Electronic Supplementary Information for

Potential singlet fission chromophores of azulene-containing tetracene analogue: a theoretical study

Tianyu Li,[a] Li shen,[*,b] Xianyuan Wang,[a] Xiaonan Fan,[a] Boce Cui,[a] Yanli Chen,[a] Bingchuan Yang,[*,c] Heyuan Liu,[*,a] Xiyou Li[*,a]

[a] College of Chemistry and Chemical Engineering, School of Materials Science and Engineering, China University of Petroleum (East China), Qingdao, 266580, China.

[b] College of Chemical Engineering and Environmental Chemistry, Weifang University, Weifang, 261061, China.

[c] College of Chemistry and Chemical Engineering, Qilu Normal University, Shandong, 250013, China.

To whom correspondence should be addressed：*shenliren93@wfu.edu.cn, liuheyuan123@upc.edu.cn, xiyouli@upc.edu.cn*

Contents

18. HLG for α and β substituted **B4a** with respect to the $E(T_1)$ (Fig. S9).
19. E(HOMO), E(LUMO), HLG, DRC y_0, $E(S_1)$, $E(T_1)$, and ΔE_{SF} for **B4b** derivatives (Fig S10).
20. Correlation between the vertical and adiabatic energies of S_1, T_1, and the corresponding ΔE_{SF} (**A1-B6**) (Fig S11).
21. Optimized geometries of **B4a** at different basis sets (Fig S12).
22. Coordinates of the geometries.

The vertical excitation energies of model compounds have been tested with and TDA method and different functionals. These functionals include B3LYP, CAM-B3LYP, ωB97XD, M06-2X and tuned LC-BLYP. The solvation effects were evaluated by continuum model (PCM) with toluene, dichloromethane (DCM) and methanol (MeOH) used as solvents.[1] Compared to available experimental results, the functional CAM-B3LYP, ωB97XD, M06-2X and tuned LC-BLYP overestimate $E(S_1)_V$ (Table S1). The range separating parameters μ were tuned for model molecules (Table S2) with Quantum program optDFTw[2]. The functional CAM-B3LYP and ωB97XD show similar results and larger $E(S_1)_V$ and $E(T_1)_V$ than the functional B3LYP. The function M06-2X also overestimates $E(S_1)_V$ and shows similar results to CAM-B3LYP and ωB97XD, while the overestimation of $E(T_1)_V$ is more severe than the two functions. The S_1 energies of **A0** and **A1** calculated by TDA-B3LYP are within 0.1 eV of the experimental reference. To the best of our knowledge, no experimental gas-phase or solvent reference for the T_1 state of tetracene has been reported so far. If one assumes that, the gas-phase triplet energy is about 0.189 eV above the energy in the crystal, then the agreement is also good in this case.

To show how Tamm-Dancoff (TDA) approximation improves the triplet instability problem[3,4], we compare the excitation energy calculated by TD-DFT and TDA methods. The results suggest that TDA apparently remedies the triplet instability problem. It also improves the problem of underestimating the energy of S_1 state for tetracene compared to TD-DFT[5] (Table S3).

The solvation effects have similar patterns for these three model compounds. Moreover, the basis set was extended to larger basis sets, including 6-311G*, 6-311G** and cc-pVTZ. The calculated results show that solvation effects affect the SF-relevant excited state energies (Table S4), while the excitation energies are insensitive to the extension of basis set (Table S5). All test results show that our calculation method is reliable.

Singlet fission is an intrinsically multi-molecular process, and electronic coupling among adjacent molecules may affect the SF relevant excited energies. We calculated $E(S_1)$v, $E(T_1)$v and Davydov splitting energy ΔE_{DV} for these dimers at the theoretical

level of TDA-ωB97XD/6-31G* based on the geometrical without optimizations. The Davydov splitting energy is a useful indicator of the electronic coupling strength between adjacent molecules, as demonstrated in previous studies.[6,7] Three dimeric structures were selected from its crystal (Fig. S2) and the SF relevant excited state energies and Davydov splitting energies were calculated (Table S7).

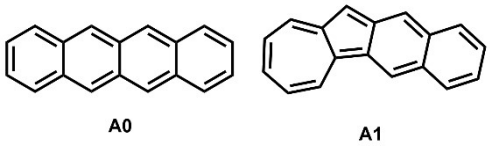

Fig. S1 Molecular structures of the involved molecules for test.

Table S1 Vertical excitation energies (eV) of model compounds with different functionals based on S_0 geometries.[a]

Compound		$E(S_1)_V$	$E(T_1)_V$
A0	B3LYP	2.740	1.438
	CAM-B3LYP	3.163	1.537
	M06-2X	3.168	1.767
	ωB97XD	3.225	1.597
	Tuned-LC-BLYP	3.147	
	Exp.	2.710[b]	1.250[c]
A1	B3LYP	2.030	1.437
	CAM-B3LYP	2.390	1.583
	M06-2X	2.377	1.730
	ωB97XD	2.412	1.627
	Tuned-LC-BLYP	2.255	
	Exp.	1.916[d]	

[a]Calcualted $E(S_1)_V$ and $E(T_1)_V$ based on the optimized S_0 geometries at the theoretical level of B3LYP/6-31G*.

[b]Reference [8]. [c]Reference [9]: 0−0 transition (crystal). [d]Reference [10]: in MeOH

Table S2 Tuned rang separating parameters μ(bohr^{-1}) in LC-BLYP/6-31G* with Quantum program optDFTw.

	A0	**A1**
μ	0.2245	0.2146

Table S3 Comparison of the excitation energies using the TDDFT with and without Tamm-Dancoff approximation (TDA).

Molecule	TD	TDA
A0	2.514/1.153	2.740/1.438
A1	1.938/1.238	2.030/1.437

Table S4 Solvation effects on vertical excitation energies (eV) of S_1 and T_1 states

Molecule	Vacuum	Toluene	DCM	MeOH
A0	2.740/1.438	2.697/1.463	2.634/1.464	2.611/1.464
A1	2.030/1.437	2.030/1.452	2.056/1.466	2.065/1.471

Table S5 Basis set effects on the vertical excitation energies (eV) of the S_1 and T_1 states of the three model compounds.

Molecule	6-31G*	6-311G*	6-311G**	cc-pVTZ
A0	2.740/1.438	2.707/1.457	2.707/1.458	2.666/1.449
A1	2.030/1.438	1.997/1.424	1.993/1.423	1.971/1.412

Table S6 Comparison of the adiabatic energies $E(T_1)$ (eV) using the TDDFT with Tamm-Dancoff approximation (TDA) and UDFT.

Compound	UDFT	TDA
A1	1.052	1.091
A2	1.196	1.229
A3	0.717	0.794
A4	0.500	0.560
A5	0.610	0.663
B1	1.425	1.463
B2	1.351	1.393
B3	0.588	0.661
B4	0.708	0.769
B5	0.606	0.674
B6	0.402	0.432

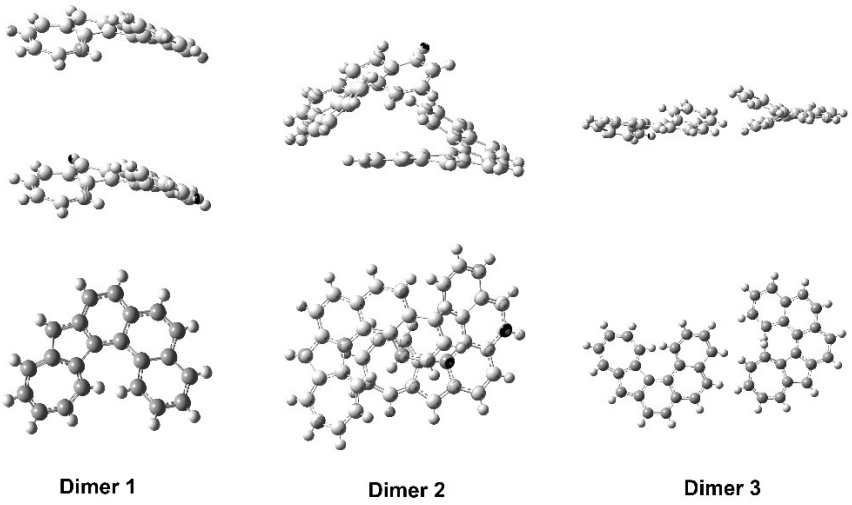

Fig. S2 Geometry structures of **[5]AzH** dimers**.**

Table S7 Effect of electronic coupling in **[5]AzH** dimers on $E(S_1)_V$ and $E(T_1)_V$ in vacuum (oscillator strengths are listed in parentheses) (in eV).

Compound	Monomer 1	Monomer 2	Dimer 1	ΔE_{DV}(1)	Dimer 2	ΔE_{DV}(2)	Dimer 3	ΔE_{DV}(3)
S_1	1.741 (0.009)	2.068 (0.008)	1.732 (0.005)	0.005	1.743 (0.010)	-	1.742 (0.010)	-
S_2	3.006 (0.009)	3.194 (0.111)	1.737 (0.011)		2.093 (0.005)		2.073 (0.008)	
S_3	3.710 (0.166)	3.832 (0.110)	2.998 (0.005)		2.950 (0.032)		3.008 (0.015)	
S_4	3.983 (0.939)	4.169 (0.925)	3.002 (0.012)		3.008 (0.032)		3.193 (0.132)	
T_1	1.268	1.630	1.260	0.004	1.279	-	1.270	-
T_2	1.917	1.896	1.264		1.662		1.634	
T_3	2.438	2.840	1.908		1.917		1.901	
T_4	2.774	2.924	1.914		1.927		1.925	

In Dimer 2 and Dimer 3, there are two distinct monomers (monomer 1 and 2), and the S1 (T_1) and S_2 (T_2) energies are originated from monomer 1 and 2, respectively. As a result, their excited states maintain the characteristics of the individual monomers and no electronic coupling is presented in dimer 2 and 3.

Table S8 Hammett constant (σ_p) of the introduced substituents.[11]

	-F	**-Cl**	**-Br**	**-CF_3**	**-CN**
σ_p	0.06	0.23	0.23	0.54	0.66
	-Me	**-OH**	**-OMe**	**-NH_2**	**-NMe_2**
σ_p	-0.17	-0.37	-0.27	-0.66	-0.83

Table S9 Difference electronic energy (eV) between open-shell symmetry-broken singlet and closed-shell RB3LYP solution ($\Delta E_{OS\text{-}CS}$), triplet-singlet gap ($\Delta E_{T\text{-}OS}$) at the B3LYP level, spin contamination for the open shell singlet (<S^2>).

Compound	**y_0**	**Stability**	**$\Delta E_{OS\text{-}CS}$**	**$\Delta E_{T\text{-}OS}$**	**<S^2>**
A1	0.223	Stable	0.000	1.052	0
A2	0.207	Stable	0.000	1.196	0
A3	0.322	Stable	0.000	0.717	0
A4	0.372	Stable	0.000	0.500	0
A5	0.320	Stable	0.000	0.610	0
A6	0.791	RHF→UHF instability	-0.127	0.003	1.069
B1	0.147	Stable	0.000	1.425	0
B2	0.141	Stable	0.000	1.351	0
B3	0.319	Stable	0.000	0.588	0
B4	0.257	Stable	0.000	0.708	0
B5	0.337	Stable	0.000	0.606	0
B6	0.621	Stable	0.000	0.402	0

Table S10 HOMO, LUMO energies and HLG values (in eV), DRC y_0 and TRC y_1.

		HOMO	LUMO	HLG	y_0	y_1
A0		-4.855	-2.079	2.776	0.283	0.033
A1		-4.755	-2.135	2.620	0.223	0.058
A2		-4.957	-2.137	2.820	0.207	0.288
A3		-4.598	-2.379	2.219	0.322	0.063
A4		-4.502	-2.495	2.007	0.372	0.027
A5		-4.586	-2.462	2.123	0.320	0.017
A6		-4.579	-2.867	1.712	0.791	0.036
B0		-5.541	-1.310	4.231	0.084	0.052
B1		-4.994	-2.077	2.917	0.147	0.107
B2		-4.998	-2.117	2.881	0.141	0.116
B3		-4.615	-2.520	2.095	0.319	0.076
B4		-4.655	-2.395	2.260	0.257	0.077
B5		-4.754	-2.446	2.308	0.337	0.034
B6		-4.383	-2.730	1.653	0.621	0.050
			B4a			
-F	α	-4.839	-2.471	2.368	0.243	0.074
	β	-4.734	-2.483	2.250	0.254	0.064
-Cl	α	-4.937	-2.655	2.282	0.259	0.073
	β	-4.868	-2.623	2.245	0.245	0.066
-Br	α	-4.932	-2.659	2.272	0.259	0.073
	β	-4.860	-2.625	2.235	0.242	0.067
-CF_3	α	-5.094	-2.828	2.266	0.258	0.070
	β	-5.189	-2.810	2.379	0.218	0.070
-CN	α	-5.237	-3.156	2.081	0.302	0.069
	β	-5.262	-3.007	2.255	0.241	0.066
-Me	α	-4.696	-2.323	2.373	0.236	0.068
	β	-4.635	-2.364	2.271	0.253	0.068
-OH	α	-4.607	-2.183	2.424	0.225	0.068
	β	-4.379	-2.268	2.111	0.279	0.059
-OMe	α	-4.566	-2.101	2.465	0.215	0.064
	β	-4.585	-2.364	2.221	0.259	0.064
-NH_2	α	-4.345	-1.954	2.391	0.221	0.064
	β	-4.156	-2.137	2.019	0.292	0.055
-NMe_2	α	-4.224	-1.864	2.360	0.215	0.062
	β	-4.681	-2.388	2.293	0.250	0.068
			B4b			
-F		-5.242	-2.782	2.461	0.212	0.094
-Cl		-5.327	-2.960	2.367	0.225	0.095
-Br		-5.319	-2.961	2.357	0.226	0.095
-CF_3		-5.478	-3.132	2.346	0.220	0.092

Table S10 HOMO, LUMO energies and HLG values (in eV), DRC y_0 and TRC y_1. (continued table).

	HOMO	**LUMO**	**HLG**	y_0	y_1
-CN	-5.611	-3.462	2.149	0.261	0.093
-Me	-5.097	-2.624	2.473	0.202	0.088
-OMe	-4.964	-2.393	2.571	0.184	0.084
-OH	-5.012	-2.485	2.527	0.195	0.088
-NH_2	-5.097	-2.624	2.473	0.191	0.081
-NMe_2	-4.629	-2.138	2.490	0.184	0.078

Table S11 Vertical excitation energies ($E(S_1)_V$ and $E(T_1)_V$), oscillator strength (f), adiabatic excitation energies ($E(S_1)$, $E(T_1)$ and $E(T_2)$) and the ΔE_{SF} and ΔE_{TTA} (in eV).[g]

		$E(S_1)_V$	f	$E(S_1)$	$E(T_1)_V$	$E(T_1)$	$E(T_2)$	ΔE_{SF}	ΔE_{TTA}
A0		2.740	0.089	2.617	1.438	1.201	2.546	0.214	0.144
A1		2.027	0.018	1.640	1.434	1.052	1.842	-0.464	-0.262
A2		2.352	0.031	1.965	1.596	1.196	2.091	-0.426	-0.300
A3		1.755	0.021	1.457	1.023	0.717	1.957	0.024	0.524
A4		1.481	0.035	0.939	0.900	0.500	1.459	-0.061	0.459
A5		1.614	0.038	1.105	0.999	0.610	1.646	-0.115	0.426
B0		3.674	0.001	3.544	2.760	2.574	3.087	-1.604	-2.061
B1		2.184	0.012	1.846	1.747	1.425	2.053	-1.005	-0.798
B2		2.158	0.024	1.754	1.719	1.351	2.055	-0.948	-0.647
B3		1.536	0.015	1.171	0.934	0.588	1.823	-0.005	0.647
B4		1.936	0.041	1.569	1.074	0.708	1.501	0.153	0.085
B5		2.002	0.037	1.499	1.050	0.606	1.525	0.287	0.314
B6		1.088	0.010	0.691	0.699	0.402	1.024	-0.112	0.221
					B4a				
-F	α	1.962	0.028	1.587	1.204	0.846	1.462	-0.105	-0.231
	β	1.896	0.037	1.533	1.066	0.716	1.474	0.101	0.042
-Cl	α	1.954	0.051	1.607	1.114	0.769	1.513	0.069	-0.025
	β	1.925	0.047	1.567	1.095	0.771	1.529	0.025	-0.013
-Br	α	1.950	0.058	1.608	1.109	0.766	1.513	0.075	-0.014
	β	1.917	0.050	1.563	1.095	0.780	1.531	0.003	-0.028
-CF_3	α	2.015	0.065	1.690	1.073	0.711	1.628	0.269	0.207
	β	2.083	0.050	1.733	1.236	0.944	1.688	-0.154	-0.199
-CN	α	1.928	0.111	1.646	0.928	0.616	1.485	0.415	0.454
	β	1.992	0.055	1.651	1.163	0.921	1.636	-0.191	-0.207
-Me	α	2.045	0.045	1.683	1.200	0.837	1.562	0.010	-0.111
	β	1.933	0.044	1.578	1.090	0.735	1.520	0.108	0.049
-OMe	α	2.064	0.032	1.675	1.314	1.003	1.474	-0.331	-0.532
	β	1.871	0.041	1.369	1.046	0.573	1.296	0.223	0.150
-OH	α	1.996	0.027	1.603	1.286	0.951	1.438	-0.298	-0.464
	β	1.739	0.032	1.392	0.933	0.590	1.327	0.212	0.147
-NH_2	α	1.949	0.028	1.565	1.303	0.965	1.525	-0.365	-0.406
	β	1.635	0.032	1.269	0.846	0.484	1.226	0.300	0.257
-NMe_2	α	1.936	0.041	1.582	1.304	1.000	1.436	-0.417	-0.563
	β	1.962	0.047	1.476	1.118	0.473	1.197	0.530	0.251
					B4b				
-F		2.089	0.031	1.736	1.360	1.028	1.671	-0.320	-0.385
-Cl		2.055	0.058	1.739	1.267	0.943	1.577	-0.146	-0.308
-Br		2.050	0.066	1.738	1.262	0.939	1.571	-0.140	-0.308
-CF_3		2.160	0.052	1.684	1.363	0.876	1.474	-0.067	-0.277
-CN		2.143	0.031	1.587	1.446	0.768	1.359	0.051	-0.177

Table S11 Vertical excitation energies ($E(S_1)_V$ and $E(T_1)_V$), oscillator strength (f), adiabatic excitation energies ($E(S_1)$, $E(T_1)$ and $E(T_2)$) and the ΔE_{SF} and ΔE_{TTA} (in eV) (continued table).[e]

	$E(S_1)_V$	f	$E(S_1)$	$E(T_1)_V$	$E(T_1)$	$E(T_2)$	ΔE_{SF}	ΔE_{TTA}
-OMe	2.075	0.010	1.830	1.228	1.192	1.660	-0.554	-0.724
-OH	2.209	0.038	1.760	1.482	1.139	1.623	-0.519	-0.656
-NH_2	2.119	0.032	1.735	1.466	1.166	1.735	-0.598	-0.598
-NMe_2	2.119	0.050	1.758	1.468	1.157	1.810	-0.556	-0.504

[e]Due to the open-shell singlet ground state of **A6**, its excitation energy was not considered.

