.321695	9.388563	0.697006
H	0.262410	9.511515	-0.656213
C	-2.966948	7.643575	1.460840

H	-4.162837	6.860896	-0.193593
H	-1.431490	10.477356	0.650828
C	-2.185170	8.710190	1.678817
H	-3.612035	7.305327	2.278479
H	-2.235127	9.184194	2.665040
C	0.714104	-6.336007	-0.228992
C	-0.062230	-7.430324	-0.053767
C	2.159961	-6.404276	-0.567564
H	-1.138939	-7.260463	0.063450
C	0.356344	-8.835939	-0.055798
C	3.132696	-6.950478	0.170019
H	2.440061	-5.905197	-1.502327
C	1.321695	-9.388563	0.697006
H	-0.262410	-9.511515	-0.656213
C	2.966948	-7.643575	1.460840
H	4.162837	-6.860896	-0.193593
H	1.431490	-10.477356	0.650828
C	2.185170	-8.710190	1.678817
H	3.612035	-7.305327	2.278479
H	2.235127	-9.184194	2.665040
C	6.521182	0.545759	-0.175927
N	7.586376	0.990859	-0.166143
C	-6.521182	-0.545759	-0.175927
N	-7.586376	-0.990859	-0.166143

SCIBA19 S0

E = -1547.68446020 a.u.

C	-0.229009	2.530972	-0.001404
C	1.239683	2.157948	-0.001318
C	1.664912	0.839714	-0.001895
C	0.652475	-0.147132	-0.002834
C	-0.652475	0.147132	-0.002790
C	0.229010	-2.530973	-0.001602
C	-1.239682	-2.157949	-0.001410
C	-1.664912	-0.839714	-0.001868
N	-1.109660	1.427262	-0.002192
N	1.109660	-1.427262	-0.002354
C	-2.899578	-0.043994	-0.000890
C	-2.522498	1.333003	-0.001019
C	-4.249527	-0.389691	0.000214
C	-3.453812	2.356747	0.000002
C	-5.200669	0.626998	0.001226
H	-4.552912	-1.436948	0.000295
C	-4.805889	1.975837	0.001160
H	-3.142945	3.400504	-0.000042
H	-6.263410	0.386450	0.002111
C	2.899578	0.043993	-0.001041
C	2.522498	-1.333003	-0.001251
C	4.249527	0.389690	0.000013
C	3.453813	-2.356747	-0.000359
C	5.200670	-0.626998	0.000896
H	4.552912	1.436948	0.000155
C	4.805889	-1.975837	0.000750
H	3.142945	-3.400504	-0.000466
H	6.263410	-0.386451	0.001739
O	0.636683	-3.663304	-0.000991
O	-0.636683	3.663303	-0.000689
C	-2.152190	-3.242886	-0.000298
C	-2.952051	-4.158012	0.000655
C	2.152190	3.242886	-0.000170
C	2.952052	4.158011	0.000793
C	-3.868533	-5.195929	0.001747
N	-4.644354	-6.054503	0.002700
C	3.868532	5.195930	0.001839
N	4.644349	6.054507	0.002757
C	5.819563	-3.001944	0.001826
N	6.634562	-3.819089	0.002742
C	-5.819562	3.001944	0.002383
N	-6.634561	3.819088	0.003421

SCIBA19 T1

E = -1547.64637756 a.u.

C	-0.229009	2.530972	-0.001404
C	1.239683	2.157948	-0.001318
C	1.664912	0.839714	-0.001895
C	0.652475	-0.147132	-0.002834
C	-0.652475	0.147132	-0.002790
C	0.229010	-2.530973	-0.001602
C	-1.239682	-2.157949	-0.001410
C	-1.664912	-0.839714	-0.001868
N	-1.109660	1.427262	-0.002192
N	1.109660	-1.427262	-0.002354
C	-2.899578	-0.043994	-0.000890
C	-2.522498	1.333003	-0.001019
C	-4.249527	-0.389691	0.000214
C	-3.453812	2.356747	0.000002
C	-5.200669	0.626998	0.001226
H	-4.552912	-1.436948	0.000295
C	-4.805889	1.975837	0.001160
H	-3.142945	3.400504	-0.000042
H	-6.263410	0.386450	0.002111
C	2.899578	0.043993	-0.001041
C	2.522498	-1.333003	-0.001251
C	4.249527	0.389690	0.000013
C	3.453813	-2.356747	-0.000359
C	5.200670	-0.626998	0.000896
H	4.552912	1.436948	0.000155
C	4.805889	-1.975837	0.000750
H	3.142945	-3.400504	-0.000466
H	6.263410	-0.386451	0.001739
O	0.636683	-3.663304	-0.000991
O	-0.636683	3.663303	-0.000689
C	-2.152190	-3.242886	-0.000298
C	-2.952051	-4.158012	0.000655
C	2.152190	3.242886	-0.000170
C	2.952052	4.158011	0.000793
C	-3.868533	-5.195929	0.001747
N	-4.644354	-6.054503	0.002700

C	3.868532	5.195930	0.001839
N	4.644349	6.054507	0.002757
C	5.819563	-3.001944	0.001826
N	6.634562	-3.819089	0.002742
C	-5.819562	3.001944	0.002383
N	-6.634561	3.819088	0.003421

SCIBA20 S0

E = -1771.88285777 a.u.

C	0.560914	-2.481790	-0.000370
C	1.837976	-1.670974	-0.000316
C	1.839558	-0.286175	-0.000345
C	0.574061	0.343068	-0.000538
C	-0.574078	-0.343105	-0.000546
C	-0.560929	2.481752	-0.000337
C	-1.837994	1.670938	-0.000308
C	-1.839576	0.286138	-0.000350
N	-0.618348	-1.701003	-0.000464
N	0.618332	1.700966	-0.000431
C	-2.774734	-0.845163	-0.000139
C	-1.994208	-2.041532	-0.000219
C	-4.167123	-0.923729	0.000177
C	-2.568618	-3.300016	-0.000027
C	-4.760661	-2.183516	0.000374
H	-4.780613	-0.020864	0.000306
C	-3.972763	-3.347737	0.000266
H	-1.955285	-4.200017	-0.000086
H	-5.846138	-2.277662	0.000626
C	2.774718	0.845122	-0.000113
C	1.994194	2.041493	-0.000174
C	4.167109	0.923683	0.000203
C	2.568607	3.299975	0.000046
C	4.760648	2.183470	0.000428
H	4.780600	0.020817	0.000307
C	3.972753	3.347693	0.000346
H	1.955276	4.199978	0.000003
H	5.846126	2.277614	0.000682
O	-0.523120	3.683906	-0.000238
O	0.523105	-3.683944	-0.000285
C	-3.067502	2.378016	-0.000168
C	-4.174315	2.865426	-0.000062
C	3.067491	-2.378038	-0.000159
C	4.174330	-2.865388	-0.000043
N	5.511714	-3.309622	0.000122
O	6.349829	-2.435062	0.001357
O	5.707337	-4.496633	-0.001042
N	-5.511669	3.309754	0.000098
O	-6.349847	2.435255	0.001489
O	-5.707207	4.496778	-0.001248
C	-4.625925	-4.633720	0.000485
N	-5.154058	-5.659846	0.000666
C	4.625917	4.633674	0.000600
N	5.154052	5.659799	0.000814

SCIBA20 T1

E = -1771.84283701 a.u.

C	0.560914	-2.481790	-0.000370
C	1.837976	-1.670974	-0.000316
C	1.839558	-0.286175	-0.000345
C	0.574061	0.343068	-0.000538
C	-0.574078	-0.343105	-0.000546
C	-0.560929	2.481752	-0.000337
C	-1.837994	1.670938	-0.000308
C	-1.839576	0.286138	-0.000350
N	-0.618348	-1.701003	-0.000464
N	0.618332	1.700966	-0.000431
C	-2.774734	-0.845163	-0.000139
C	-1.994208	-2.041532	-0.000219
C	-4.167123	-0.923729	0.000177
C	-2.568618	-3.300016	-0.000027
C	-4.760661	-2.183516	0.000374
H	-4.780613	-0.020864	0.000306
C	-3.972763	-3.347737	0.000266
H	-1.955285	-4.200017	-0.000086
H	-5.846138	-2.277662	0.000626
C	2.774718	0.845122	-0.000113
C	1.994194	2.041493	-0.000174
C	4.167109	0.923683	0.000203
C	2.568607	3.299975	0.000046
C	4.760648	2.183470	0.000428
H	4.780600	0.020817	0.000307
C	3.972753	3.347693	0.000346
H	1.955276	4.199978	0.000003
H	5.846126	2.277614	0.000682
O	-0.523120	3.683906	-0.000238
O	0.523105	-3.683944	-0.000285
C	-3.067502	2.378016	-0.000168
C	-4.174315	2.865426	-0.000062
C	3.067491	-2.378038	-0.000159
C	4.174330	-2.865388	-0.000043
N	5.511714	-3.309622	0.000122
O	6.349829	-2.435062	0.001357
O	5.707337	-4.496633	-0.001042
N	-5.511669	3.309754	0.000098
O	-6.349847	2.435255	0.001489
O	-5.707207	4.496778	-0.001248
C	-4.625925	-4.633720	0.000485
N	-5.154058	-5.659846	0.000666
C	4.625917	4.633674	0.000600
N	5.154052	5.659799	0.000814

SCIBA21 S0

E = -1979.49031106 a.u.

C	-1.916843	1.667909	-0.103873
C	-2.483841	0.261822	-0.100789
C	-1.658067	-0.848691	-0.105058
C	-0.266160	-0.612388	-0.108679

C	0.266170	0.612494	-0.108675
C	1.916854	-1.667803	-0.104004
C	2.483851	-0.261716	-0.100783
C	1.658077	0.848797	-0.105063
N	-0.505080	1.734193	-0.107034
N	0.505090	-1.734088	-0.107084
C	1.737291	2.317956	-0.103294
C	0.400058	2.820887	-0.104106
C	2.808489	3.207775	-0.102333
C	0.118768	4.176652	-0.102443
C	2.543699	4.575515	-0.100917
H	3.832426	2.832867	-0.103742
C	1.220401	5.047944	-0.100573
H	-0.909323	4.535336	-0.102817
H	3.362399	5.294573	-0.100227
C	-1.737281	-2.317850	-0.103284
C	-0.400048	-2.820781	-0.104107
C	-2.808479	-3.207670	-0.102304
C	-0.118758	-4.176547	-0.102447
C	-2.543689	-4.575409	-0.100883
H	-3.832416	-2.832761	-0.103701
C	-1.220390	-5.047839	-0.100554
H	0.909333	-4.535231	-0.102846
H	-3.362389	-5.294467	-0.100178
O	2.588441	-2.669141	-0.102394
O	-2.588431	2.669247	-0.102563
C	3.900370	-0.153961	-0.086772
C	5.111993	-0.041322	-0.080414
C	-3.900361	0.154068	-0.086806
C	-5.111982	0.041418	-0.080462
C	6.542897	0.094500	-0.013780
C	7.259343	0.186629	-1.153307
C	7.093434	0.209086	1.363688
H	6.703053	0.171362	-2.096477
C	8.712156	0.386076	-1.262006
C	8.043537	-0.562856	1.902225
H	6.598170	0.948347	2.001077
C	9.668180	-0.383162	-0.721416
H	9.025967	1.192823	-1.933018
C	8.766171	-1.666320	1.243821
H	8.278826	-0.406443	2.960707
H	10.707254	-0.151177	-0.979662
C	9.473972	-1.585120	0.109211
H	8.781279	-2.615255	1.789976
H	10.030775	-2.473050	-0.208848
C	-6.542873	-0.094540	-0.013816
C	-7.259325	-0.186674	-1.153339
C	-7.093383	-0.209241	1.363653
H	-6.703049	-0.171312	-2.096515
C	-8.712123	-0.386241	-1.262030
C	-8.043546	0.562591	1.902239
H	-6.598047	-0.948491	2.000999
C	-9.668207	0.382887	-0.721390
H	-9.025872	-1.192982	-1.933079
C	-8.766284	1.666025	1.243900
H	-8.278808	0.406105	2.960716
H	-10.707264	0.150826	-0.979635
C	-9.474092	1.584821	0.109295
H	-8.781468	2.614932	1.790103
H	-10.030976	2.472719	-0.208713
C	0.986870	6.471404	-0.098740
N	0.808666	7.611883	-0.097211
C	-0.986860	-6.471298	-0.098720
N	-0.808656	-7.611777	-0.097191

SCIBA21 T1

E = -1979.46403301 a.u.

C	-1.916843	1.667909	-0.103873
C	-2.483841	0.261822	-0.100789
C	-1.658067	-0.848691	-0.105058
C	-0.266160	-0.612388	-0.108679
C	0.266170	0.612494	-0.108675
C	1.916854	-1.667803	-0.104004
C	2.483851	-0.261716	-0.100783
C	1.658077	0.848797	-0.105063
N	-0.505080	1.734193	-0.107034
N	0.505090	-1.734088	-0.107084
C	1.737291	2.317956	-0.103294
C	0.400058	2.820887	-0.104106
C	2.808489	3.207775	-0.102333
C	0.118768	4.176652	-0.102443
C	2.543699	4.575515	-0.100917
H	3.832426	2.832867	-0.103742
C	1.220401	5.047944	-0.100573
H	-0.909323	4.535336	-0.102817
H	3.362399	5.294573	-0.100227
C	-1.737281	-2.317850	-0.103284
C	-0.400048	-2.820781	-0.104107
C	-2.808479	-3.207670	-0.102304
C	-0.118758	-4.176547	-0.102447
C	-2.543689	-4.575409	-0.100883
H	-3.832416	-2.832761	-0.103701
C	-1.220390	-5.047839	-0.100554
H	0.909333	-4.535231	-0.102846
H	-3.362389	-5.294467	-0.100178
O	2.588441	-2.669141	-0.102394
O	-2.588431	2.669247	-0.102563
C	3.900370	-0.153961	-0.086772
C	5.111993	-0.041322	-0.080414
C	-3.900361	0.154068	-0.086806
C	-5.111982	0.041418	-0.080462
C	6.542897	0.094500	-0.013780
C	7.259343	0.186629	-1.153307
C	7.093434	0.209086	1.363688
H	6.703053	0.171362	-2.096477
C	8.712156	0.386076	-1.262006
C	8.043537	-0.562856	1.902225
H	6.598170	0.948347	2.001077
C	9.668180	-0.383162	-0.721416

H	9.025967	1.192823	-1.933018
C	8.766171	-1.666320	1.243821
H	8.278826	-0.406443	2.960707
H	10.707254	-0.151177	-0.979662
C	9.473972	-1.585120	0.109211
H	8.781279	-2.615255	1.789976
H	10.030775	-2.473050	-0.208848
C	-6.542873	-0.094540	-0.013816
C	-7.259325	-0.186674	-1.153339
C	-7.093383	-0.209241	1.363653
H	-6.703049	-0.171312	-2.096515
C	-8.712123	-0.386241	-1.262030
C	-8.043546	0.562591	1.902239
H	-6.598047	-0.948491	2.000999
C	-9.668207	0.382887	-0.721390
H	-9.025872	-1.192982	-1.933079
C	-8.766284	1.666025	1.243900
H	-8.278808	0.406105	2.960716
H	-10.707264	0.150826	-0.979635
C	-9.474092	1.584821	0.109295
H	-8.781468	2.614932	1.790103
H	-10.030976	2.472719	-0.208713
C	0.986870	6.471404	-0.098740
N	0.808666	7.611883	-0.097211
C	-0.986860	-6.471298	-0.098720
N	-0.808656	-7.611777	-0.097191

SCIBA22 S0

E = -2392.83015587 a.u.

C	-1.696190	-1.864310	0.139454
C	-2.446529	-0.557339	0.217401
C	-1.755417	0.648324	0.227002
C	-0.344391	0.574112	0.315937
C	0.344348	-0.574057	0.315947
C	1.696164	1.864363	0.139540
C	2.446494	0.557384	0.217493
C	1.755375	-0.648266	0.227070
N	-0.297517	-1.772658	0.228210
N	0.297486	1.772711	0.228249
C	1.988832	-2.101771	0.063947
C	0.713208	-2.744636	0.067005
C	3.126859	-2.880339	-0.155186
C	0.556550	-4.110167	-0.108110
C	2.990263	-4.253290	-0.341836
H	4.113532	-2.421579	-0.193539
C	1.724622	-4.860390	-0.308222
H	-0.433549	-4.562087	-0.102208
H	3.870584	-4.871390	-0.516003
C	-1.988853	2.101836	0.063845
C	-0.713225	2.744697	0.067023
C	-3.126847	2.880418	-0.155426
C	-0.556538	4.110228	-0.108068
C	-2.990221	4.253370	-0.342053
H	-4.113517	2.421670	-0.193910
C	-1.724582	4.860463	-0.308290
H	0.433565	4.562136	-0.102082
H	-3.870517	4.871476	-0.516323
O	2.236610	2.939131	-0.008567
O	-2.236623	-2.939062	-0.008826
C	-3.896196	-0.639151	0.295273
C	-4.718583	0.234222	0.980028
S	-4.841392	-1.881505	-0.469845
C	-6.094933	-0.079356	0.856317
H	-4.325655	1.049804	1.587067
C	-6.320773	-1.191036	0.079682
H	-6.897616	0.481321	1.334584
C	3.896166	0.639131	0.295337
C	4.718529	-0.234433	0.979876
S	4.841413	1.881496	-0.469704
C	6.094892	0.079095	0.856179
H	4.325576	-1.050123	1.586757
C	6.320769	1.190902	0.079738
H	6.897560	-0.481711	1.334323
C	-7.634668	-1.820184	-0.265126
H	-7.807631	-1.819650	-1.351152
H	-7.682669	-2.862967	0.080103
H	-8.449557	-1.261969	0.212620
C	7.634687	1.820046	-0.264989
H	7.807639	1.819668	-1.351017
H	7.682737	2.862774	0.080397
H	8.449557	1.261723	0.212664
C	1.623241	-6.287068	-0.492977
N	1.550758	-7.429732	-0.640704
C	-1.623171	6.287139	-0.493037
N	-1.550664	7.429803	-0.640756

SCIBA22 T1

E = -2392.79854080 a.u.

C	-1.696190	-1.864310	0.139454
C	-2.446529	-0.557339	0.217401
C	-1.755417	0.648324	0.227002
C	-0.344391	0.574112	0.315937
C	0.344348	-0.574057	0.315947
C	1.696164	1.864363	0.139540
C	2.446494	0.557384	0.217493
C	1.755375	-0.648266	0.227070
N	-0.297517	-1.772658	0.228210
N	0.297486	1.772711	0.228249
C	1.988832	-2.101771	0.063947
C	0.713208	-2.744636	0.067005
C	3.126859	-2.880339	-0.155186
C	0.556550	-4.110167	-0.108110
C	2.990263	-4.253290	-0.341836
H	4.113532	-2.421579	-0.193539
C	1.724622	-4.860390	-0.308222
H	-0.433549	-4.562087	-0.102208
H	3.870584	-4.871390	-0.516003
C	-1.988853	2.101836	0.063845

C	-0.713225	2.744697	0.067023
C	-3.126847	2.880418	-0.155426
C	-0.556538	4.110228	-0.108068
C	-2.990221	4.253370	-0.342053
H	-4.113517	2.421670	-0.193910
C	-1.724582	4.860463	-0.308290
H	0.433565	4.562136	-0.102082
H	-3.870517	4.871476	-0.516323
O	2.236610	2.939131	-0.008567
O	-2.236623	-2.939062	-0.008826
C	-3.896196	-0.639151	0.295273
C	-4.718583	0.234222	0.980028
S	-4.841392	-1.881505	-0.469845
C	-6.094933	-0.079356	0.856317
H	-4.325655	1.049804	1.587067
C	-6.320773	-1.191036	0.079682
H	-6.897616	0.481321	1.334584
C	3.896166	0.639131	0.295337
C	4.718529	-0.234433	0.979876
S	4.841413	1.881496	-0.469704
C	6.094892	0.079095	0.856179
H	4.325576	-1.050123	1.586757
C	6.320769	1.190902	0.079738
H	6.897560	-0.481711	1.334323
C	-7.634668	-1.820184	-0.265126
H	-7.807631	-1.819650	-1.351152
H	-7.682669	-2.862967	0.080103
H	-8.449557	-1.261969	0.212620
C	7.634687	1.820046	-0.264989
H	7.807639	1.819668	-1.351017
H	7.682737	2.862774	0.080397
H	8.449557	1.261723	0.212664
C	1.623241	-6.287068	-0.492977
N	1.550758	-7.429732	-0.640704
C	-1.623171	6.287139	-0.493037
N	-1.550664	7.429803	-0.640756

SCIBA23 S0

E = -1749.30672303 a.u.

