SUPPORTING INFORMATION

Heavy Atom Free Singlet Oxygen Generation – Doubly Substituted Configurations Dominate S_1 States of bis-BODIPYs

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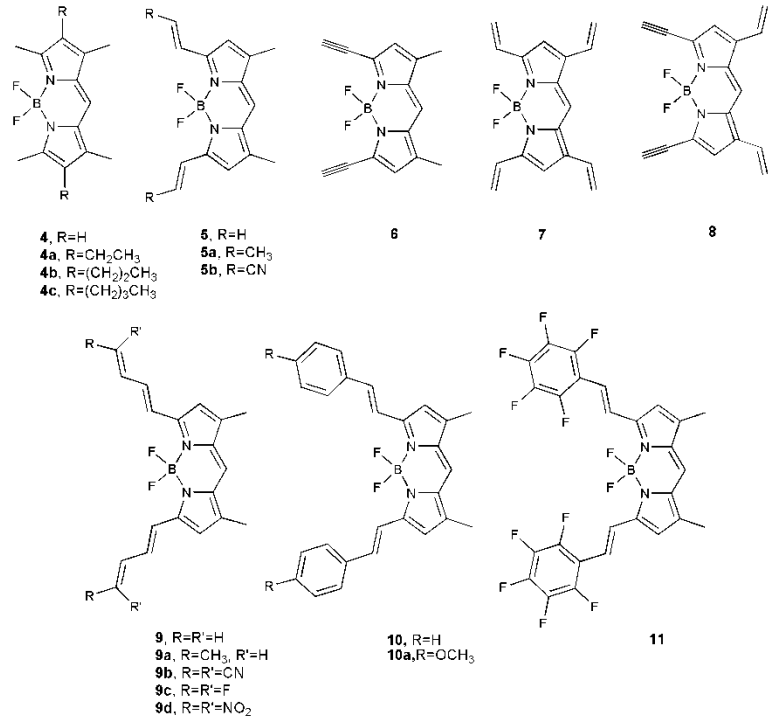


Scheme S2. Monomers of Orthogonal 8-8' 2,6-diiodo bis-BODIPYs Considered in this Work

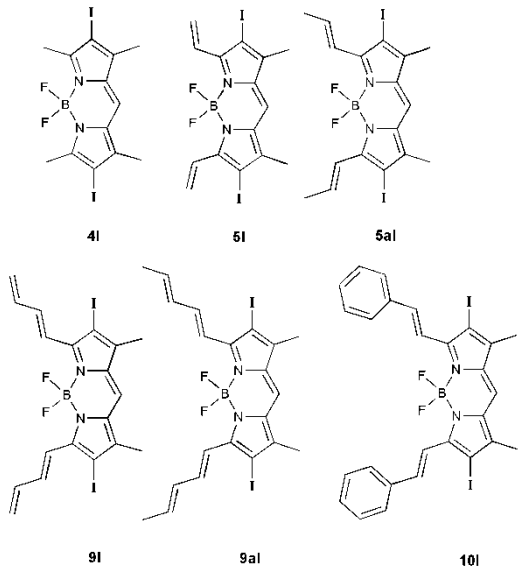


TABLE S1. Calculated HOMO-LUMO Energy Gaps (nm) for **1** and **4** at Various Levels

Theoretical level	E (HOMO -LUMO) (nm)	
	1	**4**
(U)B3LYP/STO-3G	367	379
(U)B3LYP/6-31G	397	417
(U)B3LYP/6-31G(d)	397	418
(U)B3LYP/6-31G(d,p)	398	419
(U)B3LYP/6-311G(d)	398	420
(U)B3LYP/6-311G(d,p)	399	420
(U)BHandHLYP/cc-pVDZ	255	266
(U)B3LYP/cc-pVTZ[a]	421	441
(U)B3LYP/cc-pVTZ[b]	413	433
(U)B3LYP/cc-PVTZ[c]	403	426
(U)B3LYP/cc-pVTZ[d]	412	433
(U)B3LYP/cc-pVTZ[e]	407	408
(U)B3LYP/cc-pVTZ[f]	415	436
(U)B3LYP/cc-pVTZ[g]	417	438
(R)PBE1PBE/cc-pVTZ[h]	363	382
(R)PBE1PBE/cc-pVTZ[c]	368	389
(R)B3PW91/cc-pVTZ[h]	395	417
(R)B3PW91/cc-pVTZ[c]	401	424
(U)B3LYP/CEP-31G	409	426
(UB3LYP)/CEP-31G[f]	404	421
(U)B3LYP/CEP-31G[g]	406	423
(U)B3LYP/CEP-31G(d,p)	411	428
(U)B3LYP/LANL2DZ	404	422
Experimental	499-505	505