Table S12 N^{FOD} for all compounds considered in this work at the TPSS/def2-TZVP Level.

Compound		N^{FOD}
A0		0.518
B0		0.190
C0		0.146
A1		0.627
A2		0.537
A3		0.773
A4		0.893
A5		0.822
A6		1.669
B1		0.513
B2		0.530
B3		0.846
B4		0.798
B5		0.776
B6		1.157
B4a		0.774
B4b		0.731
	B4a	
-F	α	0.771
	β	0.822
-Cl	α	0.804
	β	0.819
-Br	α	0.813
	β	0.819
-CF_3	α	0.808
	β	0.737
-CN	α	0.894
	β	0.782
-Me	α	0.755
	β	0.809
-OMe	α	0.731
	β	0.845
-OH	α	0.753
	β	0.918
-NH_2	α	0.768
	β	0.982
-NMe_2	α	0.774
	β	0.851
	B4b	
-F		0.724
-Cl		0.761

Table S12 N^{FOD} for all compounds considered in this work at the TPSS/def2-TZVP Level (continued table).

Compound	N^{FOD}
-Br	0.771
-CF_3	0.773
-CN	0.861
-Me	0.708
-OMe	0.678
-OH	0.700
-NH_2	0.704
-NMe_2	0.706

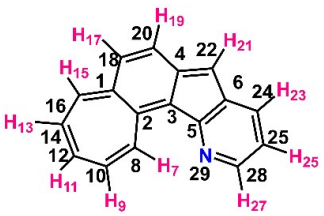

Fig. S3 Molecular structure of **B4a**.

Table S13 Mulliken spin population[12] of **B4a** calculated at PUHF/6-31G* level.

Atom site	Atom type	Spin population
1	C	0.744
2	C	0.523
3	C	-0.556
4	C	-0.698
5	C	0.744
6	C	-0.806
7	H	0.055
8	C	-0.839
9	H	-0.055
10	C	0.837
11	H	0.060
12	C	-0.892
13	H	-0.058
14	C	0.870
15	H	0.055
16	C	-0.853
17	H	0.044
18	C	-0.749
19	H	-0.043
20	C	0.745
21	H	-0.047
22	C	0.839
23	H	-0.048
24	C	0.790
25	H	0.048
26	C	-0.766
27	H	-0.051
28	C	0.746
29	N	-0.640

Table S14 Comparison of the vertical excitation energy of S_1 with the energy at the CI point (eV).

Compound	$E(S_1)$v	$E(S_1)_{CI}$	$\Delta E(S_{1CI}\text{-}S_1v)$
A1	2.319	2.305	-0.014
A2	2.501	2.746	0.245
A3	1.570	1.911	0.341
A4	1.662	1.049	-0.613
A5	1.790	1.232	-0.558
B1	2.268	2.681	0.350
B2	2.304	1.707	-0.136
B3	1.400	1.260	-0.140
B4	1.853	2.075	0.222
B5	1.945	1.787	-0.158
B6	1.062	0.661	-0.401
B4a	1.891	2.418	0.527
B4b	2.014	2.517	0.503
βCF_3-B4b	1.819	2.380	0.561

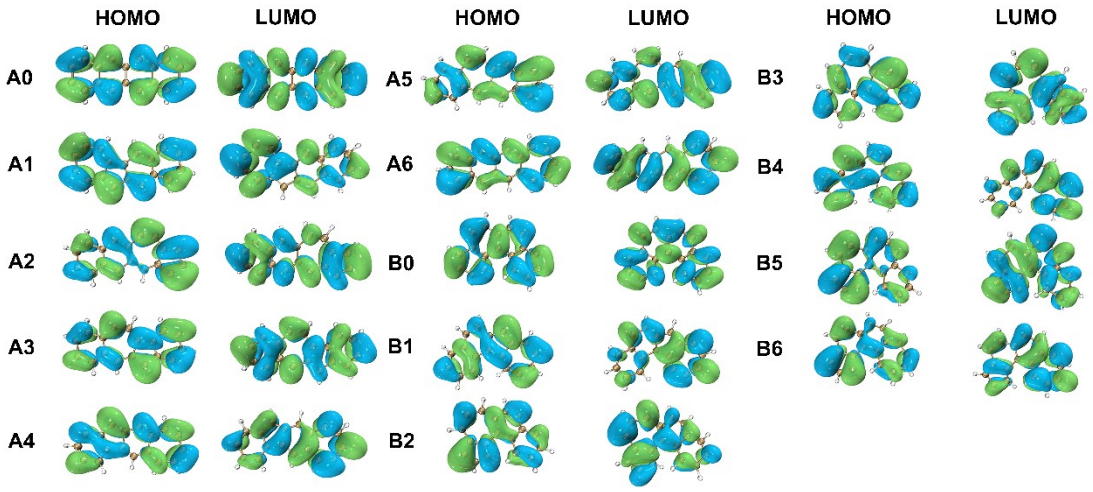

Fig. S4 Electron density distributions of HOMO and LUMO in azulene-containing analogues (**A0-B6**) (isovalue=0.02 e·bohr^{-3}).

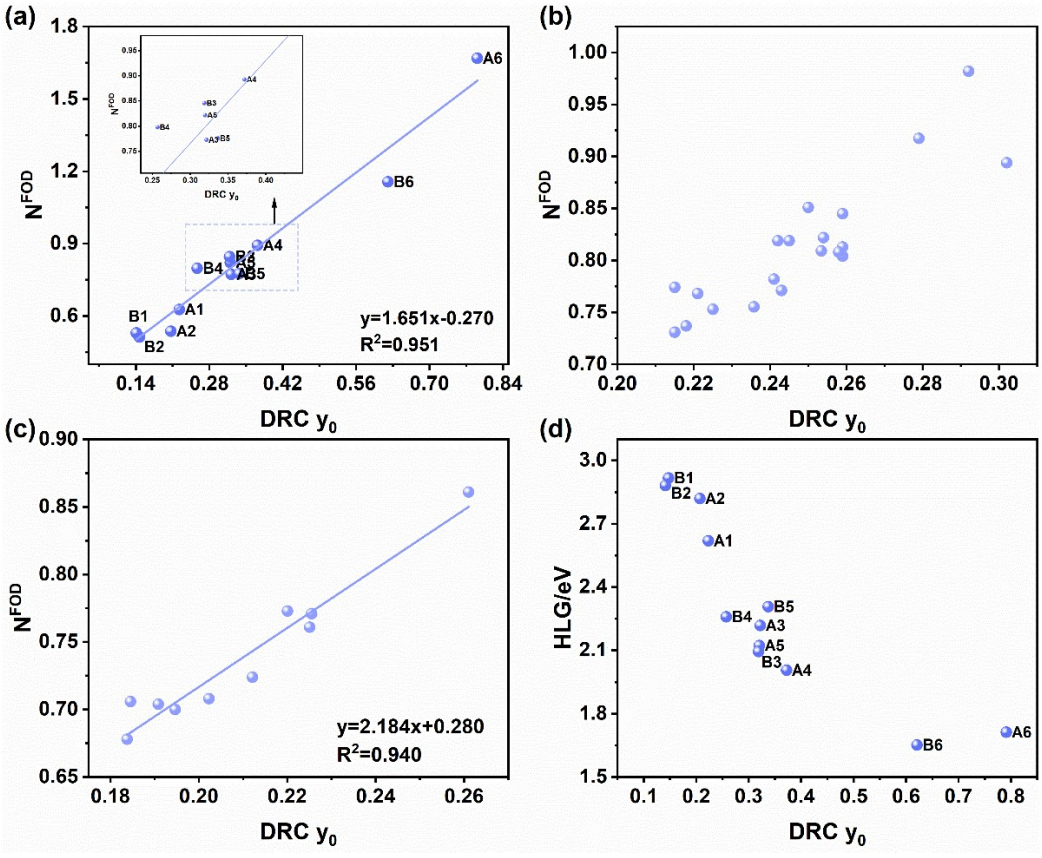

Fig. S5 Comparison of DRC y_0 and the N^{FOD} values for (a) azulene-containing analogues (**A1-B6**) (b) **B4a** derivatives and (c) **B4b** derivatives (d) HLG versus DRC y_0 for azulene-containing analogues (**A1-B6**).

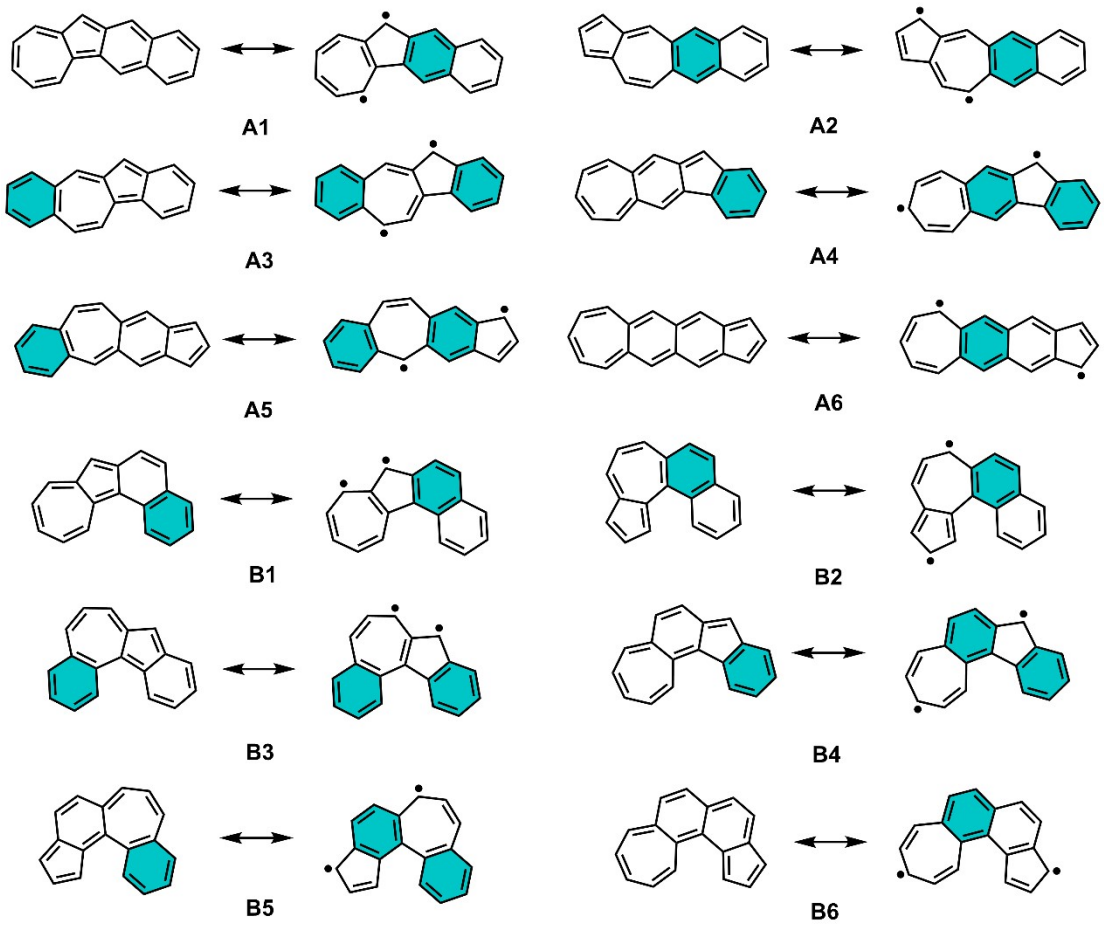

Fig. S6 Closed-shell and open-shell resonance structures of azulene-containing analogues (**A1-B6**) based on OED isosurfaces (Clar's sextets are shown by color filing.).

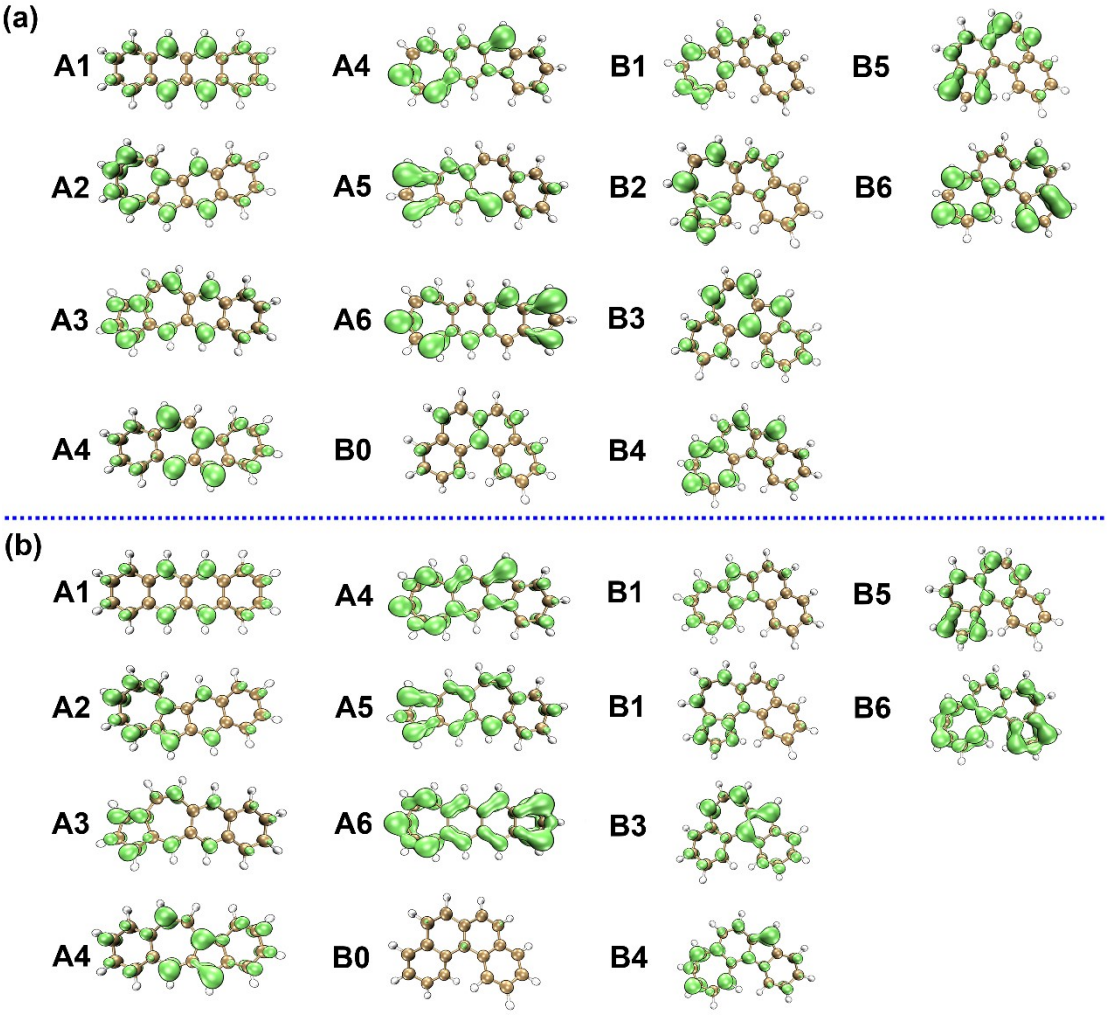

Fig. S7 (a) OED corresponding to the broken symmetry solutions obtained at the UNO/6-31G* level (isovalue=0.003 e·bohr^{-3}). (b) Isocontour plot of the FOD density calculated at FT-TPSS/def2-TZVP level (isovalue=0.002 e·bohr^{-3}).