C	1.650200	-1.916928	-0.047652
C	0.256496	-2.499373	-0.032361
C	-0.854102	-1.657060	-0.044347
C	-0.612596	-0.269612	-0.043769
C	0.612596	0.269612	-0.043769
C	-1.650200	1.916928	-0.047652
C	-0.256496	2.499373	-0.032361
C	0.854102	1.657060	-0.044347
N	1.725850	-0.512124	-0.045458
N	-1.725850	0.512124	-0.045458
C	2.330612	1.724741	-0.059254
C	2.822884	0.382508	-0.055494
C	3.253124	2.772144	-0.090538
C	4.177149	0.080787	-0.067969
C	4.617342	2.477334	-0.103351
H	2.925333	3.811049	-0.118102
C	5.069525	1.155274	-0.089157
H	4.503536	-0.957183	-0.064649
H	5.340196	3.293200	-0.129546
H	6.141628	0.954292	-0.100377
C	-2.330612	-1.724741	-0.059254
C	-2.822884	-0.382508	-0.055494
C	-3.253124	-2.772144	-0.090538
C	-4.177149	-0.080787	-0.067969
C	-4.617342	-2.477334	-0.103351
H	-2.925333	-3.811049	-0.118102
C	-5.069525	-1.155274	-0.089157
H	-4.503536	0.957183	-0.064649
H	-5.340196	-3.293200	-0.129546
H	-6.141628	-0.954292	-0.100377
O	-2.669459	2.578149	-0.058886
O	2.669459	-2.578149	-0.058886
C	-0.082415	3.933937	0.017794
C	-1.018848	4.911886	-0.059239
H	0.956203	4.254110	0.111277
H	-2.069703	4.665029	-0.198755
C	0.082415	-3.933937	0.017794
C	1.018848	-4.911886	-0.059239
H	-0.956203	-4.254110	0.111277
H	2.069703	-4.665029	-0.198755
C	0.668721	-6.312163	0.042769
C	1.585099	-7.265138	-0.226302
H	2.599663	-7.024619	-0.540108
C	-0.886953	-8.054199	0.455212
H	-0.983021	-6.165101	1.222456
C	0.056702	-8.948412	0.163136
H	-1.892101	-8.385319	0.713586
H	-0.107015	-10.022944	0.145001
C	-0.668721	6.312163	0.042769
C	-1.585099	7.265138	-0.226302
H	-2.599663	7.024619	-0.540108
C	0.886953	8.054199	0.455212
H	0.983021	6.165101	1.222456
C	-0.056702	8.948412	0.163136
H	1.892101	8.385319	0.713586
H	0.107015	10.022944	0.145001
N	0.668721	6.659304	0.387846
N	-0.668721	-6.659304	0.387846
O	-1.342305	8.601066	-0.190410
O	1.342305	-8.601066	-0.190410

SCIBA23 T1

E = -1749.28128373 a.u.

C	1.644293	-1.934313	-0.102073
C	0.258105	-2.514957	-0.081135
C	-0.892362	-1.622960	-0.095054
C	-0.633803	-0.281237	-0.083547
C	0.633803	0.281237	-0.083547
C	-1.644293	1.934313	-0.102073

C	-0.258105	2.514957	-0.081135
C	0.892362	1.622960	-0.095054
N	1.739435	-0.519834	-0.097706
N	-1.739435	0.519834	-0.097706
C	2.351034	1.692984	-0.124975
C	2.841327	0.346189	-0.121867
C	3.287592	2.737078	-0.166522
C	4.200520	0.040529	-0.145990
C	4.644243	2.434676	-0.191826
H	2.968224	3.779041	-0.192497
C	5.094992	1.105755	-0.178680
H	4.525482	-0.997737	-0.141833
H	5.372185	3.246231	-0.227001
H	6.166313	0.901945	-0.199361
C	-2.351034	-1.692984	-0.124975
C	-2.841327	-0.346189	-0.121867
C	-3.287592	-2.737078	-0.166522
C	-4.200520	-0.040529	-0.145990
C	-4.644243	-2.434676	-0.191826
H	-2.968224	-3.779041	-0.192497
C	-5.094992	-1.105755	-0.178680
H	-4.525482	0.997737	-0.141833
H	-5.372185	-3.246231	-0.227001
H	-6.166313	-0.901945	-0.199361
O	-2.662939	2.591905	-0.115799
O	2.662939	-2.591905	-0.115799
C	-0.082387	3.897886	-0.024869
C	-1.025777	4.925603	-0.056471
H	0.963120	4.210638	0.028532
H	-2.077741	4.698410	-0.210851
C	0.082387	-3.897886	-0.024869
C	1.025777	-4.925603	-0.056471
H	-0.963120	-4.210638	0.028532
H	2.077741	-4.698410	-0.210851
C	0.660026	-6.281479	0.093260
C	1.589651	-7.277362	-0.113429
H	2.612250	-7.059394	-0.415250
C	-0.892362	-8.016884	0.609545
H	-1.109662	-6.036395	1.106835
C	0.048005	-8.933911	0.377243
H	-1.894722	-8.317238	0.910437
H	-0.101930	-10.007429	0.443469
C	-0.660026	6.281479	0.093260
C	-1.589651	7.277362	-0.113429
H	-2.612250	7.059394	-0.415250
C	0.892362	8.016884	0.609545
H	1.109662	6.036395	1.106835
C	-0.048005	8.933911	0.377243
H	1.894722	8.317238	0.910437
H	0.101930	10.007429	0.443469
N	0.661470	6.647057	0.430998
N	-0.661470	-6.647057	0.430998
O	-1.328497	8.593241	-0.008849
O	1.328497	-8.593241	-0.008849

SCIBA24 S0

E = -2434.83495938 a.u.

C	1.679951	-1.890137	-0.017162
C	0.295360	-2.493456	-0.029917
C	-0.828473	-1.670350	-0.023561
C	-0.608436	-0.278570	-0.028585
C	0.608436	0.278570	-0.028585
C	-1.679951	1.890137	-0.017162
C	-0.295360	2.493456	-0.029917
C	0.828473	1.670350	-0.023561
N	1.733725	-0.484895	-0.023171
N	-1.733725	0.484895	-0.023171
C	2.304135	1.761563	-0.005831
C	2.816965	0.427374	-0.008898
C	3.209790	2.823659	0.024766
C	4.175459	0.146335	0.006658
C	4.578207	2.549673	0.040548
H	2.867541	3.858218	0.044817
C	5.050782	1.234797	0.029254
H	4.518126	-0.886353	0.003292
H	5.287899	3.376985	0.064111
H	6.125883	1.050588	0.041783
C	-2.304135	-1.761563	-0.005831
C	-2.816965	-0.427374	-0.008898
C	-3.209790	-2.823659	0.024766
C	-4.175459	-0.146335	0.006658
C	-4.578207	-2.549673	0.040548
H	-2.867541	-3.858218	0.044817
C	-5.050782	-1.234797	0.029254
H	-4.518126	0.886353	0.003292
H	-5.287899	-3.376985	0.064111
H	-6.125883	-1.050588	0.041783
O	-2.709027	2.536029	-0.002537
O	2.709027	-2.536029	-0.002537
C	-0.139940	3.932087	-0.061419
C	-1.092397	4.892307	0.003483
H	0.898011	4.257885	-0.145738
H	-2.142014	4.614577	0.096270
C	0.139940	-3.932087	-0.061419
C	1.092397	-4.892307	0.003483
H	-0.898011	-4.257885	-0.145738
H	2.142014	-4.614577	0.096270
C	0.796428	-6.311125	-0.047176
C	1.789525	-7.206675	0.101515
H	2.821282	-6.881929	0.246328
C	-0.716510	-8.492334	0.203607
C	0.450312	-9.117110	0.335630
H	-1.641832	-9.020758	0.429405
H	0.533193	-10.155038	0.656881
C	-0.796428	6.311125	-0.047176
C	-1.789525	7.206675	0.101515
H	-2.821282	6.881929	0.246328
C	0.716510	8.492334	0.203607
C	-0.450312	9.117110	0.335630

H	1.641832	9.020758	0.429405
H	-0.533193	10.155038	0.656881
O	-1.679951	8.557378	0.120629
O	1.679951	-8.557378	0.120629
S	0.896315	6.818356	-0.334822
S	-0.896315	-6.818356	-0.334822

SCIBA24 T1

E = -2434.80481275 a.u.

C	-1.662658	1.913892	-0.001230
C	-0.281619	2.511391	-0.001394
C	0.876645	1.633961	-0.002066
C	0.631155	0.288644	-0.002012
C	-0.631155	-0.288644	-0.002012
C	1.662658	-1.913892	-0.001230
C	0.281619	-2.511391	-0.001394
C	-0.876645	-1.633961	-0.002066
N	-1.744141	0.498675	-0.001923
N	1.744141	-0.498675	-0.001923
C	-2.335571	-1.720099	-0.002428
C	-2.838860	-0.379108	-0.001817
C	-3.260938	-2.774748	-0.003270
C	-4.200927	-0.086111	-0.001763
C	-4.620396	-2.485211	-0.003206
H	-2.933258	-3.814355	-0.004083
C	-5.084400	-1.160821	-0.002430
H	-4.537230	0.948493	-0.001365
H	-5.340073	-3.304664	-0.003845
H	-6.157958	-0.968101	-0.002469
C	2.335571	1.720099	-0.002428
C	2.838860	0.379108	-0.001817
C	3.260938	2.774748	-0.003270
C	4.200927	0.086111	-0.001763
C	4.620396	2.485211	-0.003206
H	2.933258	3.814355	-0.004083
C	5.084400	1.160821	-0.002430
H	4.537230	-0.948493	-0.001365
H	5.340073	3.304664	-0.003845
H	6.157958	0.968101	-0.002469
O	2.687651	-2.560652	-0.000709
O	-2.687651	2.560652	-0.000709
C	0.114157	-3.902418	-0.000926
C	1.071146	-4.908843	0.002444
H	-0.930772	-4.220330	-0.002473
H	2.127883	-4.646641	0.006089
C	-0.114157	3.902418	-0.000926
C	-1.071146	4.908843	0.002444
H	0.930772	4.220330	-0.002473
H	-2.127883	4.646641	0.006089
C	-0.748034	6.294083	0.001816
C	-1.759089	7.210232	0.009760
H	-2.798853	6.881175	0.015853
C	0.739173	8.523682	0.005028
C	-0.433391	9.152286	0.013373
H	1.657552	9.109437	0.007330
H	-0.524186	10.237050	0.022802
C	0.748034	-6.294083	0.001816
C	1.759089	-7.210232	0.009760
H	2.798853	-6.881175	0.015853
C	-0.739173	-8.523682	0.005028
C	0.433391	-9.152286	0.013373
H	-1.657552	-9.109437	0.007330
H	0.524186	-10.237050	0.022802
O	1.662658	-8.551157	0.012484
O	-1.662658	8.551157	0.012484
S	-0.974343	-6.778125	-0.011115
S	0.974343	6.778125	-0.011115

SCIBA25 S0

E = -2395.15993826 a.u.

C	1.599803	-1.958870	-0.054399
C	0.191415	-2.505260	-0.037712
C	-0.897648	-1.634700	-0.052489
C	-0.619466	-0.253832	-0.052383
C	0.619466	0.253832	-0.052383
C	-1.599803	1.958870	-0.054399
C	-0.191415	2.505260	-0.037712
C	0.897648	1.634700	-0.052489
N	1.711543	-0.556543	-0.053315
N	-1.711543	0.556543	-0.053315
C	2.375656	1.662997	-0.067980
C	2.831908	0.308241	-0.063398
C	3.327119	2.684260	-0.101996
C	4.177405	-0.030422	-0.075877
C	4.682766	2.352957	-0.114832
H	3.029216	3.731913	-0.133176
C	5.098780	1.019074	-0.098548
H	4.475435	-1.076894	-0.071793
H	5.427337	3.148910	-0.143452
H	6.164952	0.788903	-0.109978
C	-2.375656	-1.662997	-0.067980
C	-2.831908	-0.308241	-0.063398
C	-3.327119	-2.684260	-0.101996
C	-4.177405	0.030422	-0.075877
C	-4.682766	-2.352957	-0.114832
H	-3.029216	-3.731913	-0.133176
C	-5.098780	-1.019074	-0.098548
H	-4.475435	1.076894	-0.071793
H	-5.427337	-3.148910	-0.143452
H	-6.164952	-0.788903	-0.109978
O	-2.601732	2.645316	-0.065384
O	2.601732	-2.645316	-0.065384
C	0.017359	3.935658	0.020166
C	-0.897648	4.934229	-0.056957
H	1.067340	4.217584	0.114027
H	-1.948382	4.703501	-0.218273
C	-0.017359	-3.935658	0.020166
C	0.897648	-4.934229	-0.056957

H	-1.067340	-4.217584	0.114027
H	1.948382	-4.703501	-0.218273
C	0.541577	-6.339871	0.034289
C	1.447665	-7.277210	-0.320798
H	2.435236	-6.958109	-0.653105
C	-1.076130	-7.975245	0.812842
H	-1.142520	-5.970187	1.105518
C	-0.351206	-9.055049	0.515470
H	-2.004245	-8.088398	1.375686
H	-0.676794	-10.046514	0.824851
C	-0.541577	6.339871	0.034289
C	-1.447665	7.277210	-0.320798
H	-2.435236	6.958109	-0.653105
C	1.076130	7.975245	0.812842
H	1.142520	5.970187	1.105518
C	0.351206	9.055049	0.515470
H	2.004245	8.088398	1.375686
H	0.676794	10.046514	0.824851
N	0.767857	6.656069	0.458540
N	-0.767857	-6.656069	0.458540
S	-1.180257	9.011759	-0.382262
S	1.180257	-9.011759	-0.382262

SCIBA25 T1

E = -2395.13717544 a.u.

C	1.602376	-1.970420	-0.104547
C	0.203290	-2.521234	-0.080418
C	-0.927241	-1.603028	-0.095750
C	-0.639138	-0.267258	-0.083483
C	0.639138	0.267258	-0.083483
C	-1.602376	1.970420	-0.104547
C	-0.203290	2.521234	-0.080418
C	0.927241	1.603028	-0.095750
N	1.726809	-0.559064	-0.098864
N	-1.726809	0.559064	-0.098864
C	2.387557	1.639447	-0.128068
C	2.847433	0.281829	-0.124774
C	3.349020	2.660393	-0.172937
C	4.199054	-0.055058	-0.150695
C	4.698637	2.327506	-0.200058
H	3.054613	3.709616	-0.200920
C	5.118470	0.988797	-0.185814
H	4.499191	-1.100768	-0.146169
H	5.444940	3.122115	-0.237784
H	6.184693	0.760015	-0.207833
C	-2.387557	-1.639447	-0.128068
C	-2.847433	-0.281829	-0.124774
C	-3.349020	-2.660393	-0.172937
C	-4.199054	0.055058	-0.150695
C	-4.698637	-2.327506	-0.200058
H	-3.054613	-3.709616	-0.200920
C	-5.118470	-0.988797	-0.185814
H	-4.499191	1.100768	-0.146169
H	-5.444940	-3.122115	-0.237784
H	-6.184693	-0.760015	-0.207833
O	-2.607376	2.648549	-0.121285
O	2.607376	-2.648549	-0.121285
C	-0.001524	3.897433	-0.018862
C	-0.927241	4.946213	-0.048959
H	1.054326	4.175832	0.032914
H	-1.978033	4.729245	-0.219204
C	0.001524	-3.897433	-0.018862
C	0.927241	-4.946213	-0.048959
H	-1.054326	-4.175832	0.032914
H	1.978033	-4.729245	-0.219204
C	0.566981	-6.301052	0.105358
C	1.513926	-7.289258	-0.128880
H	2.515390	-6.986725	-0.432754
C	-1.160767	-7.953234	0.649374
H	-1.291255	-5.924182	0.909606
C	-0.419152	-9.049027	0.443602
H	-2.198976	-8.057312	0.968372
H	-0.834348	-10.045724	0.574852
C	-0.566981	6.301052	0.105358
C	-1.513926	7.289258	-0.128880
H	-2.515390	6.986725	-0.432754
C	1.160767	7.953234	0.649374
H	1.291255	5.924182	0.909606
C	0.419152	9.049027	0.443602
H	2.198976	8.057312	0.968372
H	0.834348	10.045724	0.574852
N	0.735979	6.648983	0.477418
N	-0.735979	-6.648983	0.477418
S	-1.275034	8.997891	-0.048201
S	1.275034	-8.997891	-0.048201

SCIBA26 BS-S0

E = -1539.27300298 a.u.

C	1.915456	1.666901	0.000073
C	2.519870	0.265222	0.000041
C	1.626313	-0.885311	0.000054
C	0.285739	-0.631642	0.000089
C	-0.285754	0.631749	0.000092
C	-1.915471	-1.666792	0.000200
C	-2.519876	-0.265121	0.000089
C	-1.626328	0.885419	0.000089
N	0.508321	1.743144	0.000077
N	-0.508336	-1.743038	0.000121
C	-1.708647	2.347053	0.000070
C	-0.367707	2.844409	0.000068
C	-2.760365	3.272884	0.000054
C	-0.068442	4.203530	0.000052
C	-2.465945	4.632726	0.000038
H	-3.800392	2.947964	0.000053
C	-1.141420	5.091240	0.000038
H	0.966868	4.537354	0.000050
H	-3.283087	5.354863	0.000026
H	-0.944566	6.163986	0.000025

C	1.708632	-2.346943	0.000033
C	0.367694	-2.844303	0.000062
C	2.760354	-3.272768	-0.000012
C	0.068435	-4.203426	0.000053
C	2.465940	-4.632611	-0.000026
H	3.800379	-2.947840	-0.000038
C	1.141418	-5.091130	0.000006
H	-0.966873	-4.537255	0.000085
H	3.283086	-5.354744	-0.000061
H	0.944568	-6.163878	-0.000002
O	-2.565929	-2.683839	-0.000017
O	2.565881	2.683967	0.000032
C	-3.881147	-0.093423	0.000027
C	-4.935825	-1.063511	0.000027
H	-4.221320	0.943400	-0.000025
H	-4.671376	-2.121307	0.000088
C	3.881140	0.093469	-0.000004
C	4.935899	1.063474	-0.000027
H	4.221251	-0.943375	-0.000027
H	4.671545	2.121290	-0.000003
C	6.252477	0.682073	-0.000079
C	7.352512	1.609761	-0.000106
B	6.924262	-0.763208	-0.000130
C	8.590040	0.925046	-0.000155
H	7.245431	2.695745	-0.000088
C	8.437332	-0.462823	-0.000169
H	6.373635	-1.831539	-0.000106
H	9.550288	1.446281	-0.000180
H	9.293435	-1.137541	-0.000202
C	-6.252436	-0.682224	-0.000043
C	-7.352392	-1.610007	-0.000039
B	-6.924345	0.763000	-0.000128
C	-8.589978	-0.925397	-0.000167
H	-7.245218	-2.695981	0.000028
C	-8.437388	0.462486	-0.000264
H	-6.373809	1.831378	-0.000210
H	-9.550182	-1.446713	-0.000211
H	-9.293548	1.137131	-0.000391

SCIBA26 T1

E = -1539.27232647 a.u.