[a]Geometry optimized with CEP-31G basis set.
[b]Geometry optimized with CEP-31G(d,p) basis set.
[c]Geometry optimized at (U)B3LYP/cc-pVDZ level of theory.
[d]Geometry optimized with LANL2DZ basis set.
[e]Geometry optimized with LANL2DZ basis set. Solvent: ethanol.
[f]Geometry optimized with CEP-31G basis set. Solvent: ethanol.
[g]Geometry optimized with CEP-31G basis set. Solvent: chloroform.
[h]Geometry optimized at (U)BHandHLYP/cc-pVDZ level of theory

TABLE S2. Calculated Oscillator Strengths for **1** and **4** at Various TD-DFT Levels with Solvent Effect Contributions

	1				**4**			
Theoretical level	**ethanol**		**chloroform**		**ethanol**		**chloroform**	
	λ (nm)	*f*	λ (nm)	*f*	λ (nm)	*f*	λ (nm)	*f*
(U)B3LYP/6-31G(d)	423	0.45	427	0.48	427	0.47	445	0.59
(U)B3LYP/6-31G(d,p)	424	0.45	428	0.48	428	0.47	446	0.59
(U)B3LYP/cc-pVTZ	434	0.48	439	0.51	453	0.58	457	0.60
(U)B3LYP/CEP-31G	418	0.49	422	0.52	431	0.61	435	0.64
(U)BHandHLYP/6-31G(d)	417	0.60	422	0.62	421	0.58	441	0.69
(R)PBE1PBE/6-31G(d)	420	0.49	424	0.52	424	0.50	442	0.61
(R)B3PW91/6-31G(d)	422	0.46	426	0.48	426	0.47	443	0.59
Experimental	499-505				505			

Geometry optimized at (U)B3LYP/CEP-31G level of theory.

TABLE S3. Selected Parameters for Modified BODIPY Cores and Associated Orthogonal bis-BODPIYs