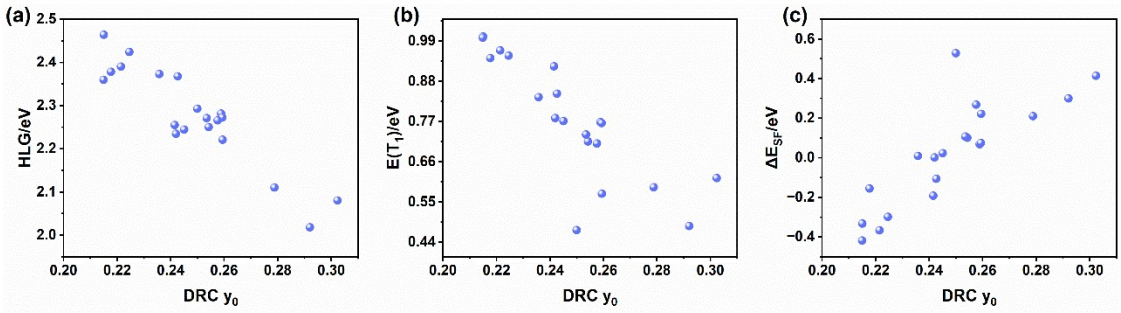

Fig. S8 (a) HLG (b) $E(T_1)$ and (c) ΔE_{SF} for α and β substituted **B4a** with respect to the DRC y_0.

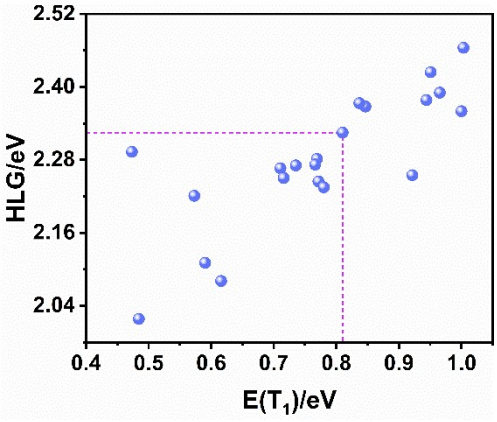

Fig. S9 HLG for α and β substituted **B4a** with respect to the $E(T_1)$ (the dashed line indicates the HLG and corresponding $E(T_1)$ of **B4a**).

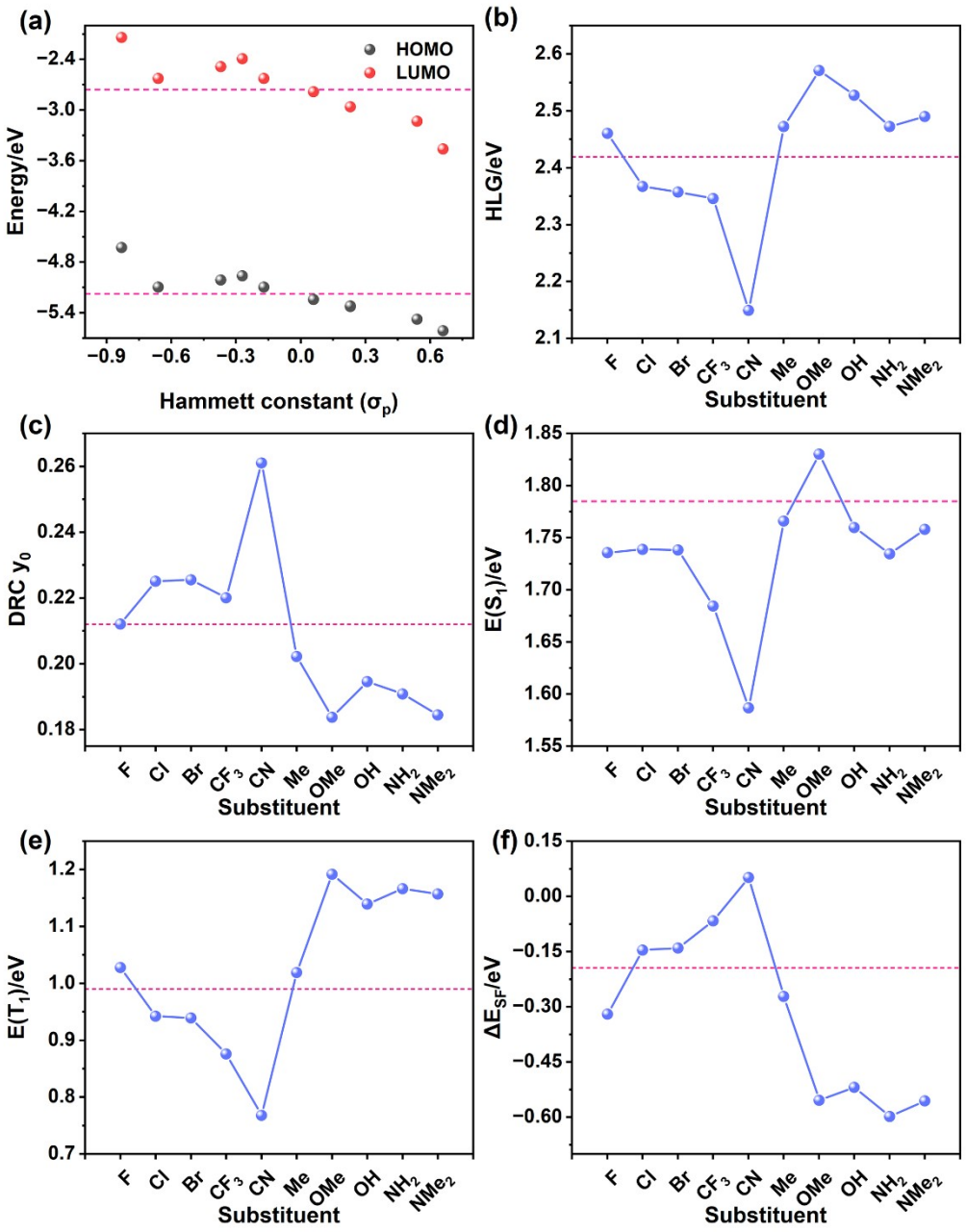

Fig. S10 (a) *E*(HOMO) and *E*(LUMO) of **B4b** derivatives with respect to Hammett constant (σ_p) of the attached substituents. (b) HLG (eV), (c) DRC y_0, (d) $E(S_1)$, (e) $E(T_1)$, and (f) ΔE_{SF} for **B4b** derivatives**.** (The solid lines are only guides for the eyes and the dashed lines indicate the corresponding values of **B4b**).

The variation trend of HOMO, LUMO and HLG of **R-B4b** is similar to that of **αR-B4a** (Fig. S9). For the same substituents, the HOMO and LUMO energies of **R-B4b** are lower than those of **R-B4a**. The electron density distribution of HOMO (4.72%) is smaller than that of LUMO (15.80%) at C15. As a result,

similar to **α-B4a**, EWGs give a narrower HLG, while EDGs give a wider HLG. The effect of substituents on DRC y_0 is also similar to **αR-B4a**.

The variations of $E(T_1)$ and $E(S_1)$ show similar trend as that of HLG. Compared to the parent **B4b**, the introduction of EWGs results in a decrease in $E(T_1)$, while the EDGs show opposite effect. Only **αMeO-B4b** shows slightly larger $E(S_1)$ than **B4b**. Consequently, relatively weaker EWGs, -Cl and -Br, achieve balance between less endothermicity and appropriate $E(T_1)$ to be SF sensitizers. Noticeably, these **B4b** derivatives suffer from significantly negative ΔE_{TTA}.

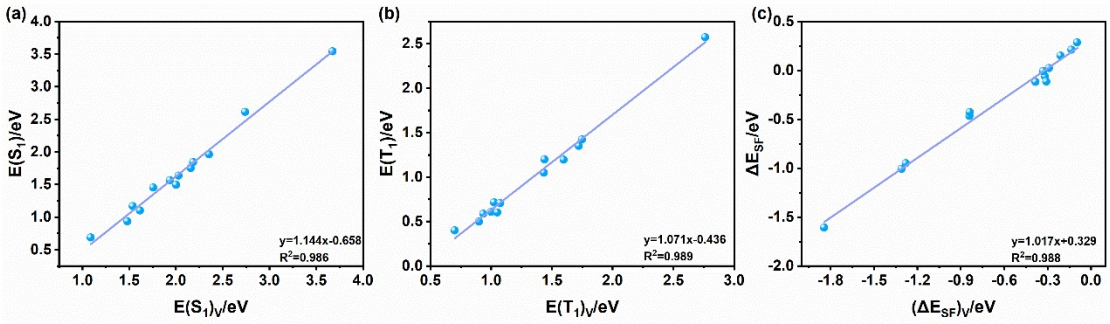

Fig. S11 Correlation between the vertical and adiabatic energies of S_1, T_1, and the corresponding ΔE_{SF}.

As shown in Fig. S11, we observed a similar linear correlation between the vertical and adiabatic energies of S_1, T_1, and ΔE_{SF}, as reported by Corminboeuf et al.[13] . This correlation further supports the notion that the trends in adiabatic and vertical excitation energies are similar.

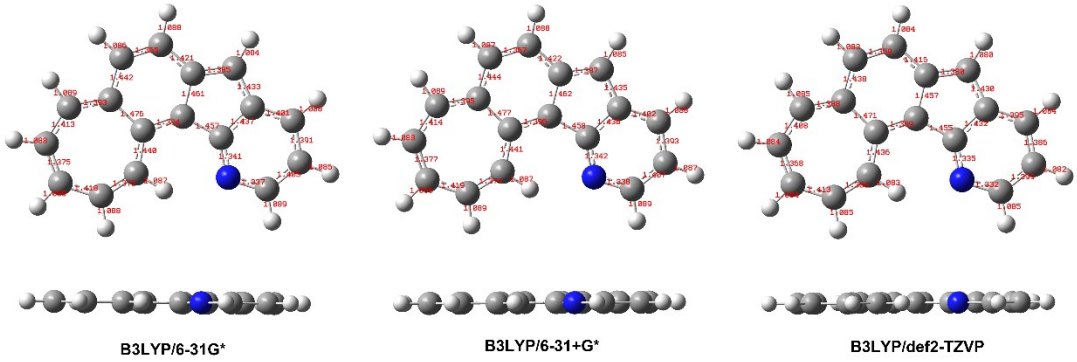

Fig S12 Optimized geometries of **B4a** at different basis sets.

The geometry optimization of polycyclic aromatic hydrocarbons is not highly

sensitive to the choice of basis set.[14] Similarly, no significant differences were observed in the optimized geometries using the method of B3LYP/6-31G*, B3LYP/6-31+G*, or B3LYP/def2-TZVP in our study. With **B4a** as an example, we optimized its structure with these three different methods and showed them in Fig. S12. We found that the optimized molecular structure of **B4a** obtained from these three methods are almost the same. Therefore, the vertical/adiabatic energies, diradical character y_0, NICS and N^{FOD} calculated with the optimized S_0 structures using different model chemistries should be reasonable.

Coordinates of the geometries.

A0

C	-4.88938700	0.71536000	0.00000000
C	-3.71162100	1.40935100	0.00000000
C	-2.45063200	0.72605900	0.00000000
C	-2.45063200	-0.72605900	0.00000000
C	-3.71162100	-1.40935100	0.00000000
C	-4.88938700	-0.71536000	0.00000000
C	-1.23566600	1.40634500	0.00000000
C	-1.23566600	-1.40634500	0.00000000
C	0.00020800	-0.72649100	0.00000000
C	0.00020800	0.72649100	0.00000000
C	1.23526500	1.40621900	0.00000000
H	1.23583500	2.49455400	0.00000000
C	1.23526500	-1.40621900	0.00000000
H	-1.23572400	2.49466100	0.00000000
H	-5.83678100	1.24775000	0.00000000
H	-3.70975200	2.49693700	0.00000000
H	-3.70975200	-2.49693700	0.00000000
H	-5.83678100	-1.24775000	0.00000000
H	-1.23572400	-2.49466100	0.00000000
H	1.23583500	-2.49455400	0.00000000
C	2.45091500	0.72603100	0.00000000
C	3.71131300	1.40905800	0.00000000
C	4.88956600	0.71503600	0.00000000
C	4.88956600	-0.71503600	0.00000000
C	3.71131300	-1.40905800	0.00000000
C	2.45091500	-0.72603100	0.00000000
H	3.71012100	2.49669400	0.00000000
H	5.83652600	1.24832700	0.00000000
H	5.83652600	-1.24832700	0.00000000
H	3.71012100	-2.49669400	0.00000000

B0

H	4.62783700	0.42251500	-0.40268400
C	3.74262900	-0.17236400	-0.18961900
C	1.46008100	-1.63928200	0.43569100
C	2.70432100	-2.24079400	0.45607000
C	3.85799700	-1.51431700	0.10446400
H	0.60656800	-2.21069600	0.77511000
H	2.79084100	-3.27891600	0.76564200
H	4.83153400	-1.99671600	0.10582300
C	-3.85799800	-1.51431700	-0.10446600

C	-3.74262900	-0.17236400	0.18961600
C	-2.48364800	0.47597400	0.18346100
C	-1.28901200	-0.28025700	-0.05670100
C	-1.46008100	-1.63928200	-0.43568800
C	-2.70432100	-2.24079400	-0.45606900
C	-2.40671400	1.89315400	0.34190200
C	0.00000000	0.39520300	0.00000100
C	0.00000000	1.81357800	0.00000100
C	-1.21786100	2.53872500	0.18872100
C	1.21786200	2.53872500	-0.18872000
H	1.16735100	3.62395500	-0.23259600
C	2.40671400	1.89315400	-0.34190200
C	2.48364800	0.47597400	-0.18346200
C	1.28901200	-0.28025600	0.05670300
H	-3.32306000	2.44848000	0.52625100
H	-4.83153500	-1.99671600	-0.10582800
H	-4.62783600	0.42251700	0.40268000
H	-0.60656800	-2.21069800	-0.77510400
H	-2.79084200	-3.27891600	-0.76564100
H	-1.16735000	3.62395500	0.23259800
H	3.32306000	2.44848100	-0.52625200

A1

C	-4.69287700	0.89943300	0.00000000
C	-3.66494500	1.80542400	0.00000100
C	-2.25664300	1.56076500	0.00000000
C	-4.63613100	-0.53066500	-0.00000100
C	-1.59043400	0.36768600	0.00000000
C	-3.54043500	-1.35096200	0.00000000
C	-2.15255200	-1.01033300	0.00000000
H	-5.69737200	1.31871300	0.00000000
H	-3.94867500	2.85573400	0.00000100
H	-1.63668800	2.45628300	0.00000000
H	-5.60315000	-1.02912700	0.00000000
H	-3.74252800	-2.42171800	-0.00000100
C	-1.11165200	-1.91361500	0.00000000
H	-1.22176600	-2.99230500	0.00000000
C	-0.14258800	0.20523100	0.00000000
C	0.88251800	1.13116300	0.00000000
C	2.22860200	0.69660200	0.00000000
C	2.51740300	-0.71870900	0.00000000
C	1.45592300	-1.65304600	0.00000000
C	0.14315000	-1.20994700	0.00000000
H	3.08767700	2.68304100	0.00000000

H	0.67837800	2.20021000	0.00000000
C	3.31336300	1.61878500	0.00000000
C	3.88214500	-1.12812400	0.00000100
H	1.68524800	-2.71639900	0.00000000
C	4.90250200	-0.20716300	0.00000000
C	4.61703900	1.18407000	-0.00000100
H	4.10254300	-2.19322800	0.00000000
H	5.93656200	-0.54169200	0.00000000
H	5.43344500	1.90092000	-0.00000100

A2

C	-4.88989300	0.38370300	0.00000000
C	-3.79200600	1.20941800	0.00000000
C	-2.47457800	0.66625800	0.00000000
C	-2.31629000	-0.76017600	0.00000000
C	-3.47660400	-1.58692300	0.00000000
C	-4.73200200	-1.02995500	0.00000000
H	-1.45140000	2.54967900	0.00000000
H	-5.89012200	0.80806700	0.00000000
H	-3.91200400	2.29006000	0.00000000
C	-1.32134300	1.46975500	0.00000000
C	-1.01207100	-1.28025600	-0.00000100
H	-3.34911100	-2.66685300	0.00000000
H	-5.61259200	-1.66608100	0.00000100
C	0.13893500	-0.48314300	0.00000000
C	-0.01808600	0.96136500	-0.00000100
H	-0.89066900	-2.36129000	0.00000000
C	1.04584400	1.94203200	0.00000000
C	2.40334800	1.80786500	0.00000000
C	3.19118900	0.62391200	0.00000000
C	1.38980500	-1.20307000	0.00000000
C	2.68161800	-0.76862300	0.00000000
H	0.68063700	2.96720600	0.00000000
H	2.97254600	2.73695800	0.00000000
H	1.26638400	-2.28623900	-0.00000100
C	4.56886700	0.54545400	0.00000000
H	5.24772600	1.39088600	0.00000000
C	4.96263300	-0.84138400	0.00000100
H	5.98881500	-1.19241200	0.00000000
C	3.84171000	-1.63207700	0.00000000
H	3.80334200	-2.71491900	0.00000100