C	1.917868	1.665219	-0.000027
C	2.521726	0.261458	-0.000069
C	1.622926	-0.890142	-0.000069
C	0.285610	-0.633437	-0.000092
C	-0.285617	0.633480	-0.000092
C	-1.917876	-1.665176	-0.000140
C	-2.521729	-0.261417	-0.000100
C	-1.622933	0.890185	-0.000089
N	0.511117	1.743741	-0.000064
N	-0.511124	-1.743698	-0.000107
C	-1.703749	2.351233	-0.000062
C	-0.362132	2.846653	-0.000073
C	-2.754326	3.278685	-0.000051
C	-0.060923	4.205614	-0.000064
C	-2.457814	4.637854	-0.000045
H	-3.794869	2.955325	-0.000057
C	-1.132451	5.094671	-0.000050
H	0.974732	4.538346	-0.000063
H	-3.273876	5.361226	-0.000040
H	-0.934174	6.167148	-0.000044
C	1.703742	-2.351189	-0.000051
C	0.362125	-2.846611	-0.000075
C	2.754321	-3.278639	-0.000027
C	0.060919	-4.205572	-0.000073
C	2.457811	-4.637809	-0.000023
H	3.794863	-2.955276	-0.000020
C	1.132448	-5.094628	-0.000043
H	-0.974736	-4.538306	-0.000095
H	3.273874	-5.361179	-0.000007
H	0.934173	-6.167104	-0.000042
O	-2.569731	-2.680671	-0.000040
O	2.569710	2.680722	-0.000104
C	-3.878134	-0.087597	-0.000075
C	-4.939783	-1.058612	-0.000101
H	-4.218064	0.949383	-0.000039
H	-4.676654	-2.116777	-0.000208
C	3.878133	0.087615	-0.000056
C	4.939815	1.058596	-0.000065
H	4.218038	-0.949373	-0.000040
H	4.676724	2.116769	-0.000143
C	6.250581	0.673739	0.000015
C	7.357002	1.608059	0.000089
B	6.921067	-0.768452	0.000141
C	8.587475	0.928578	0.000291
H	7.246193	2.693696	0.000035
C	8.431642	-0.465108	0.000353
H	6.372567	-1.837965	0.000023
H	9.548760	1.447481	0.000386
H	9.288552	-1.139069	0.000565
C	-6.250563	-0.673800	-0.000002
C	-7.356952	-1.608157	0.000065
B	-6.921098	0.768369	0.000171
C	-8.587448	-0.928718	0.000308
H	-7.246107	-2.693790	-0.000019
C	-8.431663	0.464974	0.000406
H	-6.372634	1.837900	0.000059
H	-9.548715	-1.447654	0.000406
H	-9.288595	1.138906	0.000657

SCIBA27 S0

E = -1539.26979388 a.u.

C	1.963280	1.595278	0.013349
C	2.506035	0.183313	0.005505
C	1.633073	-0.904686	-0.008832
C	0.251489	-0.620883	-0.006352
C	-0.251487	0.620890	0.006178
C	-1.963279	-1.595271	-0.013433

C	-2.506033	-0.183306	-0.005600
C	-1.633071	0.904691	0.008710
N	0.560532	1.709902	0.015138
N	-0.560531	-1.709896	-0.015270
C	-1.656105	2.383065	0.024534
C	-0.300129	2.833715	0.026507
C	-2.673455	3.339518	0.041489
C	0.045214	4.177415	0.040296
C	-2.336404	4.693146	0.055269
H	-3.722760	3.047612	0.046861
C	-1.000385	5.103057	0.053960
H	1.092763	4.471390	0.041027
H	-3.129611	5.440874	0.068540
H	-0.765613	6.168203	0.065375
C	1.656106	-2.383061	-0.024617
C	0.300130	-2.833710	-0.026545
C	2.673454	-3.339518	-0.041519
C	-0.045215	-4.177410	-0.040254
C	2.336401	-4.693146	-0.055207
H	3.722760	-3.047615	-0.046892
C	1.000382	-5.103055	-0.053869
H	-1.092765	-4.471383	-0.040966
H	3.129608	-5.440875	-0.068425
H	0.765608	-6.168201	-0.065216
O	-2.649984	-2.594949	-0.018704
O	2.649982	2.594957	0.018684
C	-3.935471	0.032006	-0.019290
C	-4.941182	-0.878198	-0.005849
H	-4.225488	1.084203	-0.034675
H	-4.704771	-1.940000	0.043632
C	3.935474	-0.031999	0.019229
C	4.941187	0.878204	0.005914
H	4.225491	-1.084198	0.034528
H	4.704783	1.940011	-0.043482
C	-6.345832	-0.499337	-0.035015
C	-6.916884	0.708832	-0.281164
C	-7.416446	-1.548909	0.228300
H	-6.346630	1.604885	-0.528412
B	-8.470459	0.502849	-0.170614
C	-8.654106	-1.038216	0.167559
H	-7.143125	-2.586413	0.443192
H	-9.329935	1.330433	-0.309128
H	-9.555912	-1.626883	0.333476
C	6.345833	0.499334	0.035106
C	6.916870	-0.708852	0.281205
C	7.416458	1.548909	-0.228150
H	6.346602	-1.604914	0.528388
B	8.470444	-0.502887	0.170668
C	8.654114	1.038207	-0.167399
H	7.143146	2.586431	-0.442968
H	9.329912	-1.330490	0.309112
H	9.555933	1.626877	-0.333235

SCIBA27 T1

E = -1539.25865370 a.u.

C	1.958589	1.615583	-0.000010
C	2.527308	0.199495	0.000072
C	1.602049	-0.929693	0.000040
C	0.270295	-0.639942	0.000093
C	-0.270298	0.639962	0.000075
C	-1.958592	-1.615563	-0.000195
C	-2.527310	-0.199476	-0.000081
C	-1.602052	0.929714	-0.000059
N	0.553445	1.729400	0.000031
N	-0.553448	-1.729380	-0.000024
C	-1.644880	2.392630	-0.000206
C	-0.290965	2.853697	-0.000114
C	-2.669356	3.348977	-0.000448
C	0.045836	4.204384	-0.000215
C	-2.338272	4.699924	-0.000559
H	-3.718077	3.053803	-0.000581
C	-1.001318	5.121671	-0.000439
H	1.089983	4.509432	-0.000147
H	-3.135009	5.444491	-0.000752
H	-0.774754	6.188473	-0.000531
C	1.644877	-2.392609	-0.000114
C	0.290962	-2.853677	-0.000124
C	2.669354	-3.348955	-0.000268
C	-0.045838	-4.204365	-0.000254
C	2.338271	-4.699903	-0.000407
H	3.718074	-3.053780	-0.000298
C	1.001317	-5.121650	-0.000397
H	-1.089985	-4.509413	-0.000268
H	3.135009	-5.444468	-0.000530
H	0.774754	-6.188453	-0.000511
O	-2.634034	-2.615815	-0.000381
O	2.634026	2.615838	-0.000135
C	-3.883851	0.003721	0.000097
C	-4.953656	-0.944303	0.000168
H	-4.187106	1.051758	0.000240
H	-4.710390	-2.004908	0.000130
C	3.883850	-0.003713	0.000225
C	4.953669	0.944295	0.000312
H	4.187093	-1.051753	0.000315
H	4.710421	2.004904	0.000405
C	-6.280262	-0.572539	0.000279
C	-6.862314	0.737690	0.000282
C	-7.385284	-1.568550	0.000404
H	-6.262947	1.647928	0.000068
B	-8.407483	0.558866	0.000495
C	-8.612230	-0.995576	0.000554
H	-7.170261	-2.641026	0.000406
H	-9.240224	1.422784	0.000629
H	-9.530674	-1.583276	0.000707
C	6.280270	0.572508	0.000298
C	6.862299	-0.737728	0.000126
C	7.385308	1.568503	0.000467
H	6.262918	-1.647956	-0.000109
B	8.407471	-0.558929	0.000208

C	8.612245	0.995509	0.000419
H	7.170302	2.640982	0.000600
H	9.240199	-1.422862	0.000142
H	9.530699	1.583194	0.000529

SCIBA28 S0

E = -1707.13563451 a.u.

C	1.712979	-1.872412	-0.101574
C	0.324122	-2.474163	-0.098902
C	-0.813546	-1.674322	-0.105689
C	-0.607259	-0.282548	-0.109223
C	0.607259	0.282548	-0.109223
C	-1.712979	1.872412	-0.101574
C	-0.324122	2.474163	-0.098902
C	0.813546	1.674322	-0.105689
N	1.747931	-0.464516	-0.107814
N	-1.747931	0.464516	-0.107814
C	2.277627	1.789396	-0.106346
C	2.815659	0.466499	-0.106446
C	3.144436	2.880168	-0.111334
C	4.181506	0.223616	-0.107732
C	4.519656	2.643110	-0.113196
H	2.742287	3.893895	-0.116951
C	5.024764	1.338681	-0.110551
H	4.554559	-0.798957	-0.107832
H	5.211326	3.486030	-0.118432
H	6.104646	1.183662	-0.112507
C	-2.277627	-1.789396	-0.106346
C	-2.815659	-0.466499	-0.106446
C	-3.144436	-2.880168	-0.111334
C	-4.181506	-0.223616	-0.107732
C	-4.519656	-2.643110	-0.113196
H	-2.742287	-3.893895	-0.116951
C	-5.024764	-1.338681	-0.110551
H	-4.554559	0.798957	-0.107832
H	-5.211326	-3.486030	-0.118432
H	-6.104646	-1.183662	-0.112507
O	-2.730388	2.526893	-0.095452
O	2.730388	-2.526893	-0.095452
C	-0.277290	3.884019	-0.077711
C	-0.236105	5.103643	-0.046083
C	0.277290	-3.884019	-0.077711
C	0.236105	-5.103643	-0.046083
C	-0.301763	6.515624	-0.009529
C	0.785298	7.283354	0.241607
H	1.763183	6.829278	0.392869
C	-1.682531	8.432459	0.285615
H	-2.349220	6.517352	-0.045172
C	-0.607259	9.182991	0.535618
H	1.453339	9.135789	0.781151
H	-2.689825	8.814867	0.440773
H	-0.678078	10.204645	0.900473
C	0.301763	-6.515624	-0.009529
C	-0.785298	-7.283354	0.241607
H	-1.763183	-6.829278	0.392869
C	1.682531	-8.432459	0.285615
H	2.349220	-6.517352	-0.045172
C	0.607259	-9.182991	0.535618
H	-1.453339	-9.135789	0.781151
H	2.689825	-8.814867	0.440773
H	0.678078	-10.204645	0.900473
N	1.569398	-7.132588	-0.251680
N	-1.569398	7.132588	-0.251680
N	-0.696503	-8.666086	0.302080
N	0.696503	8.666086	0.302080

SCIBA28 T1

E = -1707.12304975 a.u.

C	1.502180	-2.051346	-0.000141
C	0.076509	-2.501031	-0.000102
C	-1.015026	-1.544648	-0.000177
C	-0.652901	-0.227731	-0.000223
C	0.652901	0.227731	-0.000223
C	-1.502180	2.051346	-0.000141
C	-0.076509	2.501031	-0.000102
C	1.015026	1.544648	-0.000177
N	1.704868	-0.656570	-0.000189
N	-1.704868	0.656570	-0.000189
C	2.467123	1.508650	-0.000187
C	2.863676	0.131457	-0.000311
C	3.459628	2.497759	-0.000143
C	4.202659	-0.254545	-0.000419
C	4.795045	2.112375	-0.000242
H	3.178536	3.551951	-0.000037
C	5.160703	0.755597	-0.000378
H	4.463237	-1.310977	-0.000487
H	5.574837	2.875429	-0.000206
H	6.217937	0.486224	-0.000437
C	-2.467123	-1.508650	-0.000187
C	-2.863676	-0.131457	-0.000311
C	-3.459628	-2.497759	-0.000143
C	-4.202659	0.254545	-0.000419
C	-4.795045	-2.112375	-0.000242
H	-3.178536	-3.551951	-0.000037
C	-5.160703	-0.755597	-0.000378
H	-4.463237	1.310977	-0.000487
H	-5.574837	-2.875429	-0.000206
H	-6.217937	-0.486224	-0.000437
O	-2.468241	2.802190	-0.000157
O	2.468241	-2.802190	-0.000157
C	0.001195	3.867637	-0.000004
C	-0.220427	5.087832	0.000041
C	-0.001195	-3.867637	-0.000004
C	0.220427	-5.087832	0.000041
C	-1.015026	6.215576	0.000193
C	-0.609689	7.546672	0.000154
H	0.442379	7.816875	-0.000048
C	-3.304809	6.978792	0.000622

H	-2.661671	4.966930	0.000604
C	-2.905176	8.269078	0.000494
H	-1.228788	9.512535	0.000229
H	-4.358045	6.705772	0.000809
H	-3.595610	9.106947	0.000564
C	1.015026	-6.215576	0.000193
C	0.609689	-7.546672	0.000154
H	-0.442379	-7.816875	-0.000048
C	3.304809	-6.978792	0.000622
H	2.661671	-4.966930	0.000604
C	2.905176	-8.269078	0.000494
H	1.228788	-9.512535	0.000229
H	4.358045	-6.705772	0.000809
H	3.595610	-9.106947	0.000564
N	2.392673	-5.954606	0.000583
N	-2.392673	5.954606	0.000583
N	1.539500	-8.551182	0.000352
N	-1.539500	8.551182	0.000352

SCIBA29 S0

E = -1536.79003865 a.u.

C	1.719753	1.868110	0.001441
C	2.438114	0.533096	0.001359
C	1.739231	-0.666307	0.001702
C	0.331543	-0.581204	0.002340
C	-0.331542	0.581075	0.002325
C	-1.719751	-1.868238	0.001203
C	-2.438113	-0.533226	0.001110
C	-1.739229	0.666178	0.001554
N	0.311998	1.780956	0.001961
N	-0.311997	-1.781085	0.001873
C	-1.980825	2.114873	0.000854
C	-0.709026	2.763927	0.001072
C	-3.143872	2.882564	-0.000014
C	-0.584264	4.145264	0.000414
C	-3.025455	4.273054	-0.000670
H	-4.119507	2.394936	-0.000182
C	-1.768866	4.887998	-0.000467
H	0.401696	4.606573	0.000569
H	-3.924631	4.889668	-0.001351
H	-1.707753	5.977249	-0.001004
C	1.980826	-2.115002	0.000987
C	0.709027	-2.764056	0.001057
C	3.143874	-2.882692	0.000211
C	0.584265	-4.145393	0.000343
C	3.025457	-4.273183	-0.000499
H	4.119508	-2.395065	0.000157
C	1.768868	-4.888127	-0.000442
H	-0.401695	-4.606702	0.000385
H	3.924633	-4.889796	-0.001111
H	1.707754	-5.977378	-0.001018
O	-2.281437	-2.937221	0.000701
O	2.281438	2.937092	0.001009
C	-3.851147	-0.582952	0.000173
C	-5.071030	-0.613537	-0.000572
C	3.851149	0.582822	0.000587
C	5.071031	0.613432	-0.000081
C	6.484071	0.612377	-0.001134
C	7.284153	1.706432	-0.001580
B	7.475525	-0.646439	-0.001783
C	8.734485	1.323242	-0.002723
H	6.939209	2.742402	-0.001162
C	8.917137	-0.011591	-0.003047
H	7.158240	-1.803080	-0.001071
H	9.523793	2.079478	-0.003218
H	9.898495	-0.483660	-0.003868
C	-6.484071	-0.612251	-0.001289
C	-7.284330	-1.706175	-0.001477
B	-7.475319	0.646727	-0.001745
C	-8.734600	-1.322749	-0.002338
H	-6.939555	-2.742200	-0.001054
C	-8.917035	0.012114	-0.002721
H	-7.157847	1.803316	-0.001024
H	-9.524032	-2.078856	-0.002610
H	-9.898317	0.484343	-0.003375

SCIBA29 T1

E = -1536.77160622 a.u.

C	1.749149	1.843846	0.000543
C	2.472490	0.494992	0.000506
C	1.728791	-0.727168	0.000691
C	0.351081	-0.609561	0.001004
C	-0.319264	0.580289	0.001010
C	-1.730675	-1.858491	0.000476
C	-2.435726	-0.517375	0.000516
C	-1.705314	0.688401	0.000704
N	0.339512	1.772357	0.000832
N	-0.317757	-1.796740	0.000797
C	-1.938790	2.133951	0.000358
C	-0.662264	2.771377	0.000427
C	-3.094675	2.915806	-0.000037
C	-0.521866	4.152871	0.000103
C	-2.960287	4.303153	-0.000365
H	-4.076515	2.441036	-0.000070
C	-1.696657	4.907403	-0.000303
H	0.467496	4.606499	0.000151
H	-3.852959	4.929314	-0.000674
H	-1.624956	5.995859	-0.000576
C	1.957553	-2.165783	0.000333
C	0.675784	-2.798683	0.000381
C	3.111520	-2.955809	-0.000062
C	0.529788	-4.180918	0.000023
C	2.968561	-4.340218	-0.000420
H	4.097204	-2.488710	-0.000086
C	1.700191	-4.939580	-0.000379
H	-0.461994	-4.629239	0.000051
H	3.857938	-4.971084	-0.000736
H	1.624425	-6.027772	-0.000670

O	-2.305441	-2.918279	0.000473
O	2.317271	2.903795	0.000236
C	-3.831487	-0.551905	0.000137
C	-5.058898	-0.577486	0.000001
C	3.832577	0.540773	0.000201
C	5.085375	0.564159	-0.000181
C	6.433589	0.562621	-0.000464
C	7.264592	1.765513	-0.000533
B	7.422689	-0.661749	-0.000685
C	8.610188	1.424570	-0.000872
H	6.866863	2.780559	-0.000431
C	8.805786	0.020666	-0.000967
H	7.134430	-1.826088	-0.000637
H	9.411714	2.165628	-0.001044
H	9.805342	-0.415216	-0.001247
C	-6.458900	-0.570936	-0.000406
C	-7.270128	-1.670603	-0.000484
B	-7.443500	0.692819	-0.000727
C	-8.706237	-1.279713	-0.000885
H	-6.928359	-2.707150	-0.000228
C	-8.882359	0.061193	-0.001158
H	-7.119913	1.847142	-0.000560
H	-9.501818	-2.029138	-0.001048
H	-9.862708	0.535424	-0.001580

SCIBA30 S0

E = -1536.78819574 a.u.

C	2.481988	-0.534504	0.001942
C	1.693495	-1.829251	0.001758
C	0.305783	-1.838512	0.002444
C	-0.333938	-0.580003	0.003652
C	0.333938	0.580003	0.003652
C	-2.481988	0.534504	0.001942
C	-1.693495	1.829251	0.001758
C	-0.305783	1.838512	0.002444
N	1.693495	0.634486	0.002933
N	-1.693495	-0.634486	0.002933
C	0.820214	2.780600	0.001294
C	2.023935	2.013186	0.001441
C	0.892573	4.172438	0.000121
C	3.278180	2.604729	0.000322
C	2.151044	4.774594	-0.001006
H	-0.021847	4.766660	0.000040
C	3.317782	4.002413	-0.000927
H	4.175863	1.988874	0.000424
H	2.227491	5.862090	-0.001964
H	4.287753	4.501630	-0.001844
C	-0.820214	-2.780600	0.001294
C	-2.023935	-2.013186	0.001441
C	-0.892573	-4.172438	0.000121
C	-3.278180	-2.604729	0.000322
C	-2.151044	-4.774594	-0.001006
H	0.021847	-4.766660	0.000040
C	-3.317782	-4.002413	-0.000927
H	-4.175863	-1.988874	0.000424
H	-2.227491	-5.862090	-0.001964
H	-4.287753	-4.501630	-0.001844
O	-3.687513	0.479594	0.001112
O	3.687513	-0.479594	0.001112
C	-2.458962	3.018363	0.000404
C	-3.106761	4.051574	-0.000742
C	2.458962	-3.018363	0.000404
C	3.106761	-4.051574	-0.000742
C	-3.916588	5.216075	-0.002028
C	-3.515594	6.511218	-0.003602
C	-5.437105	5.106782	-0.001589
H	-2.466681	6.804678	-0.004266
B	-4.836851	7.376101	-0.003882
C	-6.014989	6.316284	-0.002563
H	-5.924979	4.129066	-0.000741
H	-4.923058	8.572867	-0.004619
H	-7.094826	6.460943	-0.002574
C	3.916588	-5.216075	-0.002028
C	3.515594	-6.511218	-0.003602
C	5.437105	-5.106782	-0.001589
H	2.466681	-6.804678	-0.004266
B	4.836851	-7.376101	-0.003882
C	6.014989	-6.316284	-0.002563
H	5.924979	-4.129066	-0.000741
H	4.923058	-8.572867	-0.004619
H	7.094826	-6.460943	-0.002574

SCIBA30 T1

E = -1536.75793082 a.u.