	MONOMER								DIMER								
	E_H (eV)	E_L (eV)	ΔE_{H-L} (nm)	ΔE_{H-L} (eV)	$q(N_1)$	$q(N_2)$	q(C)	q(B)	E_{H-1} (eV)	E_H (eV)	E_L (eV)	E_{L+1} (eV)	$\Delta E_{L-(H-1)}$ (eV)	$\Delta E_{(L+1)-H}$ (eV)	NOONs	S_1	S_1-T_1 (eV)
4'	-5.69	-2.78	426	2.91	-0.54	-0.54	-0.24	1.31	-6.04	-5.69	-3.11	-2.76	2.93	2.93	211110	DS-TR	4.16-2.35
4	-5.69	-2.78	426	2.91	-0.54	0.54	-0.24	1.31	-6.01	-5.92	-3.04	-3.04	2.97	2.88	211110	DS-TR	3.69-1.79
4a	-5.47	-2.60	432	2.87	-0.56	-0.56	-0.25	1.30	-5.71	-5.62	-2.84	-2.81	2.87	2.81	211110	DS-TR	3.90-2.28
4b	-5.46	-2.60	433	2.86	-0.57	-0.57	-0.27	1.34	-5.70	-5.60	-2.82	-2.80	2.88	2.80	211110	DS-TR	3.45-1.69
4c	-5.45	-2.59	433	2.86	-0.56	-0.56	-0.21	1.31	-5.67	-5.58	-2.81	-2.77	2.86	2.81	211110	DS-TR	3.44-1.69
4l	-5.99	-3.15	437	2.84	n/a	n/a	n/a	n/a	-6.31	-6.23	-3.51	-3.49	2.80	2.73	211110	DS-TR	3.20-1.58
5'	-5.51	-3.03	499	2.48	-0.58	-0.58	-0.30	1.34	-5.84	-5.52	-3.33	-3.02	2.51	2.50	211110	DS-TR	3.81-2.14
5	-5.51	-3.03	499	2.48	-0.58	-0.58	-0.30	1.34	-5.82	-5.75	-3.39	-3.23	2.44	2.52	211110	DS-TR	3.77-1.62
5a'	-5.22	-2.78	509	2.43	-0.39	-0.39	-0.22	1.12	-5.46	-5.21	-3.01	-2.75	2.45	2.46	211110	DS-TR	3.33-1.69
5a	-5.22	-2.78	509	2.43	-0.39	-0.39	-0.22	1.12	-5.46	-5.39	-3.07	-2.91	2.39	2.48	211110	DS-TR	3.33-1.62
5b'	-6.30	-3.97	532	2.33	-0.54	-0.54	-0.27	1.30	-6.81	-6.50	-4.44	-4.16	2.36	2.34	211110	DS-TR	3.51-1.83
5b	-6.30	-3.97	532	2.33	-0.54	-0.54	-0.27	1.30	-6.85	-6.79	-4.49	-4.34	2.36	2.45	211110	DS-TR	3.68-1.57
5l	-5.81	-3.38	510	2.43	n/a	n/a	n/a	n/a	-6.10	-6.03	-3.72	-3.53	2.37	2.50	211110	DS-TR	2.86-1.40
5al	-5.53	-3.12	514	2.41	n/a	n/a	n/a	n/a	-5.22	-5.70	-3.41	-3.34	2.36	2.36	211110	DS-TR	2.86-1.41
6'	-5.86	-3.31	487	2.55	-0.64	-0.64	-0.25	1.61	-6.44	-5.84	-3.76	-3.29	2.68	2.55	211110	DS-TR	3.41-1.71
6	-5.86	-3.31	487	2.55	-0.64	-0.64	-0.25	1.61	-6.39	-6.33	-3.79	-3.62	2.60	2.72	211110	DS-TR	3.43-1.66
7'	-5.65	-3.30	527	2.35	-0.48	-0.48	-0.21	1.26	-5.90	-5.62	-3.56	-3.30	2.34	2.33	211110	DS-TR	3.18-1.58
7	-5.65	-3.30	527	2.35	-0.48	-0.48	-0.21	1.26	-6.02	-5.87	-3.53	-3.46	2.49	2.41	211110	DS-TR	2.71-1.34