A3

C	-4.85066400	0.47439600	0.00000100

C	-3.75199200	1.29613400	0.00000100
C	-2.41011000	0.79729100	0.00000100
C	-2.24026200	-0.64284900	-0.00000100
C	-3.41838400	-1.45884800	-0.00000100
C	-4.68437800	-0.93324500	-0.00000100
H	-5.84928500	0.90264100	0.00000000
H	-3.88772700	2.37446900	0.00000100
H	-3.28322000	-2.53743500	-0.00000100
H	-5.55182200	-1.58658100	-0.00000100
C	-1.38356500	1.77239100	0.00000100
C	0.00179100	1.64675900	0.00000000
C	0.78624500	0.50011800	0.00000000
C	0.30649700	-0.91010400	-0.00000100
C	-1.01285800	-1.34446300	-0.00000100
H	-1.74749800	2.79780000	0.00000100
H	0.54665600	2.59000900	0.00000100
H	-1.12379400	-2.42906100	-0.00000200
C	2.20529500	0.43596800	0.00000000
C	2.59370600	-0.95677600	0.00000000
C	1.43212300	-1.75457300	0.00000200
H	1.39920500	-2.83776900	0.00000400
C	3.19471000	1.44732200	0.00000000
C	4.52508100	1.08658600	-0.00000100
C	4.90905600	-0.28585000	0.00000000
C	3.97164800	-1.29542600	0.00000000
H	2.91205000	2.49735500	0.00000000
H	5.29622300	1.85184200	0.00000000
H	5.96755600	-0.53388800	0.00000000
H	4.27803800	-2.33836600	0.00000200

A4

C	2.64142400	-1.64593200	0.00003900
C	1.67569000	-0.65481300	-0.00007500
C	1.91126300	0.81172200	-0.00014400
C	3.22405900	1.41163100	-0.00020900
C	4.48305200	0.88095600	0.00002800
C	4.87649700	-0.49259000	0.00020600
C	4.06506500	-1.59400800	0.00017500
C	0.30668600	-1.11017700	-0.00013300
C	-0.74083100	-0.24224300	-0.00006500
C	-0.51120100	1.21230200	-0.00002500
C	0.83051300	1.67403400	-0.00013800
C	-2.18242700	-0.44402500	-0.00004800
C	-2.78026800	0.85463600	0.00002800

C	-1.73046600	1.85437600	0.00029100
C	-2.96841200	-1.59474700	-0.00007200
C	-4.35958800	-1.46432000	-0.00002800
C	-4.95109400	-0.19183900	0.00004900
C	-4.17552700	0.96932000	0.00007900
H	2.24085000	-2.65849500	-0.00000100
H	3.18828900	2.50050400	-0.00044000
H	5.29955800	1.59955300	0.00000500
H	5.94921700	-0.67550300	0.00032800
H	4.55780800	-2.56376300	0.00024800
H	0.13525400	-2.18441700	-0.00025900
H	1.01896400	2.74530600	-0.00016900
H	-1.89174900	2.92637800	0.00045100
H	-2.51151900	-2.58196000	-0.00017500
H	-4.98694900	-2.35120400	-0.00004900
H	-6.03521000	-0.10905800	0.00011200
H	-4.65111900	1.94696200	0.00021400

A5

C	-4.91241500	-0.06087700	0.00000100
C	-3.97948800	0.96601100	0.00000000
C	-3.12106700	-1.66070000	0.00000000
C	-4.48041400	-1.39287200	0.00000100
H	-5.97377100	0.17151800	0.00000100
H	-4.32048100	1.99800400	0.00000100
H	-2.78051500	-2.69306200	0.00000000
H	-5.19877000	-2.20724300	0.00000100
C	1.99023000	1.48083600	0.00000000
C	3.10559900	0.61239500	0.00000000
C	2.87243200	-0.84635400	0.00000000
C	1.59855000	-1.32729000	-0.00000100
H	2.15611900	2.55631200	0.00000000
H	1.41090200	-2.39912100	-0.00000100
C	4.47270100	0.80917500	0.00000000
H	4.98907500	1.76211900	0.00000100
C	5.11072700	-0.48740700	0.00000100
H	6.18520000	-0.63904100	0.00000200
C	4.16469200	-1.48681500	0.00000000
H	4.34223700	-2.55509300	-0.00000100
C	-2.58847100	0.72424100	0.00000000
C	-1.72409300	1.88256600	-0.00000100
C	-0.36855700	1.98993100	0.00000000
C	-2.14522400	-0.63445100	0.00000000
C	0.68813600	1.01244800	0.00000000

C	-0.77383600	-1.07960400	-0.00000100
C	0.44874200	-0.44620600	-0.00000100
H	-2.26353700	2.82764700	-0.00000100
H	0.00305100	3.01401600	-0.00000100
H	-0.69897500	-2.16621800	-0.00000100

A6

C	4.37230900	1.23436500	0.00013300
C	3.04809100	1.56058600	0.00023500
C	4.97611000	-0.06568700	-0.00038800
C	4.35206400	-1.28267400	-0.00055900
C	2.95487000	-1.56286000	-0.00007100
H	5.06836100	2.06996100	0.00059700
H	2.83720100	2.62944700	0.00094200
H	6.06423200	-0.07652400	-0.00045900
H	4.99474500	-2.16025200	-0.00071200
H	2.71645600	-2.62510300	-0.00006100
C	1.84831500	0.75131400	0.00013600
C	0.63888600	1.41057600	0.00010300
C	-0.63530400	0.76625600	0.00007400
C	-0.63272000	-0.70036300	0.00023600
C	0.56905100	-1.37085600	0.00033300
C	1.84860400	-0.72683400	0.00015200
H	-1.83159400	2.54102200	-0.00012200
H	0.64451200	2.49886000	0.00007500
C	-1.83655000	1.45279700	-0.00008100
C	-1.88265500	-1.41711500	0.00024300
H	0.55694800	-2.45886300	0.00041600
C	-3.06093300	-0.73169500	0.00006700
C	-3.06576800	0.75159400	-0.00013500
H	-1.85681000	-2.50521800	0.00045000
C	-4.44260100	-1.16512700	-0.00005800
C	-5.22113100	-0.03430500	-0.00008600
C	-4.38942600	1.15108100	-0.00049400
H	-4.78047500	-2.19392200	0.00039200
H	-6.30624200	-0.01730300	0.00009000
H	-4.75459900	2.17158600	-0.00064100

B1

C	4.09448300	-1.40577800	-0.06722500
C	2.87428100	-2.04183200	-0.20308000
C	1.56779500	-1.50015900	-0.17409300
C	4.36505300	-0.02922100	0.08978900
C	1.15227800	-0.19304000	-0.00500300

C	3.46550500	1.01877100	0.12972700
C	2.05650000	1.00314200	0.07066000
H	4.96998400	-2.05209100	-0.10119900
H	2.91631500	-3.11935800	-0.34729600
H	0.78833000	-2.23677500	-0.33011200
H	5.41619500	0.24006400	0.16547900
H	3.90016000	2.01415300	0.21945200
C	-0.19574100	0.31597900	0.01454600
C	-0.10320900	1.74159600	0.01788500
C	1.25919100	2.13604400	0.07056000
H	1.61788900	3.15854800	0.10157400
C	-1.49430500	-0.31423700	0.03395000
C	-2.64621200	0.53905900	-0.07372600
C	-2.49199800	1.96399300	-0.12516600
C	-1.26447700	2.55823000	-0.05315000
H	-0.90558600	-2.37642900	0.37342500
C	-1.73253300	-1.70292500	0.19169400
C	-3.94105900	-0.02904600	-0.09597800
H	-3.39187300	2.57025800	-0.20071600
H	-1.16519100	3.64045700	-0.06577600
C	-4.13115800	-1.39227500	0.01375300
C	-3.01222200	-2.22899600	0.17683500
H	-4.79576400	0.63734500	-0.18942800
H	-5.13277200	-1.81260100	-0.00248600
H	-3.15071400	-3.29940300	0.30520800

B2

C	-1.55008000	2.38804200	0.15715100
C	-2.83064000	1.97037400	0.44033400
C	-3.32577700	0.65235600	0.44139200
C	-0.33025100	1.67912800	-0.05700600
C	-2.64883500	-0.50251900	0.12186100
C	-0.12662100	0.25856900	-0.03356100
C	-1.18817300	-0.69881900	-0.17053200
H	-1.42534900	3.46953700	0.13476900
H	-3.55631800	2.75535200	0.64030200
H	-4.39037600	0.54002700	0.64437900
C	-3.29199800	-1.75706000	-0.07516500
H	-4.35384500	-1.92887000	0.05432900
C	-2.35136200	-2.65414600	-0.54695500
H	-2.54548100	-3.67607100	-0.85475200
C	-1.07780400	-2.02499100	-0.59618100
H	-0.17927400	-2.49870600	-0.96416100
C	3.96682200	-1.07690600	0.21410800

C	3.67780500	0.21676100	-0.17023200
C	2.34441700	0.68630900	-0.20973500
C	1.26208000	-0.20509900	0.07131300
C	1.60457000	-1.50228900	0.53425900
C	2.91833600	-1.92892500	0.60629500
H	2.88883600	2.73690100	-0.68936900
H	4.99659000	-1.42184700	0.25150400
H	4.47791400	0.90982500	-0.41915300
C	2.06673100	2.06470000	-0.45808000
H	0.81979800	-2.16085600	0.88160100
H	3.13855600	-2.92378500	0.98353700
C	0.80091500	2.53431700	-0.31185300
H	0.60814900	3.59968200	-0.40747100

B3

C	-2.71436100	1.57797700	-0.29248800
C	-2.42066600	0.20248100	-0.14513100
C	-1.11632900	-0.40287300	0.08520500
C	-1.92346400	2.71013800	-0.15683100
C	0.13654300	0.26827900	0.02495200
C	-0.55275100	2.77715300	0.09060200
C	0.37852100	1.74232600	0.15270800
H	-2.44043000	3.66241600	-0.24977000
H	-0.13679700	3.77872200	0.19599000
C	1.43898200	-0.31708200	-0.04061900
C	2.42159500	0.73482000	0.14309400
C	1.75632700	1.96442000	0.27818400
H	2.22102900	2.93678400	0.39104300
C	1.90936600	-1.62793600	-0.33381700
C	3.26330700	-1.88550200	-0.36021500
C	4.21406200	-0.85802000	-0.10815000
C	3.80688700	0.43592000	0.12486900
H	1.22073700	-2.42424400	-0.59104100
H	3.61413400	-2.88596700	-0.59823900
H	5.27391900	-1.09890200	-0.13024700
H	4.53314400	1.23038500	0.27738300
C	-3.50706200	-2.00437700	0.01657100
C	-2.26008700	-2.57445900	0.37293400
C	-1.12717300	-1.80292000	0.40632800
C	-3.56811400	-0.65660300	-0.21280400
H	-4.40248100	-2.61688500	-0.02986500
H	-2.20203600	-3.62496000	0.64578600
H	-0.20494500	-2.25185000	0.74602000
H	-4.52642500	-0.19156200	-0.42974400

H	-3.76335800	1.78361000	-0.49966900

B4

C	2.09624900	0.92235100	-0.02186700
C	1.72794700	2.31543400	-0.00164500
C	1.01696500	-0.08595900	0.07246600
C	-0.30240700	0.35555900	0.02032200
C	-0.62444800	1.78584300	0.04252400
C	0.43062900	2.73577400	0.04572100
C	-1.58905300	-0.34151600	-0.01408600
C	-2.61309800	0.66607200	0.03916800
C	-1.99268900	1.96068600	0.07677600
C	-1.97301800	-1.68372500	-0.14987300
C	-3.32692900	-2.02072100	-0.17177800
C	-4.31970200	-1.03290100	-0.07440400
C	-3.96925800	0.30985900	0.01986700
C	3.45691000	0.66300300	-0.16097900
C	4.19996300	-0.53987400	-0.23314100
C	3.76042400	-1.82700700	-0.05091200
C	2.43348300	-2.22950500	0.26167500
C	1.28674800	-1.48273800	0.31795700
H	2.53230000	3.04504000	-0.03292000
H	0.19973700	3.79838700	0.07029300
H	-2.51616100	2.90932700	0.11480200
H	-1.24212100	-2.47546400	-0.27404600
H	-3.61429500	-3.06350700	-0.27669200
H	-5.36795800	-1.31978300	-0.09229200
H	-4.73623400	1.07930400	0.06676600
H	4.06751500	1.55921000	-0.25679800
H	5.26271000	-0.41034500	-0.42782000
H	4.50293900	-2.61948000	-0.11072100
H	2.31028300	-3.28647200	0.49048800
H	0.40898300	-2.04002100	0.62221500

B5

C	-2.79771300	-0.08599100	0.04925500
C	-1.42585900	-0.55462700	-0.19702600
C	-0.32718700	0.26157200	0.02698000
C	-0.60338600	1.68791400	0.28542000
C	-1.95036500	2.08385500	0.63809100
C	-3.01055100	1.23331100	0.52844800
H	-2.10464900	3.12057100	0.92393900
H	-4.01622800	1.57102100	0.76865400
C	1.10982300	-1.61974600	0.70952500

C	2.29335800	-2.33858200	0.77274300
C	3.46996900	-1.78889800	0.24835900
C	3.43937800	-0.50373600	-0.25766900
H	0.20651300	-2.05430700	1.11980000
H	2.30127100	-3.32350400	1.23105900
H	4.40089500	-2.34847600	0.26814200
H	4.35649600	-0.04711000	-0.62077200
C	2.43098400	1.64707600	-0.68518500
C	1.60404200	2.71089000	-0.46793200
C	0.29805400	2.72063500	0.08649100
C	2.25552800	0.27796400	-0.27966700
C	1.02675300	-0.32505300	0.14260000
H	3.40376200	1.87244400	-1.11780400
H	1.99706200	3.68937200	-0.73686100
H	-0.10105600	3.71572400	0.27580000
C	-3.66262200	-1.12583800	-0.23411600
H	-4.74267900	-1.10273500	-0.14206600
C	-2.88277500	-2.24707900	-0.69240900
H	-3.29587400	-3.19289300	-1.02582800
C	-1.54645900	-1.92504700	-0.66458800
H	-0.73136200	-2.55182400	-0.99998200

B6

C	1.94179000	0.98779800	-0.09430000
C	1.53063100	2.35004000	-0.11104500
C	0.21151400	2.69632700	0.00997200
C	-0.82821100	1.73212600	0.06504300
C	-0.48002000	0.31857400	-0.00294800
C	0.90294900	-0.04171400	0.08226700
C	-2.16313800	2.14939200	0.18583900
C	-3.21173400	1.22788200	0.20632600
C	-2.94904800	-0.12677300	0.05323300
C	-1.56448400	-0.61214000	-0.09881000
C	-3.82369800	-1.23813300	-0.07103000
C	-3.03996400	-2.35694400	-0.33174600
C	-1.66508500	-1.99184300	-0.35410200
C	1.22151800	-1.37015500	0.47619300
C	2.40566400	-2.08887100	0.49329000
C	3.68687300	-1.69351500	0.07021900
C	4.08173700	-0.41623300	-0.28982300
C	3.31121900	0.75626300	-0.28765500
H	2.29019900	3.11938300	-0.21545300
H	-0.06727200	3.74762300	0.03377800
H	-2.36960300	3.21358900	0.26376300

H	-4.23677800	1.57813100	0.31040800
H	-4.90523800	-1.19922800	-0.01830900
H	-3.41078400	-3.36084300	-0.51101500
H	-0.86303400	-2.67371800	-0.60450300
H	0.36236100	-1.92246200	0.84417500
H	2.32305500	-3.10834500	0.86381300
H	4.45597100	-2.46311600	0.06888600
H	5.12910300	-0.28568000	-0.55244300
H	3.88093600	1.66218900	-0.48864100