C	-1.749611	1.841190	-0.000159
C	-2.462151	0.495221	-0.000165
C	-1.704251	-0.734491	-0.000200
C	-0.341638	-0.606070	-0.000277
C	0.341141	0.604727	-0.000269
C	1.749449	-1.842178	-0.000132
C	2.461574	-0.496358	-0.000125
C	1.703956	0.732938	-0.000166
N	-0.335109	1.788215	-0.000211
N	0.334859	-1.789452	-0.000213
C	1.928663	2.171721	-0.000048
C	0.645263	2.798697	-0.000082
C	3.076627	2.971474	0.000083
C	0.490718	4.181981	0.000009
C	2.926240	4.353881	0.000179
H	4.064670	2.510430	0.000109
C	1.654031	4.947767	0.000143
H	-0.502874	4.626113	-0.000023
H	3.811704	4.990453	0.000281
H	1.572182	6.035359	0.000219
C	-1.928824	-2.173137	-0.000094
C	-0.645289	-2.799984	-0.000109
C	-3.076708	-2.973121	0.000015
C	-0.490597	-4.183296	-0.000021

C	-2.926113	-4.355454	0.000106
H	-4.064837	-2.512260	0.000028
C	-1.653777	-4.949203	0.000088
H	0.503062	-4.627280	-0.000037
H	-3.811481	-4.992163	0.000191
H	-1.571810	-6.036786	0.000161
O	2.324990	-2.897852	-0.000085
O	-2.324999	2.896884	-0.000105
C	3.824542	-0.545300	-0.000057
C	5.067179	-0.607139	0.000076
C	-3.824348	0.544596	-0.000124
C	-5.067445	0.607039	-0.000028
C	6.440058	-0.686797	0.000127
C	7.204032	-1.858778	0.000149
C	7.342809	0.515623	0.000125
H	6.738352	-2.843202	0.000123
B	8.704367	-1.413037	0.000250
C	8.644167	0.163753	0.000172
H	6.933938	1.528959	0.000067
H	9.674642	-2.117386	0.000241
H	9.450152	0.897447	0.000163
C	-6.439317	0.687756	0.000066
C	-7.202704	1.861560	-0.000051
C	-7.343721	-0.512720	0.000348
H	-6.735579	2.845300	-0.000245
B	-8.703293	1.417788	0.000130
C	-8.644756	-0.158800	0.000421
H	-6.936557	-1.526732	0.000464
H	-9.672673	2.123340	0.000216
H	-9.451642	-0.891525	0.000620

SCIBA-Cl S0

E = -1945.88135494 a.u.

C	2.504597	-0.415577	0.000000
C	2.227399	1.068529	0.000000
C	0.963292	1.600364	0.000000
C	-0.096510	0.659444	0.000000
C	0.096510	-0.659444	0.000000
C	-2.504597	0.415577	0.000000
C	-2.227399	-1.068529	0.000000
C	-0.963292	-1.600364	0.000000
N	1.342218	-1.210264	0.000000
N	-1.342218	1.210264	0.000000
C	-0.255793	-2.891332	0.000000
C	1.143943	-2.615405	0.000000
C	-0.696732	-4.211969	0.000000
C	2.095590	-3.623654	0.000000
C	0.255793	-5.232582	0.000000
H	-1.764753	-4.430103	0.000000
C	1.623125	-4.939832	0.000000
H	3.155953	-3.377009	0.000000
H	-0.070833	-6.272690	0.000000
H	2.344242	-5.758364	0.000000
C	0.255793	2.891332	0.000000
C	-1.143943	2.615405	0.000000
C	0.696732	4.211969	0.000000
C	-2.095590	3.623654	0.000000
C	-0.255793	5.232582	0.000000
H	1.764753	4.430103	0.000000
C	-1.623125	4.939832	0.000000
H	-3.155953	3.377009	0.000000
H	0.070833	6.272690	0.000000
H	-2.344242	5.758364	0.000000
O	-3.609313	0.900843	0.000000
O	3.609313	-0.900843	0.000000
Cl	-3.628616	-2.057799	0.000000
Cl	3.628616	2.057799	0.000000

SCIBA-Cl T1

E = -1945.83252894 a.u.

C	2.504597	-0.415577	0.000000
C	2.227399	1.068529	0.000000
C	0.963292	1.600364	0.000000
C	-0.096510	0.659444	0.000000
C	0.096510	-0.659444	0.000000
C	-2.504597	0.415577	0.000000
C	-2.227399	-1.068529	0.000000
C	-0.963292	-1.600364	0.000000
N	1.342218	-1.210264	0.000000
N	-1.342218	1.210264	0.000000
C	-0.255793	-2.891332	0.000000
C	1.143943	-2.615405	0.000000
C	-0.696732	-4.211969	0.000000
C	2.095590	-3.623654	0.000000
C	0.255793	-5.232582	0.000000
H	-1.764753	-4.430103	0.000000
C	1.623125	-4.939832	0.000000
H	3.155953	-3.377009	0.000000
H	-0.070833	-6.272690	0.000000
H	2.344242	-5.758364	0.000000
C	0.255793	2.891332	0.000000
C	-1.143943	2.615405	0.000000
C	0.696732	4.211969	0.000000
C	-2.095590	3.623654	0.000000
C	-0.255793	5.232582	0.000000
H	1.764753	4.430103	0.000000
C	-1.623125	4.939832	0.000000
H	-3.155953	3.377009	0.000000
H	0.070833	6.272690	0.000000
H	-2.344242	5.758364	0.000000
O	-3.609313	0.900843	0.000000
O	3.609313	-0.900843	0.000000
Cl	-3.628616	-2.057799	0.000000
Cl	3.628616	2.057799	0.000000

SCIBA-Br S0

E = -6173.56843112 a.u.

C	-2.307587	1.057478	0.000000
C	-1.249274	2.133321	0.000000
C	0.096931	1.867097	0.000000
C	0.448770	0.492905	0.000000
C	-0.448770	-0.492905	-0.000000
C	2.307587	-1.057478	0.000000
C	1.249274	-2.133321	0.000000
C	-0.096931	-1.867097	-0.000000
N	-1.788553	-0.251279	0.000000
N	1.788553	0.251279	0.000000
C	-1.408474	-2.538866	0.000000
C	-2.412552	-1.525121	0.000000
C	-1.788553	-3.878888	0.000000
C	-3.766552	-1.823419	0.000000
C	-3.150108	-4.187369	0.000000
H	-1.031241	-4.662809	0.000000
C	-4.116517	-3.177181	0.000000
H	-4.504193	-1.022931	0.000000
H	-3.463980	-5.231375	0.000000
H	-5.173151	-3.448367	0.000000
C	1.408474	2.538866	0.000000
C	2.412552	1.525121	0.000000
C	1.788553	3.878888	0.000000
C	3.766552	1.823419	0.000000
C	3.150108	4.187369	0.000000
H	1.031241	4.662809	0.000000
C	4.116517	3.177181	0.000000
H	4.504193	1.022931	0.000000
H	3.463980	5.231375	0.000000
H	5.173151	3.448367	0.000000
O	3.496030	-1.268106	0.000000
O	-3.496030	1.268106	-0.000000
Br	1.912241	-3.878902	0.000000
Br	-1.912241	3.878902	-0.000000

SCIBA-Br T1

E = -6173.51928466 a.u.

C	-2.307587	1.057478	0.000000
C	-1.249274	2.133321	0.000000
C	0.096931	1.867097	0.000000
C	0.448770	0.492905	0.000000
C	-0.448770	-0.492905	-0.000000
C	2.307587	-1.057478	0.000000
C	1.249274	-2.133321	0.000000
C	-0.096931	-1.867097	-0.000000
N	-1.788553	-0.251279	0.000000
N	1.788553	0.251279	0.000000
C	-1.408474	-2.538866	0.000000
C	-2.412552	-1.525121	0.000000
C	-1.788553	-3.878888	0.000000
C	-3.766552	-1.823419	0.000000
C	-3.150108	-4.187369	0.000000
H	-1.031241	-4.662809	0.000000
C	-4.116517	-3.177181	0.000000
H	-4.504193	-1.022931	0.000000
H	-3.463980	-5.231375	0.000000
H	-5.173151	-3.448367	0.000000
C	1.408474	2.538866	0.000000
C	2.412552	1.525121	0.000000
C	1.788553	3.878888	0.000000
C	3.766552	1.823419	0.000000
C	3.150108	4.187369	0.000000
H	1.031241	4.662809	0.000000
C	4.116517	3.177181	0.000000
H	4.504193	1.022931	0.000000
H	3.463980	5.231375	0.000000
H	5.173151	3.448367	0.000000
O	3.496030	-1.268106	0.000000
O	-3.496030	1.268106	-0.000000
Br	1.912241	-3.878902	0.000000
Br	-1.912241	3.878902	-0.000000

SCIBA-I S0

E = -1621.03828540 a.u.

C	-1.921356	1.655823	-0.000000
C	-0.610130	2.400055	-0.000000
C	0.610130	1.769991	-0.000000
C	0.567494	0.350050	-0.000000
C	-0.567494	-0.350050	-0.000000
C	1.921356	-1.655823	-0.000000
C	0.610130	-2.400055	-0.000000
C	-0.610130	-1.769991	-0.000000
N	-1.786272	0.254593	-0.000000
N	1.786272	-0.254593	0.000000
C	-2.059945	-2.047831	0.000000
C	-2.740689	-0.793566	0.000000
C	-2.804971	-3.225566	0.000000
C	-4.123908	-0.697855	0.000000
C	-4.198244	-3.138202	0.000000
H	-2.304266	-4.193598	0.000000
C	-4.841720	-1.897402	0.000000
H	-4.604998	0.278532	-0.000000
H	-4.792535	-4.052141	0.000000
H	-5.931970	-1.859941	0.000000
C	2.059945	2.047831	0.000000
C	2.740689	0.793566	0.000000
C	2.804971	3.225566	0.000000
C	4.123908	0.697855	0.000000
C	4.198244	3.138202	0.000000
H	2.304266	4.193598	0.000000
C	4.841720	1.897402	0.000000
H	4.604998	-0.278532	0.000000
H	4.792535	4.052141	0.000000
H	5.931970	1.859941	0.000000
O	3.008882	-2.181670	0.000000
O	-3.008882	2.181670	0.000000
I	0.798999	-4.470737	0.000000
I	-0.798999	4.470737	0.000000

SCIBA-I T1

E = -1620.98867954 a.u.

C	-1.921356	1.655823	-0.000000
C	-0.610130	2.400055	-0.000000
C	0.610130	1.769991	-0.000000
C	0.567494	0.350050	-0.000000
C	-0.567494	-0.350050	-0.000000
C	1.921356	-1.655823	-0.000000
C	0.610130	-2.400055	-0.000000
C	-0.610130	-1.769991	-0.000000
N	-1.786272	0.254593	-0.000000
N	1.786272	-0.254593	0.000000
C	-2.059945	-2.047831	0.000000
C	-2.740689	-0.793566	0.000000
C	-2.804971	-3.225566	0.000000
C	-4.123908	-0.697855	0.000000
C	-4.198244	-3.138202	0.000000
H	-2.304266	-4.193598	0.000000
C	-4.841720	-1.897402	0.000000
H	-4.604998	0.278532	-0.000000
H	-4.792535	-4.052141	0.000000
H	-5.931970	-1.859941	0.000000
C	2.059945	2.047831	0.000000
C	2.740689	0.793566	0.000000
C	2.804971	3.225566	0.000000
C	4.123908	0.697855	0.000000
C	4.198244	3.138202	0.000000
H	2.304266	4.193598	0.000000
C	4.841720	1.897402	0.000000
H	4.604998	-0.278532	0.000000
H	4.792535	4.052141	0.000000
H	5.931970	1.859941	0.000000
O	3.008882	-2.181670	0.000000
O	-3.008882	2.181670	0.000000
I	0.798999	-4.470737	0.000000
I	-0.798999	4.470737	0.000000

BCIBA0 S0

E = -720.010169207 a.u.

C	-2.417748	-0.743939	0.000016
C	-1.530249	-1.948170	-0.000003
C	-0.157816	-1.866025	-0.000002
C	0.374870	-0.549478	0.000011
C	-0.374841	0.549491	0.000011
C	2.417734	0.743864	0.000050
C	1.530231	1.948174	0.000002
C	0.157815	1.866089	0.000003
N	-1.728007	0.503885	0.000009
N	1.728066	-0.503905	0.000020
C	-1.063674	2.690050	-0.000012
C	-2.141517	1.850121	-0.000003
C	1.063627	-2.690042	-0.000012
C	2.141514	-1.850169	-0.000010
H	2.078752	2.889630	-0.000018
O	3.624523	0.783516	-0.000036
H	-2.078627	-2.889708	-0.000015
O	-3.624535	-0.783451	-0.000014
H	-1.121873	3.774478	-0.000026
H	-3.204824	2.079457	-0.000010
H	3.204808	-2.079558	-0.000014
H	1.121777	-3.774474	-0.000022

BCIBA0 T1

E = -719.973712498 a.u.

C	-2.417748	-0.743939	0.000016
C	-1.530249	-1.948170	-0.000003
C	-0.157816	-1.866025	-0.000002
C	0.374870	-0.549478	0.000011
C	-0.374841	0.549491	0.000011
C	2.417734	0.743864	0.000050
C	1.530231	1.948174	0.000002
C	0.157815	1.866089	0.000003
N	-1.728007	0.503885	0.000009
N	1.728066	-0.503905	0.000020
C	-1.063674	2.690050	-0.000012
C	-2.141517	1.850121	-0.000003
C	1.063627	-2.690042	-0.000012
C	2.141514	-1.850169	-0.000010
H	2.078752	2.889630	-0.000018
O	3.624523	0.783516	-0.000036
H	-2.078627	-2.889708	-0.000015
O	-3.624535	-0.783451	-0.000014
H	-1.121873	3.774478	-0.000026
H	-3.204824	2.079457	-0.000010
H	3.204808	-2.079558	-0.000014
H	1.121777	-3.774474	-0.000022

BCIBA2 S0

E = -1333.93281757 a.u.

C	0.910950	2.365939	0.000134
C	-0.581111	2.410740	0.000211
C	-1.357595	1.281644	0.000126
C	-0.665506	0.040703	-0.000009
C	0.665506	-0.040703	-0.000048
C	-0.910950	-2.365939	-0.000214
C	0.581111	-2.410740	-0.000244
C	1.357595	-1.281644	-0.000165
N	1.461174	1.065699	0.000026
N	-1.461174	-1.065699	-0.000084
C	2.773686	-0.856523	-0.000153
C	2.795680	0.593003	-0.000030
C	-2.773686	0.856523	0.000132
C	-2.795680	-0.593003	-0.000000
H	0.989916	-3.420884	-0.000334
O	-1.622882	-3.346826	-0.000272

H	-0.989916	3.420884	0.000323
O	1.622882	3.346826	0.000373
C	3.956424	-1.550310	-0.000227
C	5.190664	-0.841535	-0.000186
C	5.189085	0.589218	-0.000067
C	6.434160	-1.530317	-0.000261
C	6.435414	1.271643	-0.000029
C	7.621786	-0.840618	-0.000221
H	6.426722	-2.622126	-0.000351
C	7.620515	0.576027	-0.000104
H	6.431693	2.363050	0.000060
H	8.569126	-1.380928	-0.000280
H	8.568444	1.115832	-0.000074
C	-3.956424	1.550310	0.000231
C	-5.190664	0.841535	0.000203
C	-5.189085	-0.589218	0.000073
C	-6.434160	1.530317	0.000303
C	-6.435414	-1.271643	0.000049
C	-7.621786	0.840618	0.000276
H	-6.426722	2.622126	0.000402
C	-7.620515	-0.576027	0.000147
H	-6.431693	-2.363050	-0.000050
H	-8.569126	1.380928	0.000354
H	-8.568444	-1.115832	0.000127
C	3.958964	1.310152	0.000011
C	-3.958964	-1.310152	-0.000029
H	-3.936061	-2.399235	-0.000128
H	-3.964517	2.642089	0.000331
H	3.936061	2.399235	0.000099
H	3.964517	-2.642089	-0.000318

BCIBA2 T1

E = -1333.87706431 a.u.

C	0.910950	2.365939	0.000134
C	-0.581111	2.410740	0.000211
C	-1.357595	1.281644	0.000126
C	-0.665506	0.040703	-0.000009
C	0.665506	-0.040703	-0.000048
C	-0.910950	-2.365939	-0.000214
C	0.581111	-2.410740	-0.000244
C	1.357595	-1.281644	-0.000165
N	1.461174	1.065699	0.000026
N	-1.461174	-1.065699	-0.000084
C	2.773686	-0.856523	-0.000153
C	2.795680	0.593003	-0.000030
C	-2.773686	0.856523	0.000132
C	-2.795680	-0.593003	-0.000000
H	0.989916	-3.420884	-0.000334
O	-1.622882	-3.346826	-0.000272
H	-0.989916	3.420884	0.000323
O	1.622882	3.346826	0.000373
C	3.956424	-1.550310	-0.000227
C	5.190664	-0.841535	-0.000186
C	5.189085	0.589218	-0.000067
C	6.434160	-1.530317	-0.000261
C	6.435414	1.271643	-0.000029
C	7.621786	-0.840618	-0.000221
H	6.426722	-2.622126	-0.000351
C	7.620515	0.576027	-0.000104
H	6.431693	2.363050	0.000060
H	8.569126	-1.380928	-0.000280
H	8.568444	1.115832	-0.000074
C	-3.956424	1.550310	0.000231
C	-5.190664	0.841535	0.000203
C	-5.189085	-0.589218	0.000073
C	-6.434160	1.530317	0.000303
C	-6.435414	-1.271643	0.000049
C	-7.621786	0.840618	0.000276
H	-6.426722	2.622126	0.000402
C	-7.620515	-0.576027	0.000147
H	-6.431693	-2.363050	-0.000050
H	-8.569126	1.380928	0.000354
H	-8.568444	-1.115832	0.000127
C	3.958964	1.310152	0.000011
C	-3.958964	-1.310152	-0.000029
H	-3.936061	-2.399235	-0.000128
H	-3.964517	2.642089	0.000331
H	3.936061	2.399235	0.000099
H	3.964517	-2.642089	-0.000318

BCIBA2a S0

E = -1333.93282887 a.u.

C	-0.745278	2.809606	-0.000120
C	0.742442	2.666801	-0.000098
C	1.369312	1.450169	-0.000047
C	0.524772	0.304845	-0.000014
C	-0.805665	0.390388	-0.000030
C	0.461316	-2.110114	0.000074
C	-1.021712	-1.966433	0.000060
C	-1.659313	-0.747384	0.000007
N	-1.456371	1.587036	-0.000081
N	1.174308	-0.890237	0.000037
C	-2.998545	-0.130468	-0.000028
C	-2.832254	1.267450	-0.000080
C	2.720605	0.849543	-0.000010
C	2.558729	-0.590947	0.000042
H	-1.538047	-2.924911	0.000095
O	1.044688	-3.173439	0.000132
H	1.273519	3.618276	-0.000127
O	-1.322932	3.873771	-0.000161
C	-4.308749	-0.682342	-0.000017
C	-5.412479	0.224395	-0.000059
C	-4.562282	-2.078424	0.000034
C	-6.731950	-0.302778	-0.000048
C	-5.852165	-2.553839	0.000043
H	-3.721571	-2.771597	0.000066
C	-6.949644	-1.659096	0.000002
H	-7.572841	0.393643	-0.000080

H	-6.033235	-3.629550	0.000082
H	-7.967271	-2.051268	0.000009
C	-3.914963	2.168568	-0.000122
C	-5.180619	1.631197	-0.000111
C	3.981211	1.388001	-0.000015
C	3.621099	-1.449737	0.000085
H	-6.047321	2.295195	-0.000142
H	-3.724287	3.240110	-0.000161
H	3.460122	-2.527149	0.000121
C	4.933166	-0.890210	0.000084
C	6.082582	-1.725226	0.000130
C	5.116324	0.528768	0.000038
C	7.346552	-1.185694	0.000124
H	5.939850	-2.807325	0.000160
C	6.436936	1.054055	0.000045
C	7.527607	0.219317	0.000086
H	8.218440	-1.841308	0.000152
H	6.567459	2.138141	0.000009
H	8.535952	0.634896	0.000081
H	4.127413	2.470122	-0.000052

BCIBA2a T1

E = -1333.88181933 a.u.