8'	-5.95	-3.55	517	2.40	-0.53	-0.53	-0.15	1.54	-6.25	-5.88	-3.86	-3.51	2.38	2.37	211110	DS-TR	3.30-1.63
8	-5.95	-3.55	517	2.40	-0.53	-0.53	-0.15	1.54	-6.42	-6.31	-3.89	-3.82	2.53	2.49	211110	DS-TR	2.87-1.22
9'	-5.19	-3.03	574	2.16	-0.50	-0.50	-0.27	1.24	-5.39	-5.20	-3.23	-3.02	2.16	2.17	221100	SS	3.18-1.60
9	-5.19	-3.03	574	2.16	-0.50	-0.50	-0.27	1.24	-5.40	-5.35	-3.24	-3.24	2.16	2.10	221100	SS	3.48-1.51
9a'	-4.95	-2.83	584	2.12	-0.45	-0.45	-0.30	1.18	-5.09	-4.93	-2.98	-2.79	2.11	2.14	221100	SS	3.17-1.60
9a	-4.95	-2.83	584	2.12	-0.45	-0.45	-0.30	1.18	-5.10	-5.05	-2.99	-2.98	2.12	2.07	221100	SS	3.17-1.46
9b'	-6.44	-4.49	636	1.95	-0.44	-0.44	-0.22	1.17	-6.90	-6.54	-4.90	-4.57	1.99	1.96	221100	SS	3.06-1.50
9b	-6.44	-4.49	636	1.95	-0.44	-0.44	-0.22	1.17	-6.92	-6.87	-4.83	-4.83	2.09	2.05	221100	SS	3.18-1.47
9c'	-5.59	-3.42	570	2.17	-0.40	-0.40	-0.26	1.09	-5.91	-5.65	-3.72	-3.46	2.19	2.19	221100	SS	3.20-1.59
9c	-5.59	-3.42	570	2.17	-0.40	-0.40	-0.26	1.09	-5.93	-5.86	-3.74	-3.72	2.19	2.14	221100	SS	3.37-1.50
9d'	-6.91	-5.03	659	1.88	-0.43	-0.43	-0.23	1.13	-7.45	-7.05	-5.50	-5.14	1.95	1.91	221100	SS	3.10-1.51
9d	-6.91	-5.03	659	1.88	-0.43	-0.43	-0.23	1.13	-7.60	-7.47	-5.67	-5.40	1.93	2.07	221100	SS	3.19-1.38
9l	-5.42	-3.32	589	2.10	n/a	n/a	n/a	n/a	-5.59	-5.53	-3.55	-3.48	2.04	2.06	221100	SS	3.04-1.52
9al	-5.18	-3.12	599	2.07	n/a	n/a	n/a	n/a	-5.36	-5.30	-3.33	-3.25	2.04	2.05	221100	SS	3.21-1.49
10'	-5.09	-2.97	584	2.12	-0.54	-0.54	-0.31	1.31	-5.25	-5.09	-3.13	-2.95	2.12	2.15	221100	SS	3.17-1.61
10	-5.09	-2.97	584	2.12	-0.54	-0.54	-0.31	1.31	-5.28	-5.23	-3.16	-3.14	2.12	2.09	221100	SS	3.26-1.54
10a'	-4.84	-2.78	604	2.05	-0.48	-0.48	-0.29	1.22	-4.92	-4.82	-2.89	-2.75	2.04	2.08	221100	SS	3.14-1.59
10a	-4.84	-2.78	604	2.05	-0.48	-0.48	-0.29	1.22	-4.91	-4.85	-2.92	-2.88	1.99	1.97	221100	SS	2.76-1.55
10l	-5.33	-3.23	592	2.10	n/a	n/a	n/a	n/a	-5.62	-5.56	-3.50	-3.42	2.12	2.15	221100	SS	2.76-1.54
11'	-5.98	-3.81	570	2.18	-0.36	-0.36	-0.24	1.05	-6.35	-6.09	-4.16	-3.90	2.19	2.19	221100	SS	2.52-1.54
11	-5.98	-3.81	570	2.18	-0.36	-0.36	-0.24	1.05	-6.30	-6.25	-4.12	-4.10	2.17	2.15	221100	SS	2.56-1.53