B4a

C	-2.07316800	0.92736500	0.00004100
C	-0.99550000	-0.08131500	0.00026300
C	0.32175100	0.37544700	0.00024600
C	0.65531400	1.79787600	0.00011500
C	1.59988400	-0.32327100	0.00006300
C	2.63664800	0.67158900	0.00005400
H	-0.29749700	-2.07456000	0.00037700
C	-1.22254700	-1.50333500	0.00024200
H	-2.22841200	-3.32572300	0.00044000
C	-2.37574200	-2.24738300	0.00027600
H	-4.47881900	-2.61116800	0.00026600
C	-3.72913400	-1.82280400	0.00013600
H	-5.26964400	-0.39490100	-0.00038500
C	-4.18969100	-0.52730400	-0.00020200
H	-4.05848400	1.56985800	-0.00067100
C	-3.44295000	0.67173300	-0.00032200
H	-2.50514800	3.05073200	-0.00022100
C	-1.70039600	2.32076900	-0.00010800
H	-0.17680200	3.80978600	0.00000600
C	-0.40298900	2.74586700	-0.00003300
H	2.55532400	2.91779400	0.00063200
C	2.02941800	1.97000700	0.00039100
H	4.79240900	0.94185100	-0.00010100
C	3.96711600	0.23357300	-0.00016200
H	5.21273600	-1.53077600	-0.00043500
C	4.20002800	-1.13791700	-0.00033300
H	3.28962500	-3.10193000	-0.00044800
C	3.11249200	-2.02769600	-0.00036300
N	1.83164300	-1.64431100	-0.00018300

B4b

C	2.07427077	0.92813764	-0.01400720
C	1.03085475	-0.12284168	0.03205541

C	-0.30436603	0.28319742	0.00638299
C	-0.66815887	1.69974632	0.02549703
C	-1.59198448	-0.39326173	-0.01049184
C	-2.55361462	0.67089212	0.02303989
C	-2.04915958	-1.71827732	-0.08242874
C	-3.42019672	-1.96976301	-0.08921188
C	-4.35248361	-0.91852042	-0.03362929
C	-3.92864839	0.40469019	0.01714659
H	-1.36861693	-2.56103308	-0.15567010
H	-3.77254380	-2.99625092	-0.14499220
H	-5.41532120	-1.14598224	-0.04061108
H	-4.63370400	1.23000669	0.04570808
H	0.45037219	-2.13404802	0.30288297
C	1.33008456	-1.52011306	0.15344547
H	2.40435478	-3.30476293	0.24450472
C	2.50815255	-2.22767350	0.13177225
H	4.61241314	-2.51862926	-0.04495694
C	3.83487723	-1.75836429	-0.02028396
H	5.31197886	-0.27585111	-0.21114141
C	4.24214360	-0.44768664	-0.11613835
H	4.03014457	1.64060799	-0.13293072
C	3.45031426	0.72057922	-0.08392684
H	2.44282037	3.06077444	-0.02030996
C	1.66127619	2.30649371	-0.00201409
H	0.06554731	3.73752505	0.04322645
C	0.35057995	2.68959379	0.02761627
N	-1.97301353	1.92952440	0.04647828

αF-B4a

C	1.60373800	1.35301300	-0.00009100
C	0.68423400	0.20044800	0.00001400
C	-0.68467200	0.45789500	0.00000000
C	-1.22405100	1.81784100	-0.00010400
C	-1.84596500	-0.42174300	0.00006100
C	-3.01674500	0.40960900	0.00001700
H	0.27773500	-1.87518100	0.00027000
C	1.11127500	-1.17669300	0.00014600
C	2.35321400	-1.75071000	0.00012600
C	3.61554400	-1.11159000	-0.00003000
C	3.91144900	0.22640700	-0.00014000
C	2.99640500	1.29818200	-0.00014200
C	1.03191800	2.67691100	-0.00016600
C	-0.31350000	2.90924800	-0.00017600
H	-3.26813200	2.64355400	-0.00014000

C	-2.60750100	1.78433400	-0.00008600
H	-5.18893100	0.35679800	0.00004200
C	-4.26762300	-0.22094100	0.00007600
H	-5.23819300	-2.14990800	0.00022400
C	-4.29458200	-1.61187400	0.00017600
H	-3.10408300	-3.42045000	0.00029500
C	-3.08798300	-2.33199700	0.00021500
N	-1.87841000	-1.76232400	0.00015800
H	4.96853700	0.47598700	-0.00023200
H	2.40083900	-2.83650600	0.00024200
H	3.47732100	2.27425600	-0.00021500
H	1.72177300	3.51641200	-0.00022500
H	-0.69122000	3.92907500	-0.00023500
F	4.66692300	-1.95864400	-0.00005600

βF-B4a

C	-2.14102700	0.98852800	-0.00002100
C	-1.18923400	-0.13920100	-0.00005900
C	0.17150400	0.15903200	-0.00003300
C	0.65737200	1.53746700	0.00001200
C	1.36194100	-0.68420600	0.00001100
C	2.51316500	0.17458100	-0.00001200
H	-0.73190100	-2.20362000	-0.00012000
C	-1.58258400	-1.52731100	-0.00005900
H	-2.79365400	-3.21763300	-0.00003700
C	-2.81369000	-2.12942800	-0.00001200
C	-4.11064000	-1.54935900	0.00005100
C	-4.41390000	-0.20997400	0.00006300
H	-4.03734700	1.85822000	0.00004100
C	-3.53082500	0.89458600	0.00002200
H	-2.32513900	3.14923500	0.00003800
C	-1.60915200	2.33227500	0.00002000
H	0.08070000	3.63534900	0.00004700
C	-0.27329100	2.60804300	0.00003300
C	2.03498000	1.51793300	-0.00002700
H	4.68283400	0.21551900	-0.00003200
C	3.78784600	-0.40038400	-0.00001400
H	4.81924000	-2.29700600	-0.00000400
C	3.85933000	-1.78922900	0.00000300
H	2.72833600	-3.63444600	0.00003700
C	2.67509200	-2.54723100	0.00003300
N	1.44516600	-2.02181700	0.00003500
H	-4.94705500	-2.24477900	0.00008800
H	-5.47055800	0.04971600	0.00010900

F	2.83300600	2.60282300	-0.00005300

αCl-B4a

C	1.09755600	1.64213200	-0.00005600
C	0.32133800	0.38953300	0.00003100
C	-1.06738400	0.48426200	0.00001900
C	-1.76179600	1.77101100	-0.00007000
C	-2.11836300	-0.52561300	0.00010600
C	-3.37843500	0.16231000	0.00001900
H	0.17220600	-1.71812600	0.00038200
C	0.91473900	-0.92352700	0.00021500
C	2.21509000	-1.35278800	0.00016700
C	3.40763000	-0.57912100	-0.00007400
C	3.52515700	0.79022600	-0.00018400
C	2.48686400	1.74569200	-0.00011900
C	0.37643700	2.88994500	-0.00009000
C	-0.98741300	2.96240700	-0.00010700
H	-3.88861300	2.35188300	-0.00015000
C	-3.13215200	1.57569600	-0.00008200
H	-5.52963700	-0.14339500	-0.00000200
C	-4.54714900	-0.60946200	0.00006000
H	-5.28509100	-2.63910800	0.00022200
C	-4.41111200	-1.99421500	0.00018600
H	-3.01700400	-3.65033200	0.00036400
C	-3.12859100	-2.56754900	0.00026600
N	-1.99345500	-1.86015800	0.00022500
H	4.53346100	1.19278100	-0.00033000
H	2.36012800	-2.42892900	0.00032400
H	2.85349600	2.77042400	-0.00017000
H	0.96366600	3.80422600	-0.00012600
H	-1.48320000	3.93053200	-0.00014900
Cl	4.90589800	-1.50673500	-0.00021400

βCl-B4a

C	2.19735300	-1.12688000	0.00001800
C	1.41923800	0.12576400	0.00009700
C	0.02753500	0.02759300	0.00006400
C	-0.65510200	-1.26240300	-0.00000900
C	-1.02431300	1.03575900	-0.00004700
C	-2.28796000	0.35553300	-0.00000800
H	1.26312700	2.23291600	0.00010000
C	2.00722200	1.44062900	0.00005100
H	3.45136700	2.93892200	0.00009200
C	3.31397000	1.85936400	0.00005200

C	4.51098000	1.09817000	0.00002900
C	4.61934800	-0.27242700	-0.00005000
H	3.94759400	-2.26331600	-0.00017700
C	3.58699000	-1.23611100	-0.00007900
H	2.06477900	-3.29008200	-0.00012200
C	1.47671800	-2.37671000	-0.00007300
H	-0.38540200	-3.41909000	-0.00007600
C	0.11415600	-2.45427800	-0.00006900
C	-2.02260900	-1.05018300	0.00009500
H	-4.43725600	0.64156300	-0.00000800
C	-3.46050700	1.11732100	-0.00005500
H	-4.19954200	3.14531200	-0.00014700
C	-3.32506200	2.50141600	-0.00013200
H	-1.93207500	4.15840000	-0.00022800
C	-2.04216200	3.07549900	-0.00018900
N	-0.90595900	2.37118200	-0.00014500
H	5.43950200	1.66493900	0.00006400
H	5.62779200	-0.68075600	-0.00009400
Cl	-3.24899700	-2.28678900	0.00020200

αBr-B4a

C	0.29411500	1.87918500	-0.00005600
C	-0.34324800	0.55020900	0.00004500
C	-1.73397700	0.49562800	0.00003600
C	-2.56243900	1.70023000	-0.00006000
C	-2.67017300	-0.62132100	0.00009600
C	-3.99686000	-0.07274600	0.00005800
H	-0.26573900	-1.56181400	0.00031200
C	0.38701600	-0.69189000	0.00017600
C	1.72628600	-0.97930000	0.00014200
C	2.82693300	-0.08131800	-0.00003600
C	2.79886800	1.29218000	-0.00014000
C	1.66415400	2.13144300	-0.00011500
C	-0.55657900	3.04245600	-0.00011900
C	-1.92043800	2.96775500	-0.00012600
H	-4.73938500	2.04938800	-0.00008600
C	-3.90392100	1.35889300	-0.00003900
H	-6.10275100	-0.60758100	0.00008800
C	-5.07591300	-0.96549400	0.00011700
H	-5.59138600	-3.06270800	0.00025900
C	-4.79180900	-2.32759200	0.00021200
H	-3.22771700	-3.82427500	0.00032100
C	-3.45503200	-2.75975000	0.00024500
N	-2.40243400	-1.93470000	0.00018700

H	3.75724200	1.80166300	-0.00025000
H	1.98479900	-2.03363000	0.00026400
H	1.91914200	3.18954700	-0.00018200
H	-0.07128300	4.01448300	-0.00017400
H	-2.51704600	3.87698700	-0.00017800
Br	4.55855000	-0.90887300	-0.00012300

βBr-B4a

C	-2.38752800	-1.32603800	0.00002500
C	-1.86941100	0.05470400	-0.00004900
C	-0.48533300	0.23027800	-0.00002900
C	0.43525700	-0.90169200	0.00003700
C	0.35067900	1.42390700	0.00005900
C	1.72173300	1.00064000	0.00004300
H	-2.12673300	2.15175900	-0.00005100
C	-2.70212100	1.22955400	-0.00001200
H	-4.41103500	2.41739000	-0.00005900
C	-4.06556200	1.38541500	-0.00002000
C	-5.09070600	0.40521900	-0.00000400
H	-5.83906400	-1.55745100	0.00011600
C	-4.92958300	-0.96038900	0.00007700
H	-3.88270800	-2.78201200	0.00021100
C	-3.72928400	-1.70421900	0.00011500
H	-1.83525700	-3.42195100	0.00015000
C	-1.43696700	-2.41129900	0.00010500
H	0.59711900	-3.06576300	0.00009800
C	-0.08566900	-2.22049500	0.00009600
C	1.73456000	-0.42820700	-0.00008100
H	3.77452800	1.68927600	0.00006200
C	2.72566700	1.97305200	0.00009900
H	3.06060600	4.10556900	0.00019400
C	2.32672300	3.30510900	0.00016900
H	0.64041000	4.66257200	0.00024600
C	0.95696200	3.62113000	0.00020500
N	-0.02281100	2.71147400	0.00015100
H	-6.11203200	0.77980900	-0.00004500
Br	3.29935300	-1.48627300	-0.00020000

αCF_3-B4a

C	-0.36970300	1.87497100	0.00020700
C	0.27810800	0.54784000	0.00004100
C	1.66795600	0.50624700	-0.00001100
C	2.48607900	1.71676600	0.00009300
C	2.61559300	-0.60403000	-0.00016300

C	3.93675800	-0.04432500	-0.00014600
H	0.21309000	-1.56490200	-0.00019100
C	-0.44501000	-0.69987300	-0.00007100
C	-1.78284400	-0.98593400	-0.00005300
C	-2.90369300	-0.10535800	0.00008900
C	-2.86694400	1.26741600	0.00023300
C	-1.73982300	2.11993500	0.00028200
C	0.47284200	3.04529400	0.00030400
C	1.83654000	2.98045200	0.00025100
H	4.65915700	2.08547000	0.00005900
C	3.82997400	1.38735200	0.00001200
H	6.04777200	-0.55652200	-0.00027100
C	5.02472700	-0.92495200	-0.00027700
H	5.56031800	-3.01771800	-0.00052100
C	4.75389700	-2.29026200	-0.00041600
H	3.20395200	-3.80056900	-0.00052800
C	3.42170200	-2.73412100	-0.00042000
N	2.36049700	-1.91895000	-0.00029700
H	-3.82527400	1.77650100	0.00032000
H	-2.02813100	-2.04502500	-0.00016200
H	-2.00028200	3.17654300	0.00040300
H	-0.02008600	4.01329100	0.00042500
H	2.42732900	3.89350400	0.00032900
C	-4.24947100	-0.79592900	0.00007700
F	-4.38700700	-1.59298800	1.08525000
F	-4.38707400	-1.59284100	-1.08519300
F	-5.28830200	0.06395900	0.00016900

βCF$_3$-B4a

C	2.38565200	-1.29362400	-0.01183500
C	1.83197100	0.07148600	-0.00817700
C	0.44025900	0.21067200	-0.01932400
C	-0.45583500	-0.93646700	-0.03707600
C	-0.41611000	1.38690300	-0.01356600
C	-1.77575000	0.93803400	-0.03024700
H	2.03115300	2.17168900	0.01196700
C	2.63055200	1.26453000	0.00945000
H	4.30999300	2.49759200	0.03468700
C	3.99234600	1.45693000	0.02330400
C	5.03939100	0.50582000	0.02443200
H	5.84176000	-1.43783900	0.01661800
C	4.91623500	-0.86636700	0.01299000
H	3.91719800	-2.71246900	-0.00756000
C	3.73780300	-1.63869100	-0.00229000

H	1.88477700	-3.39977800	-0.02674900
C	1.46386200	-2.39829000	-0.02582600
H	-0.54117800	-3.11174100	-0.05259800
C	0.10711800	-2.24300400	-0.04022300
C	-1.77928900	-0.50044100	-0.05585700
H	-3.83753700	1.61859300	-0.05058100
C	-2.79105700	1.90449800	-0.03107300
H	-3.15517000	4.03004800	-0.00505300
C	-2.40925700	3.24069800	-0.00790600
H	-0.74226600	4.62254200	0.02286800
C	-1.04484900	3.57695600	0.00745500
N	-0.05579000	2.67989900	0.00322300
H	6.05070800	0.90649100	0.03609000
C	-2.99904700	-1.33969700	0.01612300
F	-4.02760000	-0.79903000	-0.68837900
F	-3.45942100	-1.49576800	1.28661800
F	-2.80329800	-2.59232500	-0.47205900

αCN-B4a

C	1.24256100	1.59179000	-0.00004600
C	0.44753000	0.34785100	0.00005000
C	-0.93766800	0.46697300	0.00006100
C	-1.61014600	1.76324600	-0.00000100
C	-2.00759500	-0.52638800	0.00012100
C	-3.25546700	0.18159500	0.00010800
H	0.26680000	-1.75871400	0.00035900
C	1.02109700	-0.97602300	0.00018000
C	2.31441100	-1.41977900	0.00008000
C	3.53526400	-0.67265700	-0.00017600
C	3.65353900	0.70781500	-0.00026600
C	2.63592900	1.67885100	-0.00015700
C	0.54293700	2.84904600	-0.00005400
C	-0.82113700	2.94242000	-0.00004100
H	-3.72728500	2.38000500	0.00001100
C	-2.98442600	1.59067700	0.00003400
H	-5.41175300	-0.08328700	0.00015600
C	-4.43818300	-0.56736800	0.00016700
H	-5.21095300	-2.58441700	0.00028700
C	-4.32632500	-1.95456600	0.00024000
H	-2.96034500	-3.63314600	0.00031100
C	-3.05385500	-2.54882800	0.00025100
N	-1.90553000	-1.86151800	0.00019200
H	4.66706900	1.09987700	-0.00043400
H	2.44056600	-2.49927600	0.00020600

H	3.01484800	2.69875200	-0.00021100
H	1.14348700	3.75412200	-0.00009400
H	-1.30216100	3.91769800	-0.00005800
C	4.75241400	-1.43285100	-0.00033000
N	5.73616500	-2.05597500	-0.00045700