C	-0.745278	2.809606	-0.000120
C	0.742442	2.666801	-0.000098
C	1.369312	1.450169	-0.000047
C	0.524772	0.304845	-0.000014
C	-0.805665	0.390388	-0.000030
C	0.461316	-2.110114	0.000074
C	-1.021712	-1.966433	0.000060
C	-1.659313	-0.747384	0.000007
N	-1.456371	1.587036	-0.000081
N	1.174308	-0.890237	0.000037
C	-2.998545	-0.130468	-0.000028
C	-2.832254	1.267450	-0.000080
C	2.720605	0.849543	-0.000010
C	2.558729	-0.590947	0.000042
H	-1.538047	-2.924911	0.000095
O	1.044688	-3.173439	0.000132
H	1.273519	3.618276	-0.000127
O	-1.322932	3.873771	-0.000161
C	-4.308749	-0.682342	-0.000017
C	-5.412479	0.224395	-0.000059
C	-4.562282	-2.078424	0.000034
C	-6.731950	-0.302778	-0.000048
C	-5.852165	-2.553839	0.000043
H	-3.721571	-2.771597	0.000066
C	-6.949644	-1.659096	0.000002
H	-7.572841	0.393643	-0.000080
H	-6.033235	-3.629550	0.000082
H	-7.967271	-2.051268	0.000009
C	-3.914963	2.168568	-0.000122
C	-5.180619	1.631197	-0.000111
C	3.981211	1.388001	-0.000015
C	3.621099	-1.449737	0.000085
H	-6.047321	2.295195	-0.000142
H	-3.724287	3.240110	-0.000161
H	3.460122	-2.527149	0.000121
C	4.933166	-0.890210	0.000084
C	6.082582	-1.725226	0.000130
C	5.116324	0.528768	0.000038
C	7.346552	-1.185694	0.000124
H	5.939850	-2.807325	0.000160
C	6.436936	1.054055	0.000045
C	7.527607	0.219317	0.000086
H	8.218440	-1.841308	0.000152
H	6.567459	2.138141	0.000009
H	8.535952	0.634896	0.000081
H	4.127413	2.470122	-0.000052

BCIBA2b S0

E = -1333.92635650 a.u.

C	-1.280482	-1.972070	0.000095
C	0.200055	-2.169564	0.000123
C	1.096404	-1.141864	0.000079
C	0.526379	0.159318	0.000004
C	-0.792114	0.376511	-0.000024
C	1.041756	2.530545	-0.000109
C	-0.427479	2.734739	-0.000148
C	-1.318487	1.691228	-0.000103
N	-1.735407	-0.621049	0.000016
N	1.436058	1.173544	-0.000038
C	-2.761452	1.456206	-0.000112
C	-3.004248	0.067563	-0.000039
C	2.547162	-0.871052	0.000079
C	2.716378	0.567113	0.000003
H	-0.733125	3.780626	-0.000211
O	1.866734	3.419664	-0.000161
H	0.482295	-3.221760	0.000182
O	-2.025731	-2.926018	0.000137
C	-3.811187	2.399191	-0.000180
C	-5.101870	1.949597	-0.000174
C	-4.345842	-0.431169	-0.000032
C	-5.391390	0.554808	-0.000102
C	-4.721051	-1.804600	0.000038
C	-6.745839	0.127812	-0.000099
C	-6.044820	-2.174816	0.000038
H	-3.941485	-2.559895	0.000092
C	-7.072103	-1.204958	-0.000031
H	-7.526257	0.890989	-0.000153
H	-6.300807	-3.235098	0.000092
H	-8.117938	-1.515205	-0.000031
C	3.650145	-1.684839	0.000133
C	3.947008	1.160742	-0.000017
H	3.545279	-2.771618	0.000191
H	-3.578288	3.464558	-0.000235
H	-5.936587	2.652108	-0.000225
C	4.951164	-1.107208	0.000117

C	6.116318	-1.920957	0.000171
C	5.096567	0.316087	0.000047
C	7.368949	-1.357628	0.000154
H	5.995734	-3.006173	0.000220
C	6.406425	0.865887	0.000038
C	7.513546	0.051479	0.000090
H	8.255594	-1.992698	0.000192
H	6.515174	1.951935	-0.000012
H	8.512117	0.490721	0.000078
H	4.036353	2.246281	-0.000074

BCIBA2b T1

E = -1333.87460666 a.u.

C	-1.280482	-1.972070	0.000095
C	0.200055	-2.169564	0.000123
C	1.096404	-1.141864	0.000079
C	0.526379	0.159318	0.000004
C	-0.792114	0.376511	-0.000024
C	1.041756	2.530545	-0.000109
C	-0.427479	2.734739	-0.000148
C	-1.318487	1.691228	-0.000103
N	-1.735407	-0.621049	0.000016
N	1.436058	1.173544	-0.000038
C	-2.761452	1.456206	-0.000112
C	-3.004248	0.067563	-0.000039
C	2.547162	-0.871052	0.000079
C	2.716378	0.567113	0.000003
H	-0.733125	3.780626	-0.000211
O	1.866734	3.419664	-0.000161
H	0.482295	-3.221760	0.000182
O	-2.025731	-2.926018	0.000137
C	-3.811187	2.399191	-0.000180
C	-5.101870	1.949597	-0.000174
C	-4.345842	-0.431169	-0.000032
C	-5.391390	0.554808	-0.000102
C	-4.721051	-1.804600	0.000038
C	-6.745839	0.127812	-0.000099
C	-6.044820	-2.174816	0.000038
H	-3.941485	-2.559895	0.000092
C	-7.072103	-1.204958	-0.000031
H	-7.526257	0.890989	-0.000153
H	-6.300807	-3.235098	0.000092
H	-8.117938	-1.515205	-0.000031
C	3.650145	-1.684839	0.000133
C	3.947008	1.160742	-0.000017
H	3.545279	-2.771618	0.000191
H	-3.578288	3.464558	-0.000235
H	-5.936587	2.652108	-0.000225
C	4.951164	-1.107208	0.000117
C	6.116318	-1.920957	0.000171
C	5.096567	0.316087	0.000047
C	7.368949	-1.357628	0.000154
H	5.995734	-3.006173	0.000220
C	6.406425	0.865887	0.000038
C	7.513546	0.051479	0.000090
H	8.255594	-1.992698	0.000192
H	6.515174	1.951935	-0.000012
H	8.512117	0.490721	0.000078
H	4.036353	2.246281	-0.000074

BCIBA2c S0

E = -1333.93243161 a.u.

C	2.523768	-0.178484	0.000000
C	2.133063	1.261486	0.000000
C	0.825658	1.683778	0.000000
C	-0.153174	0.648541	0.000000
C	0.153174	-0.648541	0.000000
C	-2.523768	0.178484	0.000000
C	-2.133063	-1.261486	0.000000
C	-0.825658	-1.683778	0.000000
N	1.439558	-1.088178	0.000000
N	-1.439558	1.088178	0.000000
C	0.008906	-2.900090	0.000000
C	1.358083	-2.499317	0.000000
C	-0.008906	2.900090	0.000000
C	-1.358083	2.499317	0.000000
H	-2.992042	-1.930337	0.000000
O	-3.670526	0.569477	0.000000
H	2.992042	1.930337	0.000000
O	3.670526	-0.569477	0.000000
C	-0.313056	-4.284464	0.000000
C	0.768680	-5.218234	0.000000
C	-1.645456	-4.772256	0.000000
C	0.473773	-6.608161	0.000000
C	-1.894014	-6.124328	0.000000
H	-2.472040	-4.062265	0.000000
C	-0.825658	-7.053506	0.000000
H	1.303294	-7.318072	0.000000
H	-2.923224	-6.485847	0.000000
H	-1.038801	-8.123032	0.000000
C	2.430136	-3.412105	0.000000
C	2.115262	-4.750826	0.000000
C	0.313056	4.284464	0.000000
C	-0.768680	5.218234	0.000000
C	1.645456	4.772256	0.000000
C	-0.473773	6.608161	0.000000
C	1.894014	6.124328	0.000000
H	2.472040	4.062265	0.000000
C	0.825658	7.053506	0.000000
H	-1.303294	7.318072	0.000000
H	2.923224	6.485847	0.000000
H	1.038801	8.123032	0.000000
C	-2.430136	3.412105	0.000000
C	-2.115262	4.750826	0.000000
H	2.916559	-5.492554	0.000000
H	3.453237	-3.040514	0.000000
H	-3.453237	3.040514	0.000000
H	-2.916559	5.492554	0.000000

BCIBA2c T1

E = -1333.88567740 a.u.

C	2.523768	-0.178484	0.000000
C	2.133063	1.261486	0.000000
C	0.825658	1.683778	0.000000
C	-0.153174	0.648541	0.000000
C	0.153174	-0.648541	0.000000
C	-2.523768	0.178484	0.000000
C	-2.133063	-1.261486	0.000000
C	-0.825658	-1.683778	0.000000
N	1.439558	-1.088178	0.000000
N	-1.439558	1.088178	0.000000
C	0.008906	-2.900090	0.000000
C	1.358083	-2.499317	0.000000
C	-0.008906	2.900090	0.000000
C	-1.358083	2.499317	0.000000
H	-2.992042	-1.930337	0.000000
O	-3.670526	0.569477	0.000000
H	2.992042	1.930337	0.000000
O	3.670526	-0.569477	0.000000
C	-0.313056	-4.284464	0.000000
C	0.768680	-5.218234	0.000000
C	-1.645456	-4.772256	0.000000
C	0.473773	-6.608161	0.000000
C	-1.894014	-6.124328	0.000000
H	-2.472040	-4.062265	0.000000
C	-0.825658	-7.053506	0.000000
H	1.303294	-7.318072	0.000000
H	-2.923224	-6.485847	0.000000
H	-1.038801	-8.123032	0.000000
C	2.430136	-3.412105	0.000000
C	2.115262	-4.750826	0.000000
C	0.313056	4.284464	0.000000
C	-0.768680	5.218234	0.000000
C	1.645456	4.772256	0.000000
C	-0.473773	6.608161	0.000000
C	1.894014	6.124328	0.000000
H	2.472040	4.062265	0.000000
C	0.825658	7.053506	0.000000
H	-1.303294	7.318072	0.000000
H	2.923224	6.485847	0.000000
H	1.038801	8.123032	0.000000
C	-2.430136	3.412105	0.000000
C	-2.115262	4.750826	0.000000
H	2.916559	-5.492554	0.000000
H	3.453237	-3.040514	0.000000
H	-3.453237	3.040514	0.000000
H	-2.916559	5.492554	0.000000

BCIBA2d S0

E = -1333.91884166 a.u.

C	2.404512	-0.789198	0.000000
C	2.364027	0.694393	0.000000
C	1.203236	1.412405	0.000000
C	-0.001791	0.669452	0.000000
C	0.001791	-0.669452	0.000000
C	-2.404512	0.789198	0.000000
C	-2.364027	-0.694393	0.000000
C	-1.203236	-1.412405	0.000000
N	1.136840	-1.442595	0.000000
N	-1.136840	1.442595	0.000000
C	-0.742893	-2.797184	0.000000
C	0.664890	-2.809611	0.000000
C	0.742893	2.797184	0.000000
C	-0.664890	2.809611	0.000000
H	-3.354523	-1.147773	0.000000
O	-3.459912	1.383688	0.000000
H	3.354523	1.147773	0.000000
O	3.459912	-1.383688	0.000000
C	-1.507621	-3.982910	0.000000
C	-0.856708	-5.184287	0.000000
C	1.373331	-4.054277	0.000000
C	0.566462	-5.244967	0.000000
C	2.788788	-4.208052	0.000000
C	1.203236	-6.514057	0.000000
C	3.364444	-5.456416	0.000000
H	3.411284	-3.319199	0.000000
C	2.570927	-6.624569	0.000000
H	0.573622	-7.405680	0.000000
H	4.451998	-5.539755	0.000000
H	3.042941	-7.608076	0.000000
C	1.507621	3.982910	0.000000
C	0.856708	5.184287	0.000000
C	-1.373331	4.054277	0.000000
C	-2.788788	4.208052	0.000000
C	-0.566462	5.244967	0.000000
C	-3.364444	5.456416	0.000000
H	-3.411284	3.319199	0.000000
C	-1.203236	6.514057	0.000000
C	-2.570927	6.624569	0.000000
H	-4.451998	5.539755	0.000000
H	-0.573622	7.405680	0.000000
H	-3.042941	7.608076	0.000000
H	1.414882	6.121768	0.000000
H	2.596460	3.922150	0.000000
H	-2.596460	-3.922150	0.000000
H	-1.414882	-6.121768	0.000000

BCIBA2d T1

E = -1333.87073034 a.u.

C	2.404512	-0.789198	0.000000
C	2.364027	0.694393	0.000000
C	1.203236	1.412405	0.000000
C	-0.001791	0.669452	0.000000
C	0.001791	-0.669452	0.000000
C	-2.404512	0.789198	0.000000

C	-2.364027	-0.694393	0.000000
C	-1.203236	-1.412405	0.000000
N	1.136840	-1.442595	0.000000
N	-1.136840	1.442595	0.000000
C	-0.742893	-2.797184	0.000000
C	0.664890	-2.809611	0.000000
C	0.742893	2.797184	0.000000
C	-0.664890	2.809611	0.000000
H	-3.354523	-1.147773	0.000000
O	-3.459912	1.383688	0.000000
H	3.354523	1.147773	0.000000
O	3.459912	-1.383688	0.000000
C	-1.507621	-3.982910	0.000000
C	-0.856708	-5.184287	0.000000
C	1.373331	-4.054277	0.000000
C	0.566462	-5.244967	0.000000
C	2.788788	-4.208052	0.000000
C	1.203236	-6.514057	0.000000
C	3.364444	-5.456416	0.000000
H	3.411284	-3.319199	0.000000
C	2.570927	-6.624569	0.000000
H	0.573622	-7.405680	0.000000
H	4.451998	-5.539755	0.000000
H	3.042941	-7.608076	0.000000
C	1.507621	3.982910	0.000000
C	0.856708	5.184287	0.000000
C	-1.373331	4.054277	0.000000
C	-2.788788	4.208052	0.000000
C	-0.566462	5.244967	0.000000
C	-3.364444	5.456416	0.000000
H	-3.411284	3.319199	0.000000
C	-1.203236	6.514057	0.000000
C	-2.570927	6.624569	0.000000
H	-4.451998	5.539755	0.000000
H	-0.573622	7.405680	0.000000
H	-3.042941	7.608076	0.000000
H	1.414882	6.121768	0.000000
H	2.596460	3.922150	0.000000
H	-2.596460	-3.922150	0.000000
H	-1.414882	-6.121768	0.000000

BCIBA2e S0

E = -1333.92612617 a.u.

C	0.890388	2.972559	0.000054
C	-0.594698	2.991824	0.000059
C	-1.346362	1.846018	0.000041
C	-0.657619	0.605967	0.000013
C	0.677070	0.554491	0.000004
C	-0.842911	-1.782483	-0.000070
C	0.648410	-1.792204	-0.000050
C	1.417381	-0.659921	-0.000027
N	1.452876	1.673804	0.000025
N	-1.467156	-0.499614	-0.000013
C	2.812610	-0.191366	-0.000022
C	2.789920	1.214476	0.000001
C	-2.748750	1.431261	0.000039
C	-2.814055	0.023629	0.000010
H	1.045088	-2.805850	-0.000072
O	-1.463415	-2.822740	-0.000065
H	-1.027253	3.991872	0.000079
O	1.592448	3.960139	0.000065
C	4.056696	-0.878094	-0.000039
C	5.248430	-0.090291	-0.000033
C	4.163728	-2.292839	-0.000064
C	6.506196	-0.751273	-0.000052
C	5.397591	-2.899051	-0.000083
H	3.255635	-2.895308	-0.000070
C	6.581902	-2.122836	-0.000077
H	7.414658	-0.145695	-0.000048
H	5.466308	-3.987741	-0.000103
H	7.553385	-2.618338	-0.000092
C	3.959358	1.999212	0.000010
C	5.162611	1.332648	-0.000011
C	-3.908841	2.234265	0.000061
C	-5.132553	1.624906	0.000064
C	-4.080842	-0.640872	0.000015
C	-4.278195	-2.051004	0.000003
C	-5.243170	0.204897	0.000041
C	-5.544246	-2.586049	0.000014
H	-3.408472	-2.700695	-0.000020
C	-6.532346	-0.390792	0.000050
C	-6.686321	-1.754245	0.000037
H	-5.663636	-3.670243	0.000003
H	-7.403509	0.266889	0.000070
H	-7.684350	-2.194734	0.000046
H	-6.049463	2.216038	0.000084
H	-3.812304	3.320458	0.000081
H	3.879918	3.084518	0.000029
H	6.093399	1.903304	-0.000006

BCIBA2e T1

E = -1333.87863451 a.u.

C	0.890388	2.972559	0.000054
C	-0.594698	2.991824	0.000059
C	-1.346362	1.846018	0.000041
C	-0.657619	0.605967	0.000013
C	0.677070	0.554491	0.000004
C	-0.842911	-1.782483	-0.000070
C	0.648410	-1.792204	-0.000050
C	1.417381	-0.659921	-0.000027
N	1.452876	1.673804	0.000025
N	-1.467156	-0.499614	-0.000013
C	2.812610	-0.191366	-0.000022
C	2.789920	1.214476	0.000001
C	-2.748750	1.431261	0.000039
C	-2.814055	0.023629	0.000010
H	1.045088	-2.805850	-0.000072
O	-1.463415	-2.822740	-0.000065

H	-1.027253	3.991872	0.000079
O	1.592448	3.960139	0.000065
C	4.056696	-0.878094	-0.000039
C	5.248430	-0.090291	-0.000033
C	4.163728	-2.292839	-0.000064
C	6.506196	-0.751273	-0.000052
C	5.397591	-2.899051	-0.000083
H	3.255635	-2.895308	-0.000070
C	6.581902	-2.122836	-0.000077
H	7.414658	-0.145695	-0.000048
H	5.466308	-3.987741	-0.000103
H	7.553385	-2.618338	-0.000092
C	3.959358	1.999212	0.000010
C	5.162611	1.332648	-0.000011
C	-3.908841	2.234265	0.000061
C	-5.132553	1.624906	0.000064
C	-4.080842	-0.640872	0.000015
C	-4.278195	-2.051004	0.000003
C	-5.243170	0.204897	0.000041
C	-5.544246	-2.586049	0.000014
H	-3.408472	-2.700695	-0.000020
C	-6.532346	-0.390792	0.000050
C	-6.686321	-1.754245	0.000037
H	-5.663636	-3.670243	0.000003
H	-7.403509	0.266889	0.000070
H	-7.684350	-2.194734	0.000046
H	-6.049463	2.216038	0.000084
H	-3.812304	3.320458	0.000081
H	3.879918	3.084518	0.000029
H	6.093399	1.903304	-0.000006

BCIBA3 S0

E = -1640.86251526 a.u.