n/a indicates that ESP charges are not available for iodine.

Scheme S3. Molecular Structure of **2** and **3**

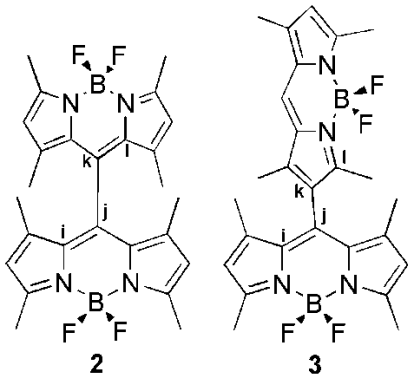


TABLE S4. Calculated Inter Plane Angles for **2** and **3**

States	2	3	2	3	Exp
	CAS(6,6)/CEP-31G		B3LYP/CEP-31G		
S_0	91.2°	89.8°	91.0°	89.9°	90 ± 0.5°
S_1	90.5°	90.0°	n/a	n/a	n/a
T_1	91.3°	90.4°	90.6°	90.0°	n/a

Measurement of inter plane dihedral angle is via the i, j, k, l sequence as shown in Scheme S3 above.

TABLE S5. Spin Orbit Coupling Constants For Species **5**, **9** and **10** and Associated Dimers

	MONOMER		DIMER	
Species	**States**	**SOCC (cm^{-1})**	**States**	**SOCC (cm^{-1})**
4	S_1-T_1	0.06	S_1-T_1	0.78
5	S_1-T_1	0.00	S_1-T_1	0.11
9	S_1-T_1	0.04	S_1-T_1	0.04
10	S_1-T_1	0.07	S_1-T_1	0.03

CAS(2,2) for monomers and CAS(4,4) for the dimers is used.

TABLE S6. Photophysical Properties (λ_{ab} and Oscillator Strength) of Compound **8** at TD-UB3LYP/cc-pVTZ Level of Theory

Species	λ (nm)	*f*
	550	0.89
8	454	0.13
	339	0.13

Geometry optimized at UB3LYP/CEP-31G
λ_{ab} values in chloroform.
Excitations with oscillator strength below 0.1 are neglected.

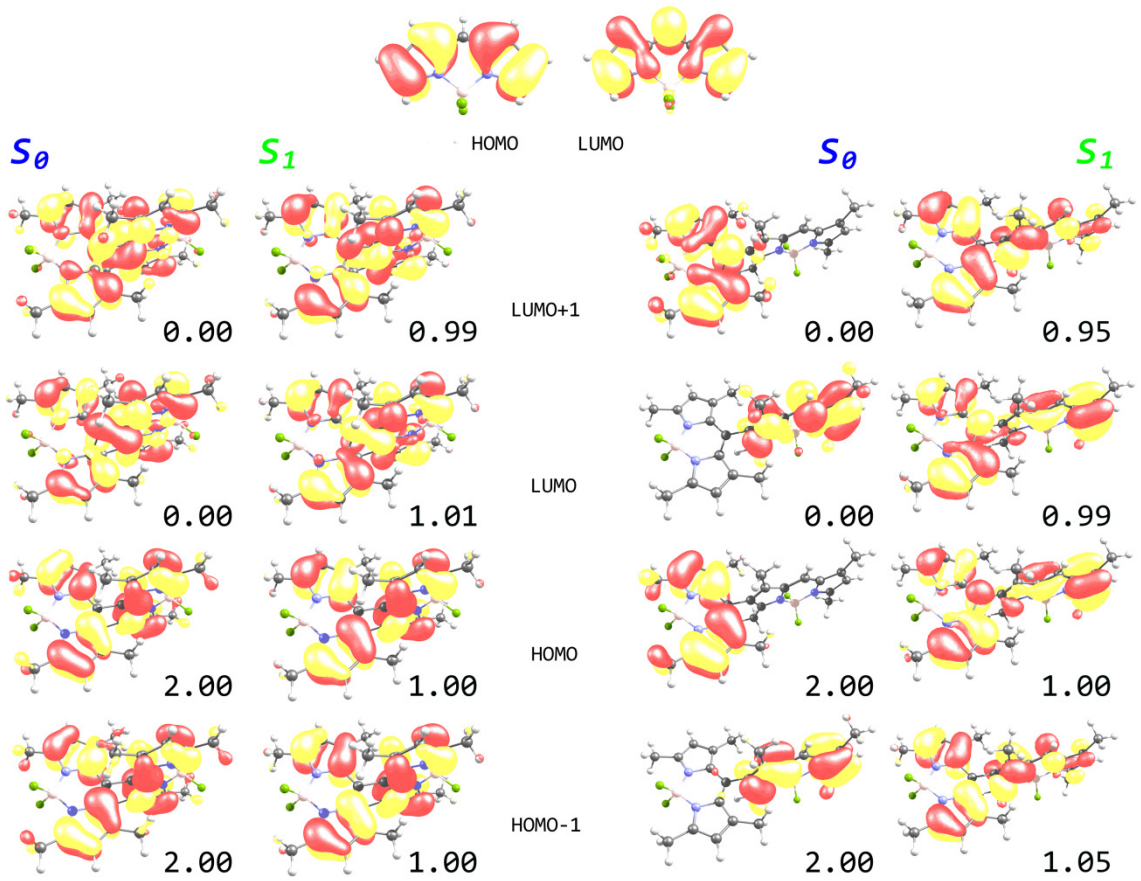