βCN-B4a

C	-2.14061700	1.13140000	-0.00002300
C	-1.34175300	-0.10610200	-0.00010300
C	0.05264500	0.01978300	-0.00006700
C	0.70297800	1.31355900	0.00003800
C	1.12336000	-0.96855000	-0.00001300
C	2.36863400	-0.26617200	0.00000300
H	-1.13632100	-2.20527100	-0.00021400
C	-1.89769400	-1.42876800	-0.00011300
H	-3.31402800	-2.95824700	-0.00009700
C	-3.19876700	-1.87636400	-0.00005500
C	-4.40551700	-1.13982600	0.00002500
C	-4.54435400	0.23189900	0.00005100
H	-3.91537100	2.23372500	0.00006400
C	-3.53521800	1.21372200	0.00002200
H	-2.05001900	3.29546800	0.00012000
C	-1.44681200	2.39222200	0.00007700
H	0.40128700	3.46485700	0.00014400
C	-0.08336700	2.49210400	0.00010600
C	2.09438200	1.15086400	-0.00007500
H	4.52375100	-0.51412500	0.00002900
C	3.55495600	-1.00646400	0.00003900
H	4.33086400	-3.02030100	0.00005700
C	3.44470700	-2.39270900	0.00005200
H	2.08210400	-4.07499700	0.00005200
C	2.17234300	-2.99031400	0.00005300
N	1.02440300	-2.30684500	0.00002100
H	-5.32308900	-1.72409000	0.00006300
H	-5.56153500	0.61705700	0.00010400
C	3.05432700	2.18664800	-0.00010800
N	3.84944800	3.04175100	0.00001000

αMe-B4a

C	1.54692600	1.40556800	-0.00032300
C	0.65698400	0.23381000	-0.00037500
C	-0.71812800	0.45843300	-0.00011900
C	-1.28741700	1.80438600	0.00015000
C	-1.85887900	-0.44760500	-0.00006100

C	-3.04907200	0.35723200	0.00034300
H	0.31647700	-1.84970400	-0.00177800
C	1.12895800	-1.12708100	-0.00107700
H	2.41311300	-2.75500000	-0.00137100
C	2.38821000	-1.66578400	-0.00080100
C	3.67405900	-1.04411100	0.00021500
C	3.87950000	0.31962700	0.00050100
H	3.39966800	2.35988000	-0.00009800
C	2.93864000	1.37323500	-0.00008100
H	1.61817200	3.57240500	-0.00054300
C	0.94677400	2.71799600	-0.00038500
H	-0.80594000	3.92866200	-0.00005900
C	-0.40319400	2.91828300	-0.00008800
H	-3.34990600	2.58492100	0.00060200
C	-2.67044400	1.74037600	0.00040500
H	-5.21933700	0.25665900	0.00082900
C	-4.28544700	-0.30073100	0.00052700
H	-5.21325000	-2.25114500	0.00040200
C	-4.28181600	-1.69215600	0.00028100
H	-3.05136300	-3.47318200	-0.00031400
C	-3.05933900	-2.38445300	-0.00011900
N	-1.86215500	-1.78861000	-0.00027200
H	4.91755100	0.64699600	0.00120000
C	4.86788900	-1.97140300	0.00094300
H	4.85588300	-2.62632600	0.88191500
H	4.85636100	-2.62708200	-0.87947100
H	5.81242800	-1.42054900	0.00097100

βMe-B4a

C	-2.13341500	1.01950000	-0.00015000
C	-1.20587200	-0.12809000	-0.00001400
C	0.16084300	0.14107000	0.00022700
C	0.69525500	1.50144800	0.00002600
C	1.32687700	-0.73210100	0.00010500
C	2.49073700	0.10538900	-0.00005800
H	-0.79557700	-2.20165400	-0.00072300
C	-1.63089500	-1.50618400	-0.00040500
H	-2.88106700	-3.16883000	-0.00022700
C	-2.87589400	-2.08039300	-0.00006700
C	-4.15884100	-1.47088700	0.00041900
C	-4.43294400	-0.12488000	0.00027300
H	-4.00842300	1.93442300	-0.00040600
C	-3.52478600	0.95891300	-0.00017000
H	-2.26116000	3.18281000	-0.00034700

C	-1.56722300	2.34669900	-0.00033100
C	-0.22363700	2.58626900	-0.00021700
C	2.08463700	1.48779800	0.00008400
H	4.66392800	0.07285800	-0.00008200
C	3.74711000	-0.51205800	-0.00009700
H	4.73553100	-2.43381300	0.00001700
C	3.78753600	-1.90353100	-0.00010800
H	2.61103600	-3.71981100	-0.00005500
C	2.58663200	-2.63133200	-0.00006400
N	1.37143200	-2.07212600	0.00007900
H	-5.01083900	-2.14735500	0.00082300
H	-5.48364200	0.15809400	0.00050300
H	0.14075000	3.61078400	-0.00029500
C	3.01773400	2.65875900	0.00036600
H	2.47757700	3.61067500	0.00041700
H	3.67428500	2.65402200	0.88185100
H	3.67446000	2.65433900	-0.88095300

αOMe-B4a

C	1.10098200	1.55262100	0.00003400
C	0.28571600	0.33243900	0.00003900
C	-1.10026900	0.46896900	0.00000900
C	-1.75387700	1.77782200	-0.00002600
C	-2.18131800	-0.50793800	0.00000400
C	-3.41939100	0.22048000	-0.00003700
H	0.07126200	-1.77150800	0.00011200
C	0.83827000	-1.00065100	0.00008700
C	2.12133100	-1.46341900	0.00008100
C	3.35867200	-0.74678200	0.00003700
C	3.50700600	0.62711500	0.00004500
C	2.49287900	1.60663800	0.00005500
C	0.42068200	2.82615100	0.00001500
C	-0.93850200	2.94428200	-0.00001700
H	-3.86170200	2.42446300	-0.00008000
C	-3.12938700	1.62534000	-0.00005300
H	-5.57880700	-0.01946700	-0.00008500
C	-4.61103200	-0.51576500	-0.00005300
H	-5.41283200	-2.52112500	-0.00003900
C	-4.51859700	-1.90422400	-0.00002800
H	-3.17746600	-3.60405200	0.00003400
C	-3.25496300	-2.51808500	0.00001300
N	-2.09872200	-1.84632700	0.00002800
H	4.51673300	1.02209900	0.00012600
H	2.25116200	-2.54281900	0.00011300

H	2.88829500	2.62122400	0.00008300
H	1.03837000	3.72047600	0.00002100
H	-1.40205100	3.92818800	-0.00003500
O	4.41560000	-1.60093600	0.00003700
C	5.74230900	-1.08942200	-0.00019500
H	6.39370100	-1.96446300	-0.00033500
H	5.93807200	-0.48731100	-0.89602500
H	5.93843900	-0.48735800	0.89557000

βOMe-B4a

C	2.21649600	-1.14212400	-0.06695900
C	1.44029000	0.11221600	-0.01298800
C	0.05139500	0.01828300	-0.06844800
C	-0.63333800	-1.26526900	-0.16922600
C	-1.00298100	1.02614700	-0.04544400
C	-2.26469000	0.34722200	-0.13918400
H	1.29095700	2.21693100	0.11765900
C	2.03301200	1.42326100	0.09488600
H	3.47792000	2.91116100	0.24725400
C	3.33817200	1.83435800	0.17147700
C	4.53541800	1.06926600	0.16532300
H	5.64558900	-0.71064200	0.08808800
C	4.63894900	-0.29744600	0.07834500
H	3.96375400	-2.28234500	-0.07775100
C	3.60432300	-1.25610100	-0.02340800
H	2.08073000	-3.30063600	-0.21822800
C	1.49303900	-2.38780100	-0.17526700
H	-0.37355200	-3.41706300	-0.31319400
C	0.13125900	-2.45884600	-0.22542500
C	-2.00372900	-1.06651300	-0.20451800
H	-4.41058600	0.65393500	-0.28304800
C	-3.43274700	1.11680000	-0.17996400
H	-4.17048900	3.14606300	-0.12756200
C	-3.29813700	2.49958500	-0.10081200
H	-1.90679100	4.14811800	0.07346200
C	-2.01786800	3.06714700	0.00788800
N	-0.88335500	2.35901700	0.03015700
H	5.46417500	1.63111300	0.23661200
O	-2.93439200	-2.06200100	-0.34345900
C	-3.74729300	-2.29267600	0.80942000
H	-4.31274000	-1.39723200	1.09523600
H	-4.44449600	-3.08986400	0.54061800
H	-3.13526900	-2.61170900	1.66324800

αOH-B4a

C	1.58711851	1.36336369	0.00002555
C	0.67677679	0.21115934	0.00002997
C	-0.69450927	0.45881676	0.00000617
C	-1.24099988	1.81638096	-0.00003114
C	-1.85031003	-0.42728103	0.00000802
C	-3.02588459	0.39840085	-0.00002835
H	0.28641814	-1.86642565	0.00006097
C	1.11612668	-1.16324741	0.00006236
C	2.35634248	-1.73473036	0.00004744
C	3.63903576	-1.11346756	0.00002472
C	3.90021580	0.24305402	0.00008983
C	2.98005837	1.30685694	0.00006543
C	1.01133338	2.68592892	-0.00000444
C	-0.33475366	2.91260211	-0.00003447
H	-3.29022704	2.63044061	-0.00007898
C	-2.62459896	1.77504222	-0.00005173
H	-5.19780243	0.33224488	-0.00006109
C	-4.27302678	-0.24014290	-0.00003393
H	-5.23306565	-2.17437535	-0.00000470
C	-4.29226742	-1.63117205	-0.00000302
H	-3.09192930	-3.43355001	0.00005814
C	-3.08173546	-2.34490083	0.00003216
N	-1.87564942	-1.76831720	0.00003726
H	4.95054636	0.53497195	0.00019811
H	2.39656499	-2.82100605	0.00000327
H	3.45882844	2.28459877	0.00009315
H	1.69819472	3.52834382	-0.00000313
H	-0.71738623	3.93077719	-0.00005855
O	4.65841335	-2.01520554	-0.00013738
H	5.50856699	-1.54613753	-0.00059630

βOH-B4a

C	2.13978865	0.99785142	0.00016170
C	1.19513240	-0.13475579	0.00018456
C	-0.16700314	0.15740866	-0.00001137
C	-0.66586256	1.52907342	-0.00006667
C	-1.35017861	-0.69362673	-0.00013155
C	-2.50662069	0.16074825	-0.00011450
H	0.75446216	-2.20458863	0.00136120
C	1.59952387	-1.52190119	0.00078852
H	2.82028457	-3.20361851	0.00093683
C	2.83376165	-2.11507953	0.00045681
C	4.12923098	-1.52802264	-0.00045712

C	4.42142680	-0.18675201	-0.00070386
H	4.03137257	1.87959450	-0.00020583
C	3.53129494	0.91259562	-0.00018555
H	2.30745947	3.15933298	0.00065798
C	1.59759251	2.33692739	0.00046416
H	-0.10112715	3.62825658	0.00040053
C	0.25866943	2.60297708	0.00033183
C	-2.05061736	1.52152946	-0.00026380
H	-4.68747059	0.16389714	0.00018642
C	-3.77456417	-0.43010886	-0.00000397
H	-4.79749032	-2.33231834	-0.00013150
C	-3.84001104	-1.82017092	-0.00009832
H	-2.69465986	-3.65556165	-0.00027642
C	-2.65102184	-2.56796176	-0.00010880
N	-1.42563730	-2.03055772	-0.00004437
H	4.96979692	-2.21837967	-0.00090031
H	5.47638661	0.08086810	-0.00131172
O	-2.81868530	2.64977321	-0.00010003
H	-3.75332187	2.39384451	-0.00105886

αNH$_2$-B4a

C	-1.56844200	1.38346500	-0.00285300
C	-0.67079100	0.22974000	-0.00420700
C	0.70546500	0.46214500	-0.00103600
C	1.26346400	1.81477100	0.00153400
C	1.85056600	-0.43382500	-0.00001900
C	3.03518000	0.38197500	0.00298300
H	-0.29928600	-1.84947700	-0.01562200
C	-1.12347500	-1.13927600	-0.01106500
C	-2.36625100	-1.70324700	-0.01240400
C	-3.66124500	-1.09071100	-0.00198800
C	-3.89395600	0.28259100	0.00423100
C	-2.96638600	1.33057900	-0.00099300
C	-0.98422300	2.70002200	-0.00101700
C	0.36502800	2.91682000	0.00096200
H	3.32214000	2.60976000	0.00566700
C	2.64854400	1.76063900	0.00385500
H	5.20679800	0.29152200	0.00663400
C	4.27591700	-0.27113600	0.00444300
H	5.21670200	-2.21426700	0.00381800
C	4.28118600	-1.66170600	0.00289300
H	3.06367500	-3.45320400	-0.00101600
C	3.06327300	-2.36428600	0.00014900
N	1.86343500	-1.77621200	-0.00112700

H	-4.93942200	0.58754700	0.00867600
H	-2.38044300	-2.79279100	-0.02754000
H	-3.43674600	2.31293900	0.00308900
H	-1.66427400	3.54815800	-0.00092200
H	0.75471600	3.93235600	0.00223100
N	-4.73779100	-1.94786500	-0.04083600
H	-4.59337600	-2.91361000	0.21674400
H	-5.65312300	-1.58175600	0.17918200

βNH$_2$-B4a

C	-2.13822600	1.00565300	-0.00578300
C	-1.19796300	-0.12970900	-0.00068400
C	0.16448500	0.15462900	-0.00196400
C	0.68046100	1.52163100	-0.00324300
C	1.34089000	-0.70699300	0.00259100
C	2.50153000	0.13520900	-0.00485600
H	-0.77147100	-2.20490600	0.00897000
C	-1.61226400	-1.51726500	0.00625500
H	-2.84187500	-3.19044900	0.01557400
C	-2.84864800	-2.10172300	0.01010800
C	-4.14380100	-1.50718300	0.00687200
C	-4.42727200	-0.16565300	-0.00044500
H	-4.02424700	1.89995900	-0.01053500
C	-3.52981900	0.92999800	-0.00593300
H	-2.28842200	3.16892400	-0.01457500
C	-1.58570500	2.34041200	-0.00948700
H	0.10285200	3.62725300	-0.01857900
C	-0.24424400	2.59544900	-0.00869800
C	2.07269800	1.51076900	0.00183500
H	4.67696400	0.12593700	-0.04810900
C	3.76390700	-0.46498500	-0.02015200
H	4.77178100	-2.37676700	-0.02466200
C	3.81875600	-1.85626200	-0.01251900
H	2.65756200	-3.68112900	0.01034300
C	2.62399200	-2.59300200	0.00425400
N	1.40305900	-2.04511900	0.00892300
H	-4.98768800	-2.19343000	0.01011800
H	-5.48059500	0.10893400	-0.00206900
N	2.93997000	2.59905400	-0.05533700
H	2.52792100	3.48031600	0.22892400
H	3.82336700	2.45196100	0.42058700

αNMe$_2$-B4a

C	-0.65833200	1.79888000	0.00009800

C	0.02765500	0.51330600	0.00018300
C	1.42407900	0.50531300	0.00002200
C	2.20316300	1.74330100	-0.00022900
C	2.39863300	-0.57169600	0.00006700
C	3.70577400	0.03080100	-0.00018900
H	0.02723700	-1.59361600	0.00105200
C	-0.66096400	-0.75102000	0.00063600
C	-1.98145600	-1.10419400	0.00058400
C	-3.17445800	-0.29919100	0.00007300
C	-3.14366300	1.10399200	0.00005400
C	-2.04682300	1.97232700	0.00011900
C	0.13765700	2.99800600	-0.00007200
C	1.50488300	2.98189100	-0.00024800
H	4.36811500	2.17654900	-0.00054900
C	3.55990100	1.45432100	-0.00036300
H	5.83024300	-0.42963900	-0.00039100
C	4.81686600	-0.82507300	-0.00020200
H	5.41235000	-2.90008500	0.00004200
C	4.58480600	-2.19592400	0.00004300
H	3.07980100	-3.75388100	0.00048200
C	3.26455900	-2.68061700	0.00028900
N	2.18247700	-1.89713900	0.00029600
H	-4.09799800	1.61498600	-0.00031100
H	-2.13866200	-2.17575000	0.00115400
H	-2.34644100	3.01983900	0.00004400
H	-0.38911800	3.94906500	-0.00009000
H	2.06165300	3.91641200	-0.00039600
N	-4.39019100	-0.95007400	-0.00030100
C	-4.47882900	-2.40762200	-0.00133500
H	-5.53052300	-2.69505000	-0.00302800
H	-4.00981900	-2.84624800	-0.89087400
H	-4.01226600	-2.84755800	0.88889400
C	-5.63238900	-0.18801100	0.00065600
H	-5.71631700	0.45035600	-0.88877300
H	-6.47608800	-0.87831200	0.00168000
H	-5.71454000	0.45069300	0.88996900

βNMe$_2$-B4a

C	2.31590900	-1.25971900	0.00000400
C	1.67664800	0.07119500	0.00000400
C	0.28318700	0.12055700	0.00000800
C	-0.53440900	-1.08356800	0.00001000
C	-0.66055200	1.23106300	0.00000900
C	-1.98751600	0.68017900	0.00000600