C	-0.790798	2.396199	0.000047
C	0.689271	2.358304	0.000007
C	1.423506	1.205108	0.000052
C	0.671333	0.000724	0.000099
C	-0.671329	-0.000467	0.000092
C	0.790853	-2.395965	0.000281
C	-0.689218	-2.358084	0.000183
C	-1.423451	-1.204881	0.000121
N	-1.450150	1.131922	0.000044
N	1.450127	-1.131670	0.000149
C	-2.809260	-0.738941	0.000060
C	-2.816127	0.654149	0.000002
C	2.809321	0.739116	0.000052
C	2.816081	-0.653956	0.000081
H	-1.104466	-3.362102	0.000207
O	1.369631	-3.460506	0.000266
H	1.104510	3.362323	-0.000047
O	-1.369445	3.460810	-0.000072
C	-4.017379	-1.516520	0.000055
C	-5.258221	-0.837957	-0.000037
C	-3.989933	-2.928660	0.000146
C	-6.439829	-1.615720	-0.000032
C	-5.158245	-3.660440	0.000145
H	-3.034758	-3.445928	0.000221
C	-6.395084	-2.995088	0.000055
H	-7.414993	-1.133967	-0.000095
H	-5.119927	-4.750294	0.000216
H	-7.323851	-3.566901	0.000058
C	-4.065464	1.388065	-0.000106
C	-5.275687	0.622707	-0.000135
C	-4.158592	2.800666	-0.000200
C	-6.504806	1.318067	-0.000265
C	-5.379938	3.441377	-0.000318
H	-3.245495	3.384913	-0.000174
C	-6.566171	2.695770	-0.000355
H	-7.438249	0.760508	-0.000302
H	-5.412412	4.531413	-0.000385
H	-7.535349	3.196577	-0.000459
C	4.017544	1.516554	0.000032
C	5.258312	0.837828	0.000014
C	3.990288	2.928699	0.000046
C	6.440017	1.615443	0.000025
C	5.158695	3.660326	0.000049
H	3.035190	3.446097	0.000059
C	6.395448	2.994815	0.000042
H	7.415122	1.133570	0.000029
H	5.120519	4.750185	0.000063
H	7.324289	3.566509	0.000053
C	4.065285	-1.388036	0.000013
C	4.158127	-2.800647	-0.000052
C	5.275607	-0.622852	-0.000028
C	5.379363	-3.441568	-0.000146
H	3.244902	-3.384721	-0.000013
C	6.504601	-1.318425	-0.000127
C	6.565720	-2.696149	-0.000184
H	5.411646	-4.531610	-0.000190
H	7.438144	-0.761033	-0.000174
H	7.534815	-3.197115	-0.000267

BCIBA3 T1

E = -1640.81613526 a.u.

C	-0.790798	2.396199	0.000047
C	0.689271	2.358304	0.000007
C	1.423506	1.205108	0.000052
C	0.671333	0.000724	0.000099
C	-0.671329	-0.000467	0.000092
C	0.790853	-2.395965	0.000281
C	-0.689218	-2.358084	0.000183
C	-1.423451	-1.204881	0.000121
N	-1.450150	1.131922	0.000044
N	1.450127	-1.131670	0.000149
C	-2.809260	-0.738941	0.000060
C	-2.816127	0.654149	0.000002
C	2.809321	0.739116	0.000052
C	2.816081	-0.653956	0.000081

H	-1.104466	-3.362102	0.000207
O	1.369631	-3.460506	0.000266
H	1.104510	3.362323	-0.000047
O	-1.369445	3.460810	-0.000072
C	-4.017379	-1.516520	0.000055
C	-5.258221	-0.837957	-0.000037
C	-3.989933	-2.928660	0.000146
C	-6.439829	-1.615720	-0.000032
C	-5.158245	-3.660440	0.000145
H	-3.034758	-3.445928	0.000221
C	-6.395084	-2.995088	0.000055
H	-7.414993	-1.133967	-0.000095
H	-5.119927	-4.750294	0.000216
H	-7.323851	-3.566901	0.000058
C	-4.065464	1.388065	-0.000106
C	-5.275687	0.622707	-0.000135
C	-4.158592	2.800666	-0.000200
C	-6.504806	1.318067	-0.000265
C	-5.379938	3.441377	-0.000318
H	-3.245495	3.384913	-0.000174
C	-6.566171	2.695770	-0.000355
H	-7.438249	0.760508	-0.000302
H	-5.412412	4.531413	-0.000385
H	-7.535349	3.196577	-0.000459
C	4.017544	1.516554	0.000032
C	5.258312	0.837828	0.000014
C	3.990288	2.928699	0.000046
C	6.440017	1.615443	0.000025
C	5.158695	3.660326	0.000049
H	3.035190	3.446097	0.000059
C	6.395448	2.994815	0.000042
H	7.415122	1.133570	0.000029
H	5.120519	4.750185	0.000063
H	7.324289	3.566509	0.000053
C	4.065285	-1.388036	0.000013
C	4.158127	-2.800647	-0.000052
C	5.275607	-0.622852	-0.000028
C	5.379363	-3.441568	-0.000146
H	3.244902	-3.384721	-0.000013
C	6.504601	-1.318425	-0.000127
C	6.565720	-2.696149	-0.000184
H	5.411646	-4.531610	-0.000190
H	7.438144	-0.761033	-0.000174
H	7.534815	-3.197115	-0.000267

BCIBA3_S1 S0

E = -2411.56250266 a.u.

C	-1.380745	2.103669	0.134938
C	-2.319633	0.931884	0.034652
C	-1.828006	-0.368221	0.118221
C	-0.426233	-0.518698	0.062375
C	0.426233	0.518698	0.062375
C	1.380745	-2.103669	0.134938
C	2.319633	-0.931884	0.034652
C	1.828006	0.368221	0.118221
N	0.004789	1.818442	0.015629
N	-0.004789	-1.818442	0.015629
C	2.302706	1.755976	0.188077
C	1.205854	2.602471	0.018550
C	-2.302706	-1.755976	0.188077
C	-1.205854	-2.602471	0.018550
O	1.779847	-3.235022	0.304041
O	-1.779847	3.235022	0.304041
C	3.603238	2.304867	0.496746
C	3.802504	3.698582	0.327592
C	4.630954	1.525276	1.075392
C	5.061091	4.242033	0.670808
C	5.845844	2.086594	1.411373
H	4.448706	0.476431	1.300320
C	6.070042	3.454626	1.188635
H	5.239801	5.310175	0.562354
H	6.616332	1.467070	1.871931
H	7.026483	3.905654	1.455987
C	1.380745	4.009881	-0.260123
C	2.705018	4.532519	-0.155800
C	0.348860	4.850924	-0.741767
C	2.925203	5.876396	-0.528304
C	0.603954	6.158527	-1.098379
H	-0.659701	4.462157	-0.824323
C	1.901825	6.678912	-0.989194
H	3.930043	6.290901	-0.477928
H	-0.209253	6.781794	-1.471869
H	2.108389	7.710524	-1.277348
C	-3.603238	-2.304867	0.496746
C	-3.802504	-3.698582	0.327592
C	-4.630954	-1.525276	1.075392
C	-5.061091	-4.242033	0.670808
C	-5.845844	-2.086594	1.411373
H	-4.448706	-0.476431	1.300320
C	-6.070042	-3.454626	1.188635
H	-5.239801	-5.310175	0.562354
H	-6.616332	-1.467070	1.871931
H	-7.026483	-3.905654	1.455987
C	-1.380745	-4.009881	-0.260123
C	-0.348860	-4.850924	-0.741767
C	-2.705018	-4.532519	-0.155800
C	-0.603954	-6.158527	-1.098379
H	0.659701	-4.462157	-0.824323
C	-2.925203	-5.876396	-0.528304
C	-1.901825	-6.678912	-0.989194
H	0.209253	-6.781794	-1.471869
H	-3.930043	-6.290901	-0.477928
H	-2.108389	-7.710524	-1.277348
C	3.723025	-1.193491	-0.238201
C	4.438765	-2.330626	-0.072017
H	4.249645	-0.327707	-0.646435
H	3.972213	-3.212313	0.364576
C	5.855140	-2.436646	-0.425897
C	6.506697	-3.588182	-0.146512

C	6.470246	-1.302348	-1.163104
H	5.914507	-4.397312	0.296819
C	7.909758	-3.915945	-0.424857
C	7.539975	-0.587749	-0.797068
H	5.934827	-0.993828	-2.067619
C	8.991968	-3.213571	-0.052982
H	8.081738	-4.890298	-0.895405
C	8.384131	-0.810796	0.390458
H	7.810746	0.275774	-1.414959
H	9.972538	-3.658408	-0.254172
C	9.018953	-1.949682	0.702773
H	8.583109	0.068894	1.012074
H	9.693318	-1.934567	1.565955
C	-3.723025	1.193491	-0.238201
C	-4.438765	2.330626	-0.072017
H	-4.249645	0.327707	-0.646435
H	-3.972213	3.212313	0.364576
C	-5.855140	2.436646	-0.425897
C	-6.506697	3.588182	-0.146512
C	-6.470246	1.302348	-1.163104
H	-5.914507	4.397312	0.296819
C	-7.909758	3.915945	-0.424857
C	-7.539975	0.587749	-0.797068
H	-5.934827	0.993828	-2.067619
C	-8.991968	3.213571	-0.052982
H	-8.081738	4.890298	-0.895405
C	-8.384131	0.810796	0.390458
H	-7.810746	-0.275774	-1.414959
H	-9.972538	3.658408	-0.254172
C	-9.018953	1.949682	0.702773
H	-8.583109	-0.068894	1.012074
H	-9.693318	1.934567	1.565955

BCIBA3_S1 T1

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C	-2.319633	0.931884	0.034652
C	-1.828006	-0.368221	0.118221
C	-0.426233	-0.518698	0.062375
C	0.426233	0.518698	0.062375
C	1.380745	-2.103669	0.134938
C	2.319633	-0.931884	0.034652
C	1.828006	0.368221	0.118221
N	0.004789	1.818442	0.015629
N	-0.004789	-1.818442	0.015629
C	2.302706	1.755976	0.188077
C	1.205854	2.602471	0.018550
C	-2.302706	-1.755976	0.188077
C	-1.205854	-2.602471	0.018550
O	1.779847	-3.235022	0.304041
O	-1.779847	3.235022	0.304041
C	3.603238	2.304867	0.496746
C	3.802504	3.698582	0.327592
C	4.630954	1.525276	1.075392
C	5.061091	4.242033	0.670808
C	5.845844	2.086594	1.411373
H	4.448706	0.476431	1.300320
C	6.070042	3.454626	1.188635
H	5.239801	5.310175	0.562354
H	6.616332	1.467070	1.871931
H	7.026483	3.905654	1.455987
C	1.380745	4.009881	-0.260123
C	2.705018	4.532519	-0.155800
C	0.348860	4.850924	-0.741767
C	2.925203	5.876396	-0.528304
C	0.603954	6.158527	-1.098379
H	-0.659701	4.462157	-0.824323
C	1.901825	6.678912	-0.989194
H	3.930043	6.290901	-0.477928
H	-0.209253	6.781794	-1.471869
H	2.108389	7.710524	-1.277348
C	-3.603238	-2.304867	0.496746
C	-3.802504	-3.698582	0.327592
C	-4.630954	-1.525276	1.075392
C	-5.061091	-4.242033	0.670808
C	-5.845844	-2.086594	1.411373
H	-4.448706	-0.476431	1.300320
C	-6.070042	-3.454626	1.188635
H	-5.239801	-5.310175	0.562354
H	-6.616332	-1.467070	1.871931
H	-7.026483	-3.905654	1.455987
C	-1.380745	-4.009881	-0.260123
C	-0.348860	-4.850924	-0.741767
C	-2.705018	-4.532519	-0.155800
C	-0.603954	-6.158527	-1.098379
H	0.659701	-4.462157	-0.824323
C	-2.925203	-5.876396	-0.528304
C	-1.901825	-6.678912	-0.989194
H	0.209253	-6.781794	-1.471869
H	-3.930043	-6.290901	-0.477928
H	-2.108389	-7.710524	-1.277348
C	3.723025	-1.193491	-0.238201
C	4.438765	-2.330626	-0.072017
H	4.249645	-0.327707	-0.646435
H	3.972213	-3.212313	0.364576
C	5.855140	-2.436646	-0.425897
C	6.506697	-3.588182	-0.146512
C	6.470246	-1.302348	-1.163104
H	5.914507	-4.397312	0.296819
C	7.909758	-3.915945	-0.424857
C	7.539975	-0.587749	-0.797068
H	5.934827	-0.993828	-2.067619
C	8.991968	-3.213571	-0.052982
H	8.081738	-4.890298	-0.895405
C	8.384131	-0.810796	0.390458
H	7.810746	0.275774	-1.414959
H	9.972538	-3.658408	-0.254172
C	9.018953	-1.949682	0.702773
H	8.583109	0.068894	1.012074

H	9.693318	-1.934567	1.565955
C	-3.723025	1.193491	-0.238201
C	-4.438765	2.330626	-0.072017
H	-4.249645	0.327707	-0.646435
H	-3.972213	3.212313	0.364576
C	-5.855140	2.436646	-0.425897
C	-6.506697	3.588182	-0.146512
C	-6.470246	1.302348	-1.163104
H	-5.914507	4.397312	0.296819
C	-7.909758	3.915945	-0.424857
C	-7.539975	0.587749	-0.797068
H	-5.934827	0.993828	-2.067619
C	-8.991968	3.213571	-0.052982
H	-8.081738	4.890298	-0.895405
C	-8.384131	0.810796	0.390458
H	-7.810746	-0.275774	-1.414959
H	-9.972538	3.658408	-0.254172
C	-9.018953	1.949682	0.702773
H	-8.583109	-0.068894	1.012074
H	-9.693318	1.934567	1.565955

BCIBA3_S2 S0

E = -2257.06508896 a.u.

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C	-0.954135	-2.310243	0.119107
C	0.350197	-1.831276	0.200021
C	0.514573	-0.430885	0.145250
C	-0.514573	0.430885	0.145250
C	2.116962	1.360560	0.220561
C	0.954135	2.310243	0.119107
C	-0.350197	1.831276	0.200021
N	-1.818263	0.022074	0.098679
N	1.818263	-0.022074	0.098679
C	-1.733736	2.319561	0.267833
C	-2.590612	1.230829	0.098662
C	1.733736	-2.319561	0.267833
C	2.590612	-1.230829	0.098662
O	3.251804	1.747956	0.393053
O	-3.251804	-1.747956	0.393053
C	-2.270387	3.626987	0.567942
C	-3.660446	3.840947	0.389356
C	-1.482533	4.651034	1.143492
C	-4.190119	5.110133	0.715924
C	-2.029409	5.878305	1.459085
H	-0.439285	4.454052	1.383458
C	-3.393377	6.116287	1.224180
H	-5.255183	5.300996	0.598780
H	-1.403717	6.649936	1.909936
H	-3.833184	7.082313	1.474854
C	-3.995495	1.418771	-0.184048
C	-4.504759	2.748992	-0.088636
C	-4.845859	0.392876	-0.661980
C	-5.845574	2.980662	-0.465034
C	-6.149995	0.659247	-1.022922
H	-4.467290	-0.619990	-0.738492
C	-6.657453	1.962837	-0.921798
H	-6.250541	3.989618	-0.420749
H	-6.780578	-0.149604	-1.393517
H	-7.686396	2.178179	-1.212981
C	2.270387	-3.626987	0.567942
C	3.660446	-3.840947	0.389356
C	1.482533	-4.651034	1.143492
C	4.190119	-5.110133	0.715924
C	2.029409	-5.878305	1.459085
H	0.439285	-4.454052	1.383458
C	3.393377	-6.116287	1.224180
H	5.255183	-5.300996	0.598780
H	1.403717	-6.649936	1.909936
H	3.833184	-7.082313	1.474854
C	3.995495	-1.418771	-0.184048
C	4.845859	-0.392876	-0.661980
C	4.504759	-2.748992	-0.088636
C	6.149995	-0.659247	-1.022922
H	4.467290	0.619990	-0.738492
C	5.845574	-2.980662	-0.465034
C	6.657453	-1.962837	-0.921798
H	6.780578	0.149604	-1.393517
H	6.250541	-3.989618	-0.420749
H	7.686396	-2.178179	-1.212981
C	1.225637	3.714943	-0.145485
C	2.362652	4.421632	0.034981
H	0.366336	4.234183	-0.574912
H	3.239829	3.926631	0.448870
C	-1.225637	-3.714943	-0.145485
C	-2.362652	-4.421632	0.034981
H	-0.366336	-4.234183	-0.574912
H	-3.239829	-3.926631	0.448870
C	2.511000	5.847717	-0.283360
C	3.790533	6.420737	-0.205550
C	1.433725	6.676367	-0.646672
C	3.995495	7.767280	-0.495247
H	4.633749	5.790182	0.083952
C	1.637760	8.021394	-0.932699
H	0.420473	6.272457	-0.691388
C	2.919212	8.573175	-0.861869
H	4.999626	8.189318	-0.432486
H	0.788771	8.648205	-1.209991
H	3.074663	9.629237	-1.087073
C	-2.511000	-5.847717	-0.283360
C	-3.790533	-6.420737	-0.205550
C	-1.433725	-6.676367	-0.646672
C	-3.995495	-7.767280	-0.495247
H	-4.633749	-5.790182	0.083952
C	-1.637760	-8.021394	-0.932699
H	-0.420473	-6.272457	-0.691388
C	-2.919212	-8.573175	-0.861869
H	-4.999626	-8.189318	-0.432486
H	-0.788771	-8.648205	-1.209991
H	-3.074663	-9.629237	-1.087073

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C	-0.954135	-2.310243	0.119107
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C	0.514573	-0.430885	0.145250
C	-0.514573	0.430885	0.145250
C	2.116962	1.360560	0.220561
C	0.954135	2.310243	0.119107
C	-0.350197	1.831276	0.200021
N	-1.818263	0.022074	0.098679
N	1.818263	-0.022074	0.098679
C	-1.733736	2.319561	0.267833
C	-2.590612	1.230829	0.098662
C	1.733736	-2.319561	0.267833
C	2.590612	-1.230829	0.098662
O	3.251804	1.747956	0.393053
O	-3.251804	-1.747956	0.393053
C	-2.270387	3.626987	0.567942
C	-3.660446	3.840947	0.389356
C	-1.482533	4.651034	1.143492
C	-4.190119	5.110133	0.715924
C	-2.029409	5.878305	1.459085
H	-0.439285	4.454052	1.383458
C	-3.393377	6.116287	1.224180
H	-5.255183	5.300996	0.598780
H	-1.403717	6.649936	1.909936
H	-3.833184	7.082313	1.474854
C	-3.995495	1.418771	-0.184048
C	-4.504759	2.748992	-0.088636
C	-4.845859	0.392876	-0.661980
C	-5.845574	2.980662	-0.465034
C	-6.149995	0.659247	-1.022922
H	-4.467290	-0.619990	-0.738492
C	-6.657453	1.962837	-0.921798
H	-6.250541	3.989618	-0.420749
H	-6.780578	-0.149604	-1.393517
H	-7.686396	2.178179	-1.212981
C	2.270387	-3.626987	0.567942
C	3.660446	-3.840947	0.389356
C	1.482533	-4.651034	1.143492
C	4.190119	-5.110133	0.715924
C	2.029409	-5.878305	1.459085
H	0.439285	-4.454052	1.383458
C	3.393377	-6.116287	1.224180
H	5.255183	-5.300996	0.598780
H	1.403717	-6.649936	1.909936
H	3.833184	-7.082313	1.474854
C	3.995495	-1.418771	-0.184048
C	4.845859	-0.392876	-0.661980
C	4.504759	-2.748992	-0.088636
C	6.149995	-0.659247	-1.022922
H	4.467290	0.619990	-0.738492
C	5.845574	-2.980662	-0.465034
C	6.657453	-1.962837	-0.921798
H	6.780578	0.149604	-1.393517
H	6.250541	-3.989618	-0.420749
H	7.686396	-2.178179	-1.212981
C	1.225637	3.714943	-0.145485
C	2.362652	4.421632	0.034981
H	0.366336	4.234183	-0.574912
H	3.239829	3.926631	0.448870
C	-1.225637	-3.714943	-0.145485
C	-2.362652	-4.421632	0.034981
H	-0.366336	-4.234183	-0.574912
H	-3.239829	-3.926631	0.448870
C	2.511000	5.847717	-0.283360
C	3.790533	6.420737	-0.205550
C	1.433725	6.676367	-0.646672
C	3.995495	7.767280	-0.495247
H	4.633749	5.790182	0.083952
C	1.637760	8.021394	-0.932699
H	0.420473	6.272457	-0.691388
C	2.919212	8.573175	-0.861869
H	4.999626	8.189318	-0.432486
H	0.788771	8.648205	-1.209991
H	3.074663	9.629237	-1.087073
C	-2.511000	-5.847717	-0.283360
C	-3.790533	-6.420737	-0.205550
C	-1.433725	-6.676367	-0.646672
C	-3.995495	-7.767280	-0.495247
H	-4.633749	-5.790182	0.083952
C	-1.637760	-8.021394	-0.932699
H	-0.420473	-6.272457	-0.691388
C	-2.919212	-8.573175	-0.861869
H	-4.999626	-8.189318	-0.432486
H	-0.788771	-8.648205	-1.209991
H	-3.074663	-9.629237	-1.087073