H	1.74808600	2.18187700	0.00000400
C	2.40368200	1.31481800	0.00000100
H	4.00055000	2.64943400	-0.00000600
C	3.74765300	1.59080400	-0.00000500
C	4.85624700	0.70515600	-0.00001000
H	5.77451300	-1.18359400	-0.00001300
C	4.81584300	-0.66887100	-0.00000900
H	3.93436100	-2.57660900	-0.00000100
C	3.68555900	-1.51662400	-0.00000200
H	1.95186900	-3.39612900	0.00001700
C	1.46419200	-2.42502300	0.00001200
H	-0.51116500	-3.24993600	0.00002700
C	0.10120200	-2.35260700	0.00001700
C	-1.88554500	-0.76365800	0.00001200
H	-4.09328900	1.22568600	-0.00002800
C	-3.06521100	1.57636500	-0.00000900
H	-3.58337400	3.67264700	-0.00002200
C	-2.78225300	2.93904900	-0.00001000
H	-1.21866400	4.43590100	0.00000100
C	-1.44662100	3.37129300	0.00000000
N	-0.39514700	2.54546500	0.00000700
H	5.84043400	1.16871700	-0.00001500
N	-2.92593400	-1.73753500	0.00000200
C	-3.73616700	-1.75755300	1.21650100
H	-4.40032100	-0.88127900	1.32918000
H	-4.36593200	-2.65585500	1.21466200
H	-3.07887900	-1.80033900	2.08959100
C	-3.73612400	-1.75759200	-1.21652600
H	-4.36574000	-2.65600100	-1.21479700
H	-4.40042800	-0.88142300	-1.32914600
H	-3.07879300	-1.80018100	-2.08959400

F-B4b

C	1.61358700	1.32444200	-0.01250800
C	0.71992200	0.14556400	0.03097000
C	-0.65788200	0.36698000	0.00495300
C	-1.20842200	1.72505300	0.02137500
C	-1.84300500	-0.47505100	-0.01075800
C	-2.93784600	0.45150800	0.02126800
C	-2.11916800	-1.84994400	-0.07926900
C	-3.44371400	-2.28258600	-0.08401900
C	-4.50769400	-1.36447500	-0.03015500
C	-4.26474900	0.00358700	0.01713300
H	-1.33300700	-2.59541800	-0.15179400

H	-3.65597800	-3.34693400	-0.13719600
H	-5.53065100	-1.73175800	-0.03577000
H	-5.07387500	0.72712200	0.04438100
H	0.41002900	-1.92877400	0.28857700
C	1.19981200	-1.20173600	0.14812600
H	2.53249200	-2.82897600	0.24102300
C	2.45582500	-1.75055100	0.13417700
C	3.69358300	-1.08608800	-0.00519400
H	4.99710600	0.53521400	-0.17922500
C	3.95025600	0.25831400	-0.09698100
H	3.45998700	2.29013600	-0.12155500
C	3.00653100	1.30237600	-0.07364900
H	1.69454000	3.48640400	-0.02466900
C	1.02080800	2.63437900	-0.00599800
H	-0.75072800	3.84138100	0.03340300
C	-0.32976800	2.84034700	0.02102400
N	-2.53141000	1.77702500	0.04186900
F	4.76461100	-1.90447700	-0.02813500

Cl-B4b

C	1.12029300	1.60027600	-0.00702400
C	0.36014100	0.33210300	0.03922900
C	-1.03183400	0.40303500	0.00713400
C	-1.72538700	1.69293100	0.01734500
C	-2.11929600	-0.56276900	-0.00979200
C	-3.30787600	0.23956800	0.01572700
C	-2.24367100	-1.95889800	-0.07555400
C	-3.51427000	-2.53234000	-0.08367300
C	-4.67157700	-1.73531700	-0.03605100
C	-4.57853900	-0.34852200	0.00820000
H	-1.38053000	-2.61404700	-0.14323000
H	-3.60972500	-3.61352600	-0.13454800
H	-5.64855800	-2.21140400	-0.04420900
H	-5.46130700	0.28321100	0.03049600
H	0.28466900	-1.75934800	0.31992200
C	0.98899200	-0.95063000	0.16861100
H	2.45960100	-2.43222800	0.27714700
C	2.29645900	-1.36576100	0.15711700
C	3.46917000	-0.58298800	0.00486200
H	4.55879200	1.20283700	-0.18663000
C	3.56068000	0.78627400	-0.09434300
H	2.85501800	2.75184800	-0.12101500
C	2.50673100	1.72219500	-0.06926000
H	0.96996800	3.75880400	-0.02328200

C	0.39163100	2.83947900	-0.00441900
H	-1.50107300	3.84694900	0.02656400
C	-0.97353800	2.89771900	0.01772400
N	-3.04634700	1.60159300	0.03373800
Cl	4.97817200	-1.48719900	-0.03366900

Br-B4b

C	0.32435000	1.83410900	-0.00450800
C	-0.30380200	0.49546600	0.04253500
C	-1.69572800	0.42555900	0.00798700
C	-2.51595100	1.63872800	0.01422000
C	-2.68015800	-0.64516300	-0.00892100
C	-3.94373700	0.03309300	0.01243000
C	-2.66280700	-2.04679700	-0.07160900
C	-3.86906200	-2.74558900	-0.08115000
C	-5.10103400	-2.06944200	-0.03782800
C	-5.14855100	-0.68024500	0.00355500
H	-1.73777400	-2.61157000	-0.13569700
H	-3.85474700	-3.83100000	-0.12967400
H	-6.02494100	-2.64174700	-0.04696700
H	-6.09061800	-0.14078500	0.02263700
H	-0.16752700	-1.59315300	0.32531000
C	0.45122300	-0.71706900	0.17464000
H	2.06280700	-2.04243900	0.28803500
C	1.79431300	-0.99802000	0.16647500
C	2.88076700	-0.10029300	0.01592700
H	3.78485100	1.78709300	-0.17682200
C	2.83493900	1.27042600	-0.08542700
H	1.93479800	3.15489600	-0.11748400
C	1.69156200	2.09550100	-0.06438500
H	-0.04302000	3.96631500	-0.02516200
C	-0.52567200	2.99336900	-0.00567400
H	-2.51062400	3.80441000	0.01957000
C	-1.88980600	2.91336200	0.01364600
N	-3.82104300	1.41457100	0.02812000
Br	4.61568600	-0.91245700	-0.02205900

CF_3-B4b

C	0.39809400	1.83308700	0.00044000
C	-0.23916000	0.49564700	0.05229500
C	-1.62894100	0.43664100	0.01124000
C	-2.44183900	1.65398800	0.01431800
C	-2.62127300	-0.62940400	-0.00763200
C	-3.87995500	0.05569500	0.00995700

C	-2.61144900	-2.02979100	-0.07224300
C	-3.82323000	-2.72118600	-0.08602800
C	-5.05048700	-2.03837600	-0.04539600
C	-5.08921800	-0.64804400	-0.00305200
H	-1.68939900	-2.59915900	-0.13512900
H	-3.81515000	-3.80655800	-0.13580100
H	-5.97791700	-2.60470100	-0.05773700
H	-6.02772000	-0.10241200	0.01329000
H	-0.11631600	-1.58974000	0.36972800
C	0.50891400	-0.72162300	0.20109000
H	2.10804900	-2.04773500	0.32596400
C	1.84987400	-1.00112900	0.18832500
C	2.95369200	-0.12086300	0.01571100
H	3.84909600	1.76194000	-0.20177300
C	2.89991200	1.24717600	-0.09584900
H	2.01283000	3.14525100	-0.12404300
C	1.76395200	2.08753800	-0.06747800
H	0.04310600	3.96856300	-0.01949500
C	-0.44627200	2.99914200	-0.00014400
H	-2.42627800	3.82082200	0.02179500
C	-1.80950200	2.92699200	0.01660000
N	-3.74714400	1.43794400	0.02566900
C	4.30541600	-0.80216500	-0.02221600
F	4.52083000	-1.51307400	1.10847400
F	4.37551300	-1.67690200	-1.05128100
F	5.33016100	0.06199500	-0.15676200

CN-B4b

C	1.26466700	1.55375100	-0.00480400
C	0.48671000	0.29278700	0.04588600
C	-0.90131000	0.38533500	0.00910500
C	-1.57592700	1.68373100	0.01672900
C	-2.00462900	-0.56582700	-0.00915800
C	-3.18108200	0.25299500	0.01343400
C	-2.14858700	-1.95831000	-0.07605900
C	-3.42943300	-2.51219800	-0.08760300
C	-4.57467300	-1.69944700	-0.04224500
C	-4.46077500	-0.31353300	0.00270200
H	-1.29536400	-2.62599200	-0.14209600
H	-3.54044600	-3.59175500	-0.13918300
H	-5.55836600	-2.16096500	-0.05290900
H	-5.33348500	0.33189800	0.02287800
H	0.38117200	-1.79544000	0.35157600
C	1.09752000	-1.00010300	0.18694500

H	2.54432200	-2.49822100	0.29916800
C	2.39788900	-1.42939300	0.17045500
C	3.59651900	-0.67173900	0.00292400
H	4.69107200	1.11285600	-0.20590300
C	3.68858100	0.70662400	-0.10388800
H	3.01454800	2.68445300	-0.13187100
C	2.65382900	1.65969600	-0.07501100
H	1.14539500	3.71338500	-0.02094600
C	0.55450100	2.80242000	-0.00168100
H	-1.32583800	3.83495000	0.02731800
C	-0.81040500	2.87915400	0.01904500
N	-2.89810300	1.61120000	0.03127700
C	4.82380200	-1.41571100	-0.03270500
N	5.81436100	-2.02642500	-0.06162800

Me-B4b

C	1.55941000	1.37473200	-0.00796100
C	0.69323600	0.17970200	0.03489400
C	-0.68847100	0.37114700	0.00684800
C	-1.26708500	1.71524800	0.01860100
C	-1.85570200	-0.49680500	-0.00886900
C	-2.97028000	0.40580100	0.01684700
C	-2.10137900	-1.87707700	-0.07220300
C	-3.41671900	-2.33874600	-0.07966800
C	-4.50045400	-1.44425100	-0.03310200
C	-4.28700800	-0.07075100	0.01008400
H	-1.29767600	-2.60425100	-0.13731200
H	-3.60545700	-3.40784600	-0.12865600
H	-5.51531700	-1.83352500	-0.04048900
H	-5.11187200	0.63510800	0.03241000
H	0.44200600	-1.89913800	0.29677500
C	1.21347500	-1.15211600	0.15407700
H	2.53589300	-2.75038400	0.25229800
C	2.48405400	-1.66839300	0.13963200
C	3.74722400	-1.02419500	-0.00556200
H	4.94263100	0.69322900	-0.18411100
C	3.91639000	0.34266200	-0.09508000
H	3.38669200	2.36790700	-0.11415600
C	2.95038900	1.37139600	-0.06772300
H	1.59832200	3.53966200	-0.02118000
C	0.94100800	2.67479000	-0.00350300
H	-0.85651600	3.84253100	0.02867400
C	-0.41267500	2.85130500	0.01902900
N	-2.59155000	1.73988300	0.03491300

C	4.96145700	-1.92360400	-0.04015800
H	5.02707000	-2.52953700	0.87260100
H	4.90513900	-2.62526900	-0.88230100
H	5.88872800	-1.35274200	-0.13603400

OMe-B4b

C	1.12138500	1.50836300	0.00097200
C	0.32320900	0.27220100	0.03940400
C	-1.06728600	0.38465200	0.00755700
C	-1.72055300	1.69655500	0.01214200
C	-2.18425700	-0.54676300	-0.00940800
C	-3.34707100	0.29316100	0.00837700
C	-2.35318300	-1.93927100	-0.06629700
C	-3.64017600	-2.47388600	-0.07615200
C	-4.77170600	-1.64006200	-0.03829600
C	-4.63497500	-0.25671200	-0.00089200
H	-1.51064900	-2.62194600	-0.12396800
H	-3.76899300	-3.55205800	-0.12017400
H	-5.76359300	-2.08482000	-0.04751500
H	-5.49802800	0.40213700	0.01532600
H	0.18497900	-1.82310100	0.28170500
C	0.91418200	-1.03288800	0.15342300
H	2.35278600	-2.55207500	0.25324600
C	2.20466300	-1.48043000	0.14973700
C	3.42440300	-0.75002100	0.02335200
H	4.54463000	1.03782100	-0.13258700
C	3.54456400	0.62574300	-0.06041000
H	2.88843200	2.60413500	-0.08852000
C	2.51265400	1.58328400	-0.04496800
H	1.04200600	3.67239900	-0.02072700
C	0.43280700	2.77266200	-0.00386400
H	-1.42463000	3.84286500	0.01448400
C	-0.92848500	2.87678200	0.01113800
N	-3.04407000	1.64659100	0.02253900
O	4.49400000	-1.58378700	0.01411000
C	5.81073700	-1.05362100	-0.09508300
H	6.47515800	-1.91845200	-0.08492900
H	5.94103800	-0.50197300	-1.03380100
H	6.04788100	-0.39926900	0.75240700

OH-B4b

C	1.59747500	1.33296700	-0.01010500
C	0.71278100	0.15549300	0.02781100
C	-0.66728300	0.36810700	0.00461300

C	-1.22408600	1.72412700	0.01829800
C	-1.84823300	-0.47943800	-0.00957900
C	-2.94742400	0.44263100	0.01865000
C	-2.11848600	-1.85621300	-0.07083700
C	-3.44050800	-2.29576100	-0.07479500
C	-4.50871100	-1.38202400	-0.02665600
C	-4.27210800	-0.01279100	0.01521000
H	-1.32859700	-2.59853700	-0.13644800
H	-3.64756400	-3.36149000	-0.12229800
H	-5.53015500	-1.75391800	-0.03146600
H	-5.08495100	0.70682200	0.03933700
H	0.41764700	-1.92315200	0.25776600
C	1.20451200	-1.19003700	0.13204900
H	2.52678600	-2.81660000	0.21786000
C	2.45839000	-1.73646100	0.12121500
C	3.71849900	-1.08881500	-0.00363900
H	4.97984500	0.59353700	-0.15510700
C	3.94039100	0.27422600	-0.08226300
H	3.44267100	2.29907600	-0.10393400
C	2.99165200	1.30937000	-0.06178100
H	1.67309100	3.49599400	-0.02381100
C	1.00174500	2.64167700	-0.00669400
H	-0.77441000	3.84249200	0.02646600
C	-0.34946700	2.84308900	0.01674900
N	-2.54800100	1.76989300	0.03628400
O	4.75889900	-1.96238000	-0.02182800
H	5.59560400	-1.47531700	-0.09720500

NH_2-B4b

C	-1.57970900	1.35145000	-0.00765700
C	-0.70736600	0.17347800	0.02934500
C	0.67762400	0.37223800	0.00554500
C	1.24475100	1.72330900	0.01669200
C	1.84936900	-0.48447300	-0.00917100
C	2.95741700	0.42942000	0.01626000
C	2.10811600	-1.86454200	-0.06837200
C	3.42495500	-2.31674000	-0.07304800
C	4.50191400	-1.41160700	-0.02772500
C	4.27829500	-0.04096800	0.01205900
H	1.31079000	-2.59957100	-0.13174300
H	3.62265200	-3.38445600	-0.11897500
H	5.52003800	-1.79296500	-0.03304500
H	5.09833200	0.67068200	0.03418700
H	-0.43030700	-1.90581300	0.26022400

C	-1.21165300	-1.16635700	0.13436000
H	-2.50996500	-2.78913900	0.23812700
C	-2.46770700	-1.70649700	0.12686100
C	-3.74055400	-1.06802200	-0.00163200
H	-4.96875600	0.64313400	-0.15130600
C	-3.93416400	0.31168600	-0.07981100
H	-3.42233800	2.32481200	-0.10065100
C	-2.97960800	1.33094700	-0.05627600
H	-1.64174100	3.51334800	-0.02545600
C	-0.97681300	2.65375000	-0.00784100
H	0.80844300	3.84349800	0.02153300
C	0.37776900	2.84645500	0.01388000
N	2.57161600	1.75807600	0.03247100
N	-4.83889500	-1.89148500	0.00907800
H	-5.73684000	-1.51338600	-0.25598100
H	-4.71516300	-2.87744000	-0.16856100

NMe_2-B4b

C	-0.68661000	1.75523200	-0.00779100
C	-0.01304900	0.45892800	-0.05382700
C	1.38521400	0.43382900	-0.01065900
C	2.15933600	1.67649600	-0.00249400
C	2.40296700	-0.59875300	0.00775300
C	3.64378300	0.12573500	0.00013200
C	2.43294500	-2.00253700	0.06358600
C	3.65905200	-2.66204700	0.07665700
C	4.86867800	-1.94233700	0.04508300
C	4.87089600	-0.55332900	0.01274400
H	1.52436100	-2.59534000	0.12121400
H	3.68157100	-3.74785600	0.12014100
H	5.81162100	-2.48355600	0.05717900
H	5.79609900	0.01541700	0.00376400
H	-0.07492900	-1.61935000	-0.39105300
C	-0.72883500	-0.77405000	-0.21001400
H	-2.22902500	-2.17384300	-0.37453700
C	-2.05352000	-1.11871000	-0.20439900
C	-3.22909300	-0.31168000	-0.02713100
H	-4.12623000	1.60847000	0.14792000
C	-3.18028700	1.09032700	0.05528500
H	-2.35938400	2.99296500	0.08522200
C	-2.07442100	1.94290100	0.03374800
H	-0.41002900	3.90026600	0.03065100
C	0.11166600	2.94684800	0.00989400
H	2.06339600	3.83936400	0.00733700