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C	0.671098	0.011142	0.076762
C	-0.671098	-0.011139	0.076764
C	0.809796	-2.374475	-0.104487
C	-0.684882	-2.338793	-0.074042
C	-1.443869	-1.203846	-0.014730
N	-1.442826	1.125760	0.073337
N	1.442826	-1.125757	0.073401
C	-2.831873	-0.717043	-0.039200
C	-2.808350	0.671030	0.061361
C	2.831873	0.717042	-0.039235
C	2.808350	-0.671027	0.061392
O	1.382416	-3.422397	-0.281800
O	-1.382419	3.422382	-0.281985

C	-4.073007	-1.438827	-0.165330
C	-5.285050	-0.703125	-0.134439
C	-4.113718	-2.838428	-0.354656
C	-6.496933	-1.406902	-0.323241
C	-5.313257	-3.496859	-0.525012
H	-3.187133	-3.402715	-0.377592
C	-6.516221	-2.772767	-0.515740
H	-7.443885	-0.871671	-0.329027
H	-5.322196	-4.577057	-0.674695
H	-7.467309	-3.285920	-0.662692
C	-4.020135	1.439896	0.227291
C	-5.256439	0.734629	0.116821
C	-4.044275	2.815026	0.565511
C	-6.455581	1.459462	0.300103
C	-5.235367	3.483499	0.750763
H	-3.111521	3.357523	0.663496
C	-6.453655	2.804048	0.605349
H	-7.412444	0.948609	0.223439
H	-5.221727	4.542327	1.010903
H	-7.398993	3.329674	0.746453
C	4.073007	1.438820	-0.165399
C	5.285050	0.703120	-0.134471
C	4.113718	2.838412	-0.354793
C	6.496933	1.406889	-0.323303
C	5.313257	3.496835	-0.525177
H	3.187133	3.402698	-0.377758
C	6.516222	2.772745	-0.515866
H	7.443886	0.871659	-0.329060
H	5.322196	4.577026	-0.674912
H	7.467310	3.285891	-0.662840
C	4.020136	-1.439885	0.227353
C	4.044277	-2.815002	0.565629
C	5.256440	-0.734622	0.116853
C	5.235369	-3.483466	0.750909
H	3.111523	-3.357494	0.663635
C	6.455582	-1.459448	0.300165
C	6.453656	-2.804021	0.605468
H	5.221729	-4.542283	1.011092
H	7.412445	-0.948597	0.223479
H	7.398995	-3.329640	0.746594
F	-1.182763	-3.559709	-0.175019
F	1.182761	3.559701	-0.175207

BCIBA3_S3 T1

E = -1839.06836603 a.u.

C	-0.809797	2.374467	-0.104635
C	0.684880	2.338789	-0.074170
C	1.443868	1.203846	-0.014795
C	0.671098	0.011142	0.076762
C	-0.671098	-0.011139	0.076764
C	0.809796	-2.374475	-0.104487
C	-0.684882	-2.338793	-0.074042
C	-1.443869	-1.203846	-0.014730
N	-1.442826	1.125760	0.073337
N	1.442826	-1.125757	0.073401
C	-2.831873	-0.717043	-0.039200
C	-2.808350	0.671030	0.061361
C	2.831873	0.717042	-0.039235
C	2.808350	-0.671027	0.061392
O	1.382416	-3.422397	-0.281800
O	-1.382419	3.422382	-0.281985
C	-4.073007	-1.438827	-0.165330
C	-5.285050	-0.703125	-0.134439
C	-4.113718	-2.838428	-0.354656
C	-6.496933	-1.406902	-0.323241
C	-5.313257	-3.496859	-0.525012
H	-3.187133	-3.402715	-0.377592
C	-6.516221	-2.772767	-0.515740
H	-7.443885	-0.871671	-0.329027
H	-5.322196	-4.577057	-0.674695
H	-7.467309	-3.285920	-0.662692
C	-4.020135	1.439896	0.227291
C	-5.256439	0.734629	0.116821
C	-4.044275	2.815026	0.565511
C	-6.455581	1.459462	0.300103
C	-5.235367	3.483499	0.750763
H	-3.111521	3.357523	0.663496
C	-6.453655	2.804048	0.605349
H	-7.412444	0.948609	0.223439
H	-5.221727	4.542327	1.010903
H	-7.398993	3.329674	0.746453
C	4.073007	1.438820	-0.165399
C	5.285050	0.703120	-0.134471
C	4.113718	2.838412	-0.354793
C	6.496933	1.406889	-0.323303
C	5.313257	3.496835	-0.525177
H	3.187133	3.402698	-0.377758
C	6.516222	2.772745	-0.515866
H	7.443886	0.871659	-0.329060
H	5.322196	4.577026	-0.674912
H	7.467310	3.285891	-0.662840
C	4.020136	-1.439885	0.227353
C	4.044277	-2.815002	0.565629
C	5.256440	-0.734622	0.116853
C	5.235369	-3.483466	0.750909
H	3.111523	-3.357494	0.663635
C	6.455582	-1.459448	0.300165
C	6.453656	-2.804021	0.605468
H	5.221729	-4.542283	1.011092
H	7.412445	-0.948597	0.223479
H	7.398995	-3.329640	0.746594
F	-1.182763	-3.559709	-0.175019
F	1.182761	3.559701	-0.175207

BCIBA3a S0

E = -1640.84929957 a.u.

C	2.405920	-0.782936	0.000000
C	2.362785	0.699516	0.000000

C	1.199938	1.416397	0.000000
C	-0.002989	0.669255	0.000000
C	0.002989	-0.669255	-0.000000
C	-2.405920	0.782936	0.000000
C	-2.362785	-0.699516	0.000000
C	-1.199938	-1.416397	-0.000000
N	1.138658	-1.439782	-0.000000
N	-1.138658	1.439782	0.000000
C	-0.735214	-2.797668	-0.000000
C	0.665851	-2.805163	-0.000000
C	-1.503380	-3.993301	-0.000000
H	-2.592032	-3.931022	-0.000000
C	0.735214	2.797668	0.000000
C	-0.665851	2.805163	0.000000
C	1.503380	3.993301	0.000000
H	2.592032	3.931022	0.000000
H	-3.352371	-1.154805	-0.000000
O	-3.461982	1.377190	-0.000000
H	3.352371	1.154805	-0.000000
O	3.461982	-1.377190	-0.000000
C	0.858435	5.190006	0.000000
C	-0.858435	-5.190006	-0.000000
C	-1.385676	4.053864	0.000000
C	-0.574759	5.257974	0.000000
C	-2.779052	4.194122	0.000000
C	-1.199938	6.506835	0.000000
H	-3.403016	3.304837	-0.000000
C	1.385676	-4.053864	-0.000000
C	0.574759	-5.257974	-0.000000
C	2.779052	-4.194122	-0.000000
C	1.199938	-6.506835	-0.000000
H	3.403016	-3.304837	-0.000000
H	1.417829	6.126625	0.000000
H	-1.417829	-6.126625	-0.000000
C	3.392389	-5.453081	-0.000000
C	4.818935	-5.581932	-0.000000
C	2.591655	-6.641239	-0.000000
C	5.406897	-6.814922	-0.000000
H	5.421517	-4.671733	0.000000
C	3.242487	-7.915748	-0.000000
C	4.606314	-7.998200	-0.000000
H	6.494036	-6.904165	-0.000000
H	2.627735	-8.817976	-0.000000
H	5.094527	-8.973941	-0.000000
H	0.577454	-7.404599	-0.000000
C	-3.392389	5.453081	0.000000
C	-4.818935	5.581932	0.000000
C	-2.591655	6.641239	0.000000
C	-5.406897	6.814922	0.000000
H	-5.421517	4.671733	0.000000
C	-3.242487	7.915748	0.000000
C	-4.606314	7.998200	0.000000
H	-6.494036	6.904165	0.000000
H	-2.627735	8.817976	0.000000
H	-5.094527	8.973941	0.000000
H	-0.577454	7.404599	0.000000

BCIBA3a T1

E = -1640.80281757 a.u.

C	2.405920	-0.782936	0.000000
C	2.362785	0.699516	0.000000
C	1.199938	1.416397	0.000000
C	-0.002989	0.669255	0.000000
C	0.002989	-0.669255	-0.000000
C	-2.405920	0.782936	0.000000
C	-2.362785	-0.699516	0.000000
C	-1.199938	-1.416397	-0.000000
N	1.138658	-1.439782	-0.000000
N	-1.138658	1.439782	0.000000
C	-0.735214	-2.797668	-0.000000
C	0.665851	-2.805163	-0.000000
C	-1.503380	-3.993301	-0.000000
H	-2.592032	-3.931022	-0.000000
C	0.735214	2.797668	0.000000
C	-0.665851	2.805163	0.000000
C	1.503380	3.993301	0.000000
H	2.592032	3.931022	0.000000
H	-3.352371	-1.154805	-0.000000
O	-3.461982	1.377190	-0.000000
H	3.352371	1.154805	-0.000000
O	3.461982	-1.377190	-0.000000
C	0.858435	5.190006	0.000000
C	-0.858435	-5.190006	-0.000000
C	-1.385676	4.053864	0.000000
C	-0.574759	5.257974	0.000000
C	-2.779052	4.194122	0.000000
C	-1.199938	6.506835	0.000000
H	-3.403016	3.304837	-0.000000
C	1.385676	-4.053864	-0.000000
C	0.574759	-5.257974	-0.000000
C	2.779052	-4.194122	-0.000000
C	1.199938	-6.506835	-0.000000
H	3.403016	-3.304837	-0.000000
H	1.417829	6.126625	0.000000
H	-1.417829	-6.126625	-0.000000
C	3.392389	-5.453081	-0.000000
C	4.818935	-5.581932	-0.000000
C	2.591655	-6.641239	-0.000000
C	5.406897	-6.814922	-0.000000
H	5.421517	-4.671733	0.000000
C	3.242487	-7.915748	-0.000000
C	4.606314	-7.998200	-0.000000
H	6.494036	-6.904165	-0.000000
H	2.627735	-8.817976	-0.000000
H	5.094527	-8.973941	-0.000000
H	0.577454	-7.404599	-0.000000
C	-3.392389	5.453081	0.000000
C	-4.818935	5.581932	0.000000
C	-2.591655	6.641239	0.000000

C	-5.406897	6.814922	0.000000
H	-5.421517	4.671733	0.000000
C	-3.242487	7.915748	0.000000
C	-4.606314	7.998200	0.000000
H	-6.494036	6.904165	0.000000
H	-2.627735	8.817976	0.000000
H	-5.094527	8.973941	0.000000
H	-0.577454	7.404599	0.000000

BCIBA3b S0

E = -1640.85708223 a.u.

C	1.593716	-1.700014	0.000252
C	0.184672	-2.163254	0.000240
C	-0.882067	-1.312919	0.000119
C	-0.595844	0.073453	-0.000046
C	0.666664	0.520796	-0.000070
C	-1.514234	2.295337	-0.000456
C	-0.103933	2.754994	-0.000395
C	0.964161	1.904612	-0.000254
N	1.778159	-0.286558	0.000067
N	-1.708838	0.879871	-0.000201
C	2.420904	1.935808	-0.000229
C	2.902891	0.620562	-0.000041
C	3.284911	3.064283	-0.000370
H	2.856834	4.067176	-0.000516
C	-2.340082	-1.352229	0.000093
C	-2.839193	-0.030582	-0.000080
C	-3.194541	-2.460333	0.000224
H	-2.778611	-3.468352	0.000358
H	-0.011590	3.840348	-0.000536
O	-2.424023	3.095159	-0.000236
H	0.090988	-3.248520	0.000365
O	2.510517	-2.492288	0.000079
C	-4.552353	-2.252288	0.000186
C	4.629470	2.863509	-0.000319
C	-4.244110	0.203002	-0.000110
C	-5.100404	-0.947281	0.000025
C	-4.844737	1.512090	-0.000260
C	-6.549173	-0.763384	-0.000002
C	-6.191590	1.668266	-0.000280
H	-4.193206	2.379234	-0.000364
C	-7.085187	0.548322	-0.000155
C	-7.461175	-1.847494	0.000119
H	-6.618940	2.672866	-0.000395
C	-8.485920	0.742133	-0.000182
C	-8.825035	-1.639159	0.000090
H	-7.100378	-2.874106	0.000238
C	-9.347972	-0.332014	-0.000062
H	-8.870210	1.763999	-0.000301
H	-9.500569	-2.495593	0.000185
H	-10.427262	-0.174112	-0.000085
C	4.321990	0.367205	0.000029
C	5.179660	1.538297	-0.000120
C	4.926938	-0.895658	0.000234
C	6.566719	1.374077	-0.000062
H	4.302685	-1.784568	0.000353
H	-5.210143	-3.117540	0.000289
H	5.320853	3.707416	-0.000423
C	6.319303	-1.045524	0.000291
C	6.923771	-2.343956	0.000501
C	7.165454	0.110426	0.000140
C	8.283113	-2.479280	0.000558
H	6.271651	-3.219352	0.000614
C	8.585084	-0.069783	0.000205
C	9.124958	-1.325026	0.000408
H	8.735520	-3.471850	0.000718
H	9.225711	0.814260	0.000091
H	10.208430	-1.453622	0.000457
H	7.200062	2.264173	-0.000176

BCIBA3b T1

E = -1640.80912363 a.u.

C	1.593716	-1.700014	0.000252
C	0.184672	-2.163254	0.000240
C	-0.882067	-1.312919	0.000119
C	-0.595844	0.073453	-0.000046
C	0.666664	0.520796	-0.000070
C	-1.514234	2.295337	-0.000456
C	-0.103933	2.754994	-0.000395
C	0.964161	1.904612	-0.000254
N	1.778159	-0.286558	0.000067
N	-1.708838	0.879871	-0.000201
C	2.420904	1.935808	-0.000229
C	2.902891	0.620562	-0.000041
C	3.284911	3.064283	-0.000370
H	2.856834	4.067176	-0.000516
C	-2.340082	-1.352229	0.000093
C	-2.839193	-0.030582	-0.000080
C	-3.194541	-2.460333	0.000224
H	-2.778611	-3.468352	0.000358
H	-0.011590	3.840348	-0.000536
O	-2.424023	3.095159	-0.000236
H	0.090988	-3.248520	0.000365
O	2.510517	-2.492288	0.000079
C	-4.552353	-2.252288	0.000186
C	4.629470	2.863509	-0.000319
C	-4.244110	0.203002	-0.000110
C	-5.100404	-0.947281	0.000025
C	-4.844737	1.512090	-0.000260
C	-6.549173	-0.763384	-0.000002
C	-6.191590	1.668266	-0.000280
H	-4.193206	2.379234	-0.000364
C	-7.085187	0.548322	-0.000155
C	-7.461175	-1.847494	0.000119
H	-6.618940	2.672866	-0.000395
C	-8.485920	0.742133	-0.000182
C	-8.825035	-1.639159	0.000090
H	-7.100378	-2.874106	0.000238

C	-9.347972	-0.332014	-0.000062
H	-8.870210	1.763999	-0.000301
H	-9.500569	-2.495593	0.000185
H	-10.427262	-0.174112	-0.000085
C	4.321990	0.367205	0.000029
C	5.179660	1.538297	-0.000120
C	4.926938	-0.895658	0.000234
C	6.566719	1.374077	-0.000062
H	4.302685	-1.784568	0.000353
H	-5.210143	-3.117540	0.000289
H	5.320853	3.707416	-0.000423
C	6.319303	-1.045524	0.000291
C	6.923771	-2.343956	0.000501
C	7.165454	0.110426	0.000140
C	8.283113	-2.479280	0.000558
H	6.271651	-3.219352	0.000614
C	8.585084	-0.069783	0.000205
C	9.124958	-1.325026	0.000408
H	8.735520	-3.471850	0.000718
H	9.225711	0.814260	0.000091
H	10.208430	-1.453622	0.000457
H	7.200062	2.264173	-0.000176

BCIBA3c S0

E = -1640.86472084 a.u.

C	2.402307	-0.799940	-0.000000
C	2.365667	0.682548	0.000000
C	1.208757	1.404431	0.000000
C	-0.000797	0.670231	0.000000
C	0.000797	-0.670231	0.000000
C	-2.402307	0.799940	-0.000000
C	-2.365667	-0.682548	0.000000
C	-1.208757	-1.404431	0.000000
N	1.132830	-1.451782	-0.000000
N	-1.132830	1.451782	-0.000000
C	-0.760127	-2.791781	-0.000000
C	0.651969	-2.821092	-0.000000
C	-1.519583	-3.967003	-0.000000
H	-2.608607	-3.911352	-0.000000
C	0.760127	2.791781	-0.000000
C	-0.651969	2.821092	-0.000000
C	1.519583	3.967003	-0.000000
H	2.608607	3.911352	-0.000000
H	-3.357685	-1.132615	-0.000000
O	-3.459814	1.390563	0.000000
H	3.357685	1.132615	-0.000000
O	3.459814	-1.390563	0.000000
C	0.870356	5.177430	0.000000
C	-0.870356	-5.177430	0.000000
C	-1.341471	4.067608	0.000000
C	-0.542653	5.258614	0.000000
C	-2.775929	4.197751	0.000000
C	-1.199061	6.563434	0.000000
C	-3.372102	5.415373	0.000000
H	-3.376676	3.294862	0.000000
C	-2.614310	6.631252	0.000000
C	-0.481285	7.784845	0.000000
H	-4.461694	5.483426	0.000000
C	-3.264414	7.886987	0.000000
C	-1.132830	9.001100	0.000000
H	0.606956	7.787180	0.000000
C	-2.539525	9.058008	0.000000
H	-4.355957	7.908068	0.000000
H	-0.550710	9.923564	0.000000
H	-3.048460	10.022770	0.000000
C	1.341471	-4.067608	0.000000
C	0.542653	-5.258614	0.000000
C	2.775929	-4.197751	0.000000
C	1.199061	-6.563434	0.000000
C	3.372102	-5.415373	0.000000
H	3.376676	-3.294862	0.000000
C	2.614310	-6.631252	0.000000
C	0.481285	-7.784845	0.000000
H	4.461694	-5.483426	0.000000
C	3.264414	-7.886987	0.000000
C	1.132830	-9.001100	0.000000
H	-0.606956	-7.787180	0.000000
C	2.539525	-9.058008	0.000000
H	4.355957	-7.908068	0.000000
H	0.550710	-9.923564	0.000000
H	3.048460	-10.022770	0.000000
H	1.466597	6.086237	0.000000
H	-1.466597	-6.086237	0.000000

BCIBA3c T1

E = -1640.81503299 a.u.