C	1.48061600	2.92277000	0.00212500
N	3.47609000	1.49868900	-0.00704300
N	-4.44609300	-0.95171400	0.02843400
C	-4.54413400	-2.40881700	0.05477900
H	-5.57435700	-2.68765600	0.27808300
H	-4.27197600	-2.86283200	-0.90767800
H	-3.90590400	-2.83805400	0.83485900
C	-5.68466000	-0.18331000	0.08126400
H	-6.53150900	-0.86817500	0.03446100
H	-5.76556500	0.39858200	1.00922600
H	-5.76138300	0.50780300	-0.76695100

Dimer 1

C	6.16540000	2.74710000	17.52060000
H	6.51200000	2.24290000	16.80720000
C	6.05620000	4.14440000	17.34930000
H	6.38280000	4.53510000	16.55830000
C	5.46790000	4.97250000	18.33430000
H	5.31040000	5.88050000	18.15090000
C	5.11520000	4.43320000	19.59870000
H	4.75700000	4.95210000	20.29580000
C	5.35870000	3.00490000	19.71960000
C	5.08220000	2.50690000	21.01720000
H	4.65050000	2.99160000	21.69880000
C	5.54560000	1.15700000	21.14250000
H	5.58610000	0.85510000	22.03100000
C	5.96120000	0.17740000	20.18680000
C	6.39240000	-1.11160000	20.53560000
H	6.35440000	-1.39490000	21.43190000
C	6.87860000	-1.97480000	19.54660000
H	7.26910000	-2.79790000	19.77700000
C	6.77340000	-1.59630000	18.24860000
C	7.08840000	-2.42130000	17.12690000
H	7.52400000	-3.25420000	17.09950000
C	6.53220000	-1.59220000	15.99870000
C	6.58250000	-2.17380000	14.81560000
H	7.01500000	-3.00130000	14.70690000
C	5.97770000	-1.52830000	13.71510000
H	6.17190000	-1.98120000	12.91450000
C	5.16070000	-0.39390000	13.46670000
H	4.89680000	-0.22690000	12.57930000
C	4.72640000	0.48570000	14.44970000
H	4.12290000	1.14810000	14.16710000
C	5.06410000	0.51350000	15.78410000

H	4.67540000	1.19060000	16.30810000
C	5.93680000	-0.37640000	16.44030000
C	6.22120000	-0.34340000	17.87080000
C	5.94940000	0.62390000	18.83360000
C	5.78600000	2.05520000	18.69900000
C	14.02040000	2.74710000	17.41670000
H	14.36700000	2.24290000	16.70320000
C	13.91120000	4.14440000	17.24540000
H	14.23780000	4.53510000	16.45440000
C	13.32290000	4.97250000	18.23030000
H	13.16540000	5.88050000	18.04700000
C	12.97020000	4.43320000	19.49480000
H	12.61200000	4.95210000	20.19180000
C	13.21370000	3.00490000	19.61570000
C	12.93720000	2.50690000	20.91330000
H	12.50550000	2.99160000	21.59490000
C	13.40070000	1.15700000	21.03850000
H	13.44110000	0.85510000	21.92710000
C	13.81620000	0.17740000	20.08280000
C	14.24740000	-1.11160000	20.43170000
H	14.20940000	-1.39490000	21.32800000
C	14.73360000	-1.97480000	19.44260000
H	15.12410000	-2.79790000	19.67310000
C	14.62840000	-1.59630000	18.14470000
C	14.94340000	-2.42130000	17.02300000
H	15.37900000	-3.25420000	16.99560000
C	14.38720000	-1.59220000	15.89470000
C	14.43750000	-2.17380000	14.71170000
H	14.87000000	-3.00130000	14.60300000
C	13.83270000	-1.52830000	13.61120000
H	14.02700000	-1.98120000	12.81060000
C	13.01580000	-0.39390000	13.36280000
H	12.75180000	-0.22690000	12.47530000
C	12.58140000	0.48570000	14.34580000
H	11.97800000	1.14810000	14.06320000
C	12.91910000	0.51350000	15.68020000
H	12.53050000	1.19060000	16.20420000
C	13.79180000	-0.37640000	16.33630000
C	14.07620000	-0.34340000	17.76690000
C	13.80440000	0.62390000	18.72970000
C	13.64100000	2.05520000	18.59510000

Dimer 2

C	12.71810000	5.46850000	11.03080000

H	12.31690000	6.04560000	10.40740000
C	12.39290000	5.60150000	12.32910000
H	11.77500000	6.27030000	12.56260000
C	12.90340000	4.82710000	13.32650000
H	12.68110000	5.01630000	14.22050000
C	13.73450000	3.77940000	13.04740000
H	14.08220000	3.23070000	13.72600000
C	14.06050000	3.55250000	11.62670000
C	14.79330000	2.44500000	11.35070000
H	15.15110000	1.88610000	12.01540000
C	14.96930000	2.21090000	9.95730000
H	15.36950000	1.39240000	9.72540000
C	14.61740000	3.05750000	8.88030000
C	14.76590000	2.64810000	7.56100000
H	15.16090000	1.81210000	7.39000000
C	14.36210000	3.40810000	6.50280000
H	14.38130000	3.07870000	5.62190000
C	13.90970000	4.73020000	6.79850000
C	13.59070000	5.74900000	5.93710000
H	13.52170000	5.67370000	5.00360000
C	13.38180000	6.94620000	6.69210000
C	13.05900000	8.08780000	6.18710000
H	12.81310000	8.06310000	5.28040000
C	13.01730000	9.32830000	6.76000000
H	12.75060000	10.02720000	6.19090000
C	13.31030000	9.69540000	8.05180000
H	13.20790000	10.60900000	8.24830000
C	13.72660000	8.92000000	9.08110000
H	13.94260000	9.37360000	9.87610000
C	13.87670000	7.52470000	9.11510000
H	14.17180000	7.13970000	9.91990000
C	13.62690000	6.67610000	8.06200000
C	13.81150000	5.18080000	8.12260000
C	14.01570000	4.29600000	9.20860000
C	13.62840000	4.50640000	10.56530000
C	10.09290000	7.56500000	8.47050000
H	10.43950000	8.06920000	7.75700000
C	9.98370000	6.16770000	8.29920000
H	10.31030000	5.77700000	7.50820000
C	9.39540000	5.33960000	9.28420000
H	9.23790000	4.43160000	9.10080000
C	9.04270000	5.87890000	10.54860000
H	8.68450000	5.36000000	11.24570000
C	9.28620000	7.30720000	10.66950000

C	9.00970000	7.80520000	11.96710000
H	8.57800000	7.32050000	12.64870000
C	9.47310000	9.15510000	12.09240000
H	9.51360000	9.45700000	12.98090000
C	9.88870000	10.13470000	11.13670000
C	10.31990000	11.42370000	11.48550000
H	10.28190000	11.70700000	12.38180000
C	10.80610000	12.28690000	10.49640000
H	11.19660000	13.11000000	10.72690000
C	10.70090000	11.90840000	9.19850000
C	11.01590000	12.73340000	8.07680000
H	11.45150000	13.56630000	8.04940000
C	10.45970000	11.90430000	6.94860000
C	10.51000000	12.48590000	5.76550000
H	10.94250000	13.31340000	5.65680000
C	9.90520000	11.84040000	4.66500000
H	10.09940000	12.29330000	3.86440000
C	9.08820000	10.70600000	4.41660000
H	8.82430000	10.53900000	3.52920000
C	8.65390000	9.82640000	5.39960000
H	8.05040000	9.16400000	5.11700000
C	8.99160000	9.79860000	6.73400000
H	8.60300000	9.12150000	7.25800000
C	9.86430000	10.68850000	7.39010000
C	10.14870000	10.65550000	8.82070000
C	9.87690000	9.68820000	9.78350000
C	9.71350000	8.25690000	9.64890000

Dimer 3

C	12.71810000	5.46850000	11.03080000
H	12.31690000	6.04560000	10.40740000
C	12.39290000	5.60150000	12.32910000
H	11.77500000	6.27030000	12.56260000
C	12.90340000	4.82710000	13.32650000
H	12.68110000	5.01630000	14.22050000
C	13.73450000	3.77940000	13.04740000
H	14.08220000	3.23070000	13.72600000
C	14.06050000	3.55250000	11.62670000
C	14.79330000	2.44500000	11.35070000
H	15.15110000	1.88610000	12.01540000
C	14.96930000	2.21090000	9.95730000
H	15.36950000	1.39240000	9.72540000
C	14.61740000	3.05750000	8.88030000
C	14.76590000	2.64810000	7.56100000

H	15.16090000	1.81210000	7.39000000
C	14.36210000	3.40810000	6.50280000
H	14.38130000	3.07870000	5.62190000
C	13.90970000	4.73020000	6.79850000
C	13.59070000	5.74900000	5.93710000
H	13.52170000	5.67370000	5.00360000
C	13.38180000	6.94620000	6.69210000
C	13.05900000	8.08780000	6.18710000
H	12.81310000	8.06310000	5.28040000
C	13.01730000	9.32830000	6.76000000
H	12.75060000	10.02720000	6.19090000
C	13.31030000	9.69540000	8.05180000
H	13.20790000	10.60900000	8.24830000
C	13.72660000	8.92000000	9.08110000
H	13.94260000	9.37360000	9.87610000
C	13.87670000	7.52470000	9.11510000
H	14.17180000	7.13970000	9.91990000
C	13.62690000	6.67610000	8.06200000
C	13.81150000	5.18080000	8.12260000
C	14.01570000	4.29600000	9.20860000
C	13.62840000	4.50640000	10.56530000
C	14.02040000	2.74710000	17.41670000
H	14.36700000	2.24290000	16.70320000
C	13.91120000	4.14440000	17.24540000
H	14.23780000	4.53510000	16.45440000
C	13.32290000	4.97250000	18.23030000
H	13.16540000	5.88050000	18.04700000
C	12.97020000	4.43320000	19.49480000
H	12.61200000	4.95210000	20.19180000
C	13.21370000	3.00490000	19.61570000
C	12.93720000	2.50690000	20.91330000
H	12.50550000	2.99160000	21.59490000
C	13.40070000	1.15700000	21.03850000
H	13.44110000	0.85510000	21.92710000
C	13.81620000	0.17740000	20.08280000
C	14.24740000	-1.11160000	20.43170000
H	14.20940000	-1.39490000	21.32800000
C	14.73360000	-1.97480000	19.44260000
H	15.12410000	-2.79790000	19.67310000
C	14.62840000	-1.59630000	18.14470000
C	14.94340000	-2.42130000	17.02300000
H	15.37900000	-3.25420000	16.99560000
C	14.38720000	-1.59220000	15.89470000
C	14.43750000	-2.17380000	14.71170000

H	14.87000000	-3.00130000	14.60300000
C	13.83270000	-1.52830000	13.61120000
H	14.02700000	-1.98120000	12.81060000
C	13.01580000	-0.39390000	13.36280000
H	12.75180000	-0.22690000	12.47530000
C	12.58140000	0.48570000	14.34580000
H	11.97800000	1.14810000	14.06320000
C	12.91910000	0.51350000	15.68020000
H	12.53050000	1.19060000	16.20420000
C	13.79180000	-0.37640000	16.33630000
C	14.07620000	-0.34340000	17.76690000
C	13.80440000	0.62390000	18.72970000
C	13.64100000	2.05520000	18.59510000

Monomer 1

C	2.23790000	7.56500000	8.57440000
H	2.58450000	8.06920000	7.86100000
C	2.12870000	6.16770000	8.40310000
H	2.45530000	5.77700000	7.61210000
C	1.54040000	5.33960000	9.38810000
H	1.38290000	4.43160000	9.20480000
C	1.18770000	5.87890000	10.65250000
H	0.82950000	5.36000000	11.34960000
C	1.43120000	7.30720000	10.77340000
C	1.15470000	7.80520000	12.07100000
H	0.72300000	7.32050000	12.75270000
C	1.61810000	9.15510000	12.19630000
H	1.65860000	9.45700000	13.08480000
C	2.03370000	10.13470000	11.24060000
C	2.46490000	11.42370000	11.58940000
H	2.42690000	11.70700000	12.48570000
C	2.95110000	12.28690000	10.60040000
H	3.34160000	13.11000000	10.83080000
C	2.84590000	11.90840000	9.30240000
C	3.16090000	12.73340000	8.18070000
H	3.59650000	13.56630000	8.15330000
C	2.60470000	11.90430000	7.05250000
C	2.65500000	12.48590000	5.86950000
H	3.08750000	13.31340000	5.76070000
C	2.05020000	11.84040000	4.76890000
H	2.24440000	12.29330000	3.96830000
C	1.23320000	10.70600000	4.52060000
H	0.96930000	10.53900000	3.63310000
C	0.79890000	9.82640000	5.50350000

H	0.19540000	9.16400000	5.22090000
C	1.13660000	9.79860000	6.83800000
H	0.74790000	9.12150000	7.36190000
C	2.00930000	10.68850000	7.49410000
C	2.29370000	10.65550000	8.92460000
C	2.02190000	9.68820000	9.88740000
C	1.85850000	8.25690000	9.75280000

Monomer 2

C	12.71810000	5.46850000	11.03080000
H	12.31690000	6.04560000	10.40740000
C	12.39290000	5.60150000	12.32910000
H	11.77500000	6.27030000	12.56260000
C	12.90340000	4.82710000	13.32650000
H	12.68110000	5.01630000	14.22050000
C	13.73450000	3.77940000	13.04740000
H	14.08220000	3.23070000	13.72600000
C	14.06050000	3.55250000	11.62670000
C	14.79330000	2.44500000	11.35070000
H	15.15110000	1.88610000	12.01540000
C	14.96930000	2.21090000	9.95730000
H	15.36950000	1.39240000	9.72540000
C	14.61740000	3.05750000	8.88030000
C	14.76590000	2.64810000	7.56100000
H	15.16090000	1.81210000	7.39000000
C	14.36210000	3.40810000	6.50280000
H	14.38130000	3.07870000	5.62190000
C	13.90970000	4.73020000	6.79850000
C	13.59070000	5.74900000	5.93710000
H	13.52170000	5.67370000	5.00360000
C	13.38180000	6.94620000	6.69210000
C	13.05900000	8.08780000	6.18710000
H	12.81310000	8.06310000	5.28040000
C	13.01730000	9.32830000	6.76000000
H	12.75060000	10.02720000	6.19090000
C	13.31030000	9.69540000	8.05180000
H	13.20790000	10.60900000	8.24830000
C	13.72660000	8.92000000	9.08110000
H	13.94260000	9.37360000	9.87610000
C	13.87670000	7.52470000	9.11510000
H	14.17180000	7.13970000	9.91990000
C	13.62690000	6.67610000	8.06200000
C	13.81150000	5.18080000	8.12260000
C	14.01570000	4.29600000	9.20860000

C	13.62840000	4.50640000	10.56530000

References

1 G. Scalmani and M. J. Frisch, *J. Chem. Phys.*, 2010, **132**, 114110.

2 T. Lu optDFTw program v1.0, webpage: http://sobereva.com/346.

3 S. Ito, T. Minami and M. Nakano, *J. Phys. Chem. C*, 2012, **116**, 19729-19736.

4 M. J. G. Peach and D. J. Tozer, *J. Phys. Chem. A*, 2012, **116**, 9783-9789.

5 Y.-L. Wang and G.-S. Wu, *Int. J. Quantum Chem.*, 2008, **108**, 430-439.

6 B. S. Basel, C. Hetzer, J. Zirzlmeier, D. Thiel, R. Guldi, F. Hampel, A. Kahnt, T. Clark, D. M. Guldi and R. R. Tykwinski, *Chem. Sci.*, 2019, **10**, 3854-3863.

7 P. D. Cunningham, S. A. Díaz, B. Yurke, I. L. Medintz and J. S. Melinger, *J. Phys. Chem. B*, 2020, **124**, 8042-8049.

8 D. Biermann and W. Schmidt, *J. Am. Chem. Soc.*, 1980, **102**, 3163-3173.

9 Y. Tomkiewicz, R. P. Groff and P. Avakian, *J. Chem. Phys.*, 1971, **54**, 4504-4507.

10 M. Yasunami, P. W. Yang, Y. Kondo, Y. Noro and K. Takase, *Chem. Lett.*, 1980, **9**, 167-170.

11 C. Hansch, A. J. Leo and R. W. Taft, *Chem. Rev.*, 1991, **91**, 165-195.

12 C. F.-W. LU Tian, *Acta Chim. Sinica*, 2011, **69**, 2393-2406.

13 J. T. Blaskovits, M. Fumanal, S. Vela, Y. Cho and C. Corminboeuf, *Chem. Commun.*, 2022, **58**, 1338-1341.

14 K. H. Kim, Y.-K. Han and J. Jung, *Theor. Chem. Acc.*, 2005, **113**, 233-237.