C	2.402307	-0.799940	-0.000000
C	2.365667	0.682548	0.000000
C	1.208757	1.404431	0.000000
C	-0.000797	0.670231	0.000000
C	0.000797	-0.670231	0.000000
C	-2.402307	0.799940	-0.000000
C	-2.365667	-0.682548	0.000000
C	-1.208757	-1.404431	0.000000
N	1.132830	-1.451782	-0.000000
N	-1.132830	1.451782	-0.000000
C	-0.760127	-2.791781	-0.000000
C	0.651969	-2.821092	-0.000000
C	-1.519583	-3.967003	-0.000000
H	-2.608607	-3.911352	-0.000000
C	0.760127	2.791781	-0.000000
C	-0.651969	2.821092	-0.000000
C	1.519583	3.967003	-0.000000
H	2.608607	3.911352	-0.000000
H	-3.357685	-1.132615	-0.000000
O	-3.459814	1.390563	0.000000
H	3.357685	1.132615	-0.000000
O	3.459814	-1.390563	0.000000

C	0.870356	5.177430	0.000000
C	-0.870356	-5.177430	0.000000
C	-1.341471	4.067608	0.000000
C	-0.542653	5.258614	0.000000
C	-2.775929	4.197751	0.000000
C	-1.199061	6.563434	0.000000
C	-3.372102	5.415373	0.000000
H	-3.376676	3.294862	0.000000
C	-2.614310	6.631252	0.000000
C	-0.481285	7.784845	0.000000
H	-4.461694	5.483426	0.000000
C	-3.264414	7.886987	0.000000
C	-1.132830	9.001100	0.000000
H	0.606956	7.787180	0.000000
C	-2.539525	9.058008	0.000000
H	-4.355957	7.908068	0.000000
H	-0.550710	9.923564	0.000000
H	-3.048460	10.022770	0.000000
C	1.341471	-4.067608	0.000000
C	0.542653	-5.258614	0.000000
C	2.775929	-4.197751	0.000000
C	1.199061	-6.563434	0.000000
C	3.372102	-5.415373	0.000000
H	3.376676	-3.294862	0.000000
C	2.614310	-6.631252	0.000000
C	0.481285	-7.784845	0.000000
H	4.461694	-5.483426	0.000000
C	3.264414	-7.886987	0.000000
C	1.132830	-9.001100	0.000000
H	-0.606956	-7.787180	0.000000
C	2.539525	-9.058008	0.000000
H	4.355957	-7.908068	0.000000
H	0.550710	-9.923564	0.000000
H	3.048460	-10.022770	0.000000
H	1.466597	6.086237	0.000000
H	-1.466597	-6.086237	0.000000

BCIBA3d S0

E = -1640.88315220 a.u.

C	2.414965	-0.768323	-0.000000
C	2.371777	0.723804	-0.000000
C	1.198580	1.432490	-0.000000
C	0.001261	0.666636	-0.000000
C	-0.001261	-0.666636	0.000000
C	-2.414965	0.768323	-0.000000
C	-2.371777	-0.723804	-0.000000
C	-1.198580	-1.432490	0.000000
N	1.149822	-1.395173	-0.000000
N	-1.149822	1.395173	-0.000000
C	-0.685837	-2.818272	0.000000
C	0.751013	-2.754310	-0.000000
C	-1.294385	-4.052739	0.000000
C	1.542476	-3.876215	-0.000000
H	-2.382691	-4.138689	0.000000
H	2.622370	-3.750631	-0.000000
C	0.685837	2.818272	-0.000000
C	-0.751013	2.754310	-0.000000
C	1.294385	4.052739	-0.000000
C	-1.542476	3.876215	-0.000000
H	2.382691	4.138689	-0.000000
H	-2.622370	3.750631	-0.000000
H	-3.356210	-1.190988	0.000000
O	-3.437076	1.420551	0.000000
H	3.356210	1.190988	-0.000000
O	3.437076	-1.420551	0.000000
C	-0.914958	5.147339	0.000000
C	-1.690788	6.380620	0.000000
C	0.507657	5.228906	-0.000000
C	-3.105480	6.387657	0.000000
C	-1.012501	7.627694	0.000000
C	1.149822	6.515710	-0.000000
C	-3.813292	7.572288	0.000000
H	-3.655818	5.447871	0.000000
C	-1.758108	8.828830	0.000000
C	0.424985	7.661365	-0.000000
H	2.240990	6.547118	-0.000000
C	-3.136138	8.806644	0.000000
H	-4.903770	7.549796	0.000000
H	-1.218916	9.778216	0.000000
H	0.920824	8.633796	-0.000000
H	-3.701444	9.739506	0.000000
C	0.914958	-5.147339	0.000000
C	1.690788	-6.380620	0.000000
C	-0.507657	-5.228906	0.000000
C	3.105480	-6.387657	0.000000
C	1.012501	-7.627694	0.000000
C	-1.149822	-6.515710	0.000000
C	3.813292	-7.572288	0.000000
H	3.655818	-5.447871	0.000000
C	1.758108	-8.828830	0.000000
C	-0.424985	-7.661365	0.000000
H	-2.240990	-6.547118	0.000000
C	3.136138	-8.806644	0.000000
H	4.903770	-7.549796	0.000000
H	1.218916	-9.778216	0.000000
H	-0.920824	-8.633796	0.000000
H	3.701444	-9.739506	0.000000

BCIBA3d T1

E = -1640.82925354 a.u.

C	2.414965	-0.768323	-0.000000
C	2.371777	0.723804	-0.000000
C	1.198580	1.432490	-0.000000
C	0.001261	0.666636	-0.000000
C	-0.001261	-0.666636	0.000000
C	-2.414965	0.768323	-0.000000
C	-2.371777	-0.723804	-0.000000
C	-1.198580	-1.432490	0.000000

N	1.149822	-1.395173	-0.000000
N	-1.149822	1.395173	-0.000000
C	-0.685837	-2.818272	0.000000
C	0.751013	-2.754310	-0.000000
C	-1.294385	-4.052739	0.000000
C	1.542476	-3.876215	-0.000000
H	-2.382691	-4.138689	0.000000
H	2.622370	-3.750631	-0.000000
C	0.685837	2.818272	-0.000000
C	-0.751013	2.754310	-0.000000
C	1.294385	4.052739	-0.000000
C	-1.542476	3.876215	-0.000000
H	2.382691	4.138689	-0.000000
H	-2.622370	3.750631	-0.000000
H	-3.356210	-1.190988	0.000000
O	-3.437076	1.420551	0.000000
H	3.356210	1.190988	-0.000000
O	3.437076	-1.420551	0.000000
C	-0.914958	5.147339	0.000000
C	-1.690788	6.380620	0.000000
C	0.507657	5.228906	-0.000000
C	-3.105480	6.387657	0.000000
C	-1.012501	7.627694	0.000000
C	1.149822	6.515710	-0.000000
C	-3.813292	7.572288	0.000000
H	-3.655818	5.447871	0.000000
C	-1.758108	8.828830	0.000000
C	0.424985	7.661365	-0.000000
H	2.240990	6.547118	-0.000000
C	-3.136138	8.806644	0.000000
H	-4.903770	7.549796	0.000000
H	-1.218916	9.778216	0.000000
H	0.920824	8.633796	-0.000000
H	-3.701444	9.739506	0.000000
C	0.914958	-5.147339	0.000000
C	1.690788	-6.380620	0.000000
C	-0.507657	-5.228906	0.000000
C	3.105480	-6.387657	0.000000
C	1.012501	-7.627694	0.000000
C	-1.149822	-6.515710	0.000000
C	3.813292	-7.572288	0.000000
H	3.655818	-5.447871	0.000000
C	1.758108	-8.828830	0.000000
C	-0.424985	-7.661365	0.000000
H	-2.240990	-6.547118	0.000000
C	3.136138	-8.806644	0.000000
H	4.903770	-7.549796	0.000000
H	1.218916	-9.778216	0.000000
H	-0.920824	-8.633796	0.000000
H	3.701444	-9.739506	0.000000

BCIBA0_A S0

E = -742.053310880 a.u.

C	-1.624374	-2.589364	0.000000
C	-0.284359	-1.988461	-0.000000
C	-0.537998	-0.562410	-0.000000
C	-2.527386	-1.578732	0.000000
C	1.005731	-2.411983	0.000000
C	0.400545	0.424720	-0.000000
C	1.775938	0.043217	-0.000000
C	2.128723	-1.422772	-0.000000
C	2.714551	1.036056	0.000000
H	3.773708	0.772932	0.000000
C	2.295560	2.415538	0.000000
C	0.980780	2.785361	0.000000
C	-0.062991	1.783475	-0.000000
C	-1.425304	2.026894	-0.000000
C	-2.438830	0.974751	0.000000
H	-1.818385	3.043600	0.000000
H	1.298581	-3.462527	0.000001
H	-1.856528	-3.650095	0.000001
H	-3.614878	-1.588033	0.000000
H	3.064975	3.189033	0.000000
H	0.701705	3.840315	0.000000
O	-3.641934	1.113766	0.000000
O	3.282923	-1.795129	-0.000000
N	-1.868658	-0.330295	-0.000000

BCIBA0_A T1

E = -742.034723194 a.u.

C	-1.624374	-2.589364	0.000000
C	-0.284359	-1.988461	-0.000000
C	-0.537998	-0.562410	-0.000000
C	-2.527386	-1.578732	0.000000
C	1.005731	-2.411983	0.000000
C	0.400545	0.424720	-0.000000
C	1.775938	0.043217	-0.000000
C	2.128723	-1.422772	-0.000000
C	2.714551	1.036056	0.000000
H	3.773708	0.772932	0.000000
C	2.295560	2.415538	0.000000
C	0.980780	2.785361	0.000000
C	-0.062991	1.783475	-0.000000
C	-1.425304	2.026894	-0.000000
C	-2.438830	0.974751	0.000000
H	-1.818385	3.043600	0.000000
H	1.298581	-3.462527	0.000001
H	-1.856528	-3.650095	0.000001
H	-3.614878	-1.588033	0.000000
H	3.064975	3.189033	0.000000
H	0.701705	3.840315	0.000000
O	-3.641934	1.113766	0.000000
O	3.282923	-1.795129	-0.000000
N	-1.868658	-0.330295	-0.000000

BCIBA0_B S0

E = -764.081197758 a.u.

C	-2.999002	-1.878887	-0.000449
C	-1.783633	-2.536687	-0.000387
C	-0.560238	-1.813439	-0.000177
C	-0.609706	-0.380638	-0.000056
C	-1.861600	0.268295	-0.000104
C	-3.039967	-0.475923	-0.000293
C	0.681327	-2.472369	-0.000104
C	0.609706	0.380638	0.000094
C	1.861600	-0.268295	0.000171
C	1.940481	-1.757179	0.000149
C	3.039967	0.475923	0.000273
H	3.984870	-0.069530	0.000336
C	2.999002	1.878887	0.000292
C	1.783633	2.536687	0.000224
C	0.560238	1.813439	0.000134
C	-0.681327	2.472369	0.000074
C	-1.940481	1.757179	0.000084
H	-0.738590	3.561823	0.000054
H	0.738590	-3.561823	-0.000217
H	-3.927931	-2.449895	-0.000613
H	-1.743863	-3.627489	-0.000498
H	-3.984870	0.069530	-0.000315
H	3.927931	2.449895	0.000362
H	1.743863	3.627489	0.000242
O	-3.019749	2.343056	-0.000037
O	3.019749	-2.343056	0.000175

BCIBA0_B T1

E = -764.077645784 a.u.

C	-2.999002	-1.878887	-0.000449
C	-1.783633	-2.536687	-0.000387
C	-0.560238	-1.813439	-0.000177
C	-0.609706	-0.380638	-0.000056
C	-1.861600	0.268295	-0.000104
C	-3.039967	-0.475923	-0.000293
C	0.681327	-2.472369	-0.000104
C	0.609706	0.380638	0.000094
C	1.861600	-0.268295	0.000171
C	1.940481	-1.757179	0.000149
C	3.039967	0.475923	0.000273
H	3.984870	-0.069530	0.000336
C	2.999002	1.878887	0.000292
C	1.783633	2.536687	0.000224
C	0.560238	1.813439	0.000134
C	-0.681327	2.472369	0.000074
C	-1.940481	1.757179	0.000084
H	-0.738590	3.561823	0.000054
H	0.738590	-3.561823	-0.000217
H	-3.927931	-2.449895	-0.000613
H	-1.743863	-3.627489	-0.000498
H	-3.984870	0.069530	-0.000315
H	3.927931	2.449895	0.000362
H	1.743863	3.627489	0.000242
O	-3.019749	2.343056	-0.000037
O	3.019749	-2.343056	0.000175

BCIBA0_C S0

E = -751.987912376 a.u.

C	-2.435796	0.691047	-0.000011
C	-1.550393	1.915169	0.000002
C	-0.176218	1.850162	0.000001
C	0.367188	0.553908	-0.000007
C	-0.367183	-0.553913	-0.000007
C	2.435794	-0.691030	-0.000034
C	1.550390	-1.915169	-0.000000
C	0.176217	-1.850175	-0.000001
N	-1.710247	-0.546230	-0.000006
N	1.710256	0.546233	-0.000013
C	-1.092874	-2.622592	0.000009
C	1.092865	2.622590	0.000009
H	2.116323	-2.846337	0.000013
O	3.634987	-0.736599	0.000020
H	-2.116299	2.846353	0.000010
O	-3.634988	0.736590	0.000008
H	-1.223419	-3.703138	0.000020
H	1.223402	3.703137	0.000019
N	-2.144385	-1.853872	0.000003
N	2.144385	1.853880	0.000008

BCIBA0_C T1

E = -751.965388880 a.u.

C	-2.435796	0.691047	-0.000011
C	-1.550393	1.915169	0.000002
C	-0.176218	1.850162	0.000001
C	0.367188	0.553908	-0.000007
C	-0.367183	-0.553913	-0.000007
C	2.435794	-0.691030	-0.000034
C	1.550390	-1.915169	-0.000000
C	0.176217	-1.850175	-0.000001
N	-1.710247	-0.546230	-0.000006
N	1.710256	0.546233	-0.000013
C	-1.092874	-2.622592	0.000009
C	1.092865	2.622590	0.000009
H	2.116323	-2.846337	0.000013
O	3.634987	-0.736599	0.000020
H	-2.116299	2.846353	0.000010
O	-3.634988	0.736590	0.000008
H	-1.223419	-3.703138	0.000020
H	1.223402	3.703137	0.000019
N	-2.144385	-1.853872	0.000003
N	2.144385	1.853880	0.000008

BCIBA0_D S0

E = -752.048564947 a.u.

C	-2.431662	0.667760	-0.000018
C	-1.573358	1.906619	0.000005

C	-0.200416	1.849246	0.000000
C	0.354405	0.555850	-0.000014
C	-0.354402	-0.555852	-0.000013
C	2.431661	-0.667754	-0.000059
C	1.573357	-1.906620	-0.000003
C	0.200415	-1.849251	-0.000002
N	-1.702886	-0.578299	-0.000010
N	1.702891	0.578300	-0.000023
C	-1.969086	-1.969431	0.000001
C	1.969085	1.969435	0.000021
H	2.142230	-2.835151	0.000021
O	3.634065	-0.677209	0.000038
H	-2.142218	2.835158	0.000017
O	-3.634066	0.677205	0.000020
H	-2.997601	-2.330802	0.000011
H	2.997599	2.330809	0.000024
N	-0.912775	-2.722712	0.000022
N	0.912771	2.722711	0.000004

BCIBA0_D T1

E = -752.012061520 a.u.

C	-2.431662	0.667760	-0.000018
C	-1.573358	1.906619	0.000005
C	-0.200416	1.849246	0.000000
C	0.354405	0.555850	-0.000014
C	-0.354402	-0.555852	-0.000013
C	2.431661	-0.667754	-0.000059
C	1.573357	-1.906620	-0.000003
C	0.200415	-1.849251	-0.000002
N	-1.702886	-0.578299	-0.000010
N	1.702891	0.578300	-0.000023
C	-1.969086	-1.969431	0.000001
C	1.969085	1.969435	0.000021
H	2.142230	-2.835151	0.000021
O	3.634065	-0.677209	0.000038
H	-2.142218	2.835158	0.000017
O	-3.634066	0.677205	0.000020
H	-2.997601	-2.330802	0.000011
H	2.997599	2.330809	0.000024
N	-0.912775	-2.722712	0.000022
N	0.912771	2.722711	0.000004

BCIBA0_E S0

E = -1292.96081533 a.u.

C	2.862991	-0.699187	-0.000001
C	1.896060	-1.821324	-0.000001
C	0.518276	-1.828957	0.000001
C	-0.262188	-0.629776	0.000003
C	0.262189	0.629778	0.000002
C	-2.862989	0.699181	-0.000004
C	-1.896060	1.821323	0.000000
C	-0.518277	1.828958	0.000001
C	0.383400	2.995209	-0.000001
C	1.716882	2.722974	-0.000002
C	-0.383402	-2.995207	-0.000000
C	-1.716884	-2.722971	-0.000000
H	-2.436313	2.772592	-0.000003
O	-4.055763	0.821062	-0.000009
H	2.436310	-2.772595	-0.000002
O	4.055764	-0.821067	-0.000002
H	0.003793	4.017999	-0.000001
H	2.513551	3.462873	-0.000003
H	-2.513554	-3.462869	-0.000002
H	-0.003796	-4.017997	-0.000001
P	1.940415	0.933232	-0.000001
P	-1.940414	-0.933230	0.000008

BCIBA0_E T1

E = -1292.93288763 a.u.

C	2.862991	-0.699187	-0.000001
C	1.896060	-1.821324	-0.000001
C	0.518276	-1.828957	0.000001
C	-0.262188	-0.629776	0.000003
C	0.262189	0.629778	0.000002
C	-2.862989	0.699181	-0.000004
C	-1.896060	1.821323	0.000000
C	-0.518277	1.828958	0.000001
C	0.383400	2.995209	-0.000001
C	1.716882	2.722974	-0.000002
C	-0.383402	-2.995207	-0.000000
C	-1.716884	-2.722971	-0.000000
H	-2.436313	2.772592	-0.000003
O	-4.055763	0.821062	-0.000009
H	2.436310	-2.772595	-0.000002
O	4.055764	-0.821067	-0.000002
H	0.003793	4.017999	-0.000001
H	2.513551	3.462873	-0.000003
H	-2.513554	-3.462869	-0.000002
H	-0.003796	-4.017997	-0.000001
P	1.940415	0.933232	-0.000001
P	-1.940414	-0.933230	0.000008

CIBA-THIO S0

E = -1672.79607818 a.u.

C	-2.392633	-0.778513	0.000000
C	-2.363913	0.691005	-0.000000
C	-1.199580	1.419283	-0.000000
C	-0.000478	0.668465	-0.000000
C	0.000478	-0.668465	0.000000
C	2.392632	0.778514	-0.000000
C	2.363913	-0.691005	0.000000
C	1.199581	-1.419283	0.000000
N	-1.146325	-1.408365	0.000000
N	1.146325	1.408367	-0.000000
C	0.713503	-2.806095	0.000000
C	-0.713504	-2.770182	0.000000

C	1.379560	-4.027216	0.000000
C	-1.464373	-3.939285	0.000000
C	0.628986	-5.202924	0.000000
H	2.469877	-4.057298	0.000000
C	-0.766719	-5.151465	0.000000
H	-2.550164	-3.898501	0.000000
H	1.134917	-6.168616	0.000000
H	-1.336718	-6.081522	0.000000
C	-0.713504	2.806095	-0.000000
C	0.713503	2.770183	-0.000000
C	-1.379561	4.027216	-0.000000
C	1.464372	3.939286	-0.000000
C	-0.628987	5.202924	-0.000000
H	-2.469878	4.057300	-0.000000
C	0.766718	5.151466	-0.000000
H	2.550164	3.898501	-0.000000
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H	3.348989	-1.155857	0.000000
H	-3.348989	1.155859	-0.000000
S	3.833559	1.602173	-0.000000
S	-3.833557	-1.602176	0.000000

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E = -1672.76259698 a.u.

C	-2.392633	-0.778513	0.000000
C	-2.363913	0.691005	-0.000000
C	-1.199580	1.419283	-0.000000
C	-0.000478	0.668465	-0.000000
C	0.000478	-0.668465	0.000000
C	2.392632	0.778514	-0.000000
C	2.363913	-0.691005	0.000000
C	1.199581	-1.419283	0.000000
N	-1.146325	-1.408365	0.000000
N	1.146325	1.408367	-0.000000
C	0.713503	-2.806095	0.000000
C	-0.713504	-2.770182	0.000000
C	1.379560	-4.027216	0.000000
C	-1.464373	-3.939285	0.000000
C	0.628986	-5.202924	0.000000
H	2.469877	-4.057298	0.000000
C	-0.766719	-5.151465	0.000000
H	-2.550164	-3.898501	0.000000
H	1.134917	-6.168616	0.000000
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C	-0.713504	2.806095	-0.000000
C	0.713503	2.770183	-0.000000
C	-1.379561	4.027216	-0.000000
C	1.464372	3.939286	-0.000000
C	-0.628987	5.202924	-0.000000
H	-2.469878	4.057300	-0.000000
C	0.766718	5.151466	-0.000000
H	2.550164	3.898501	-0.000000
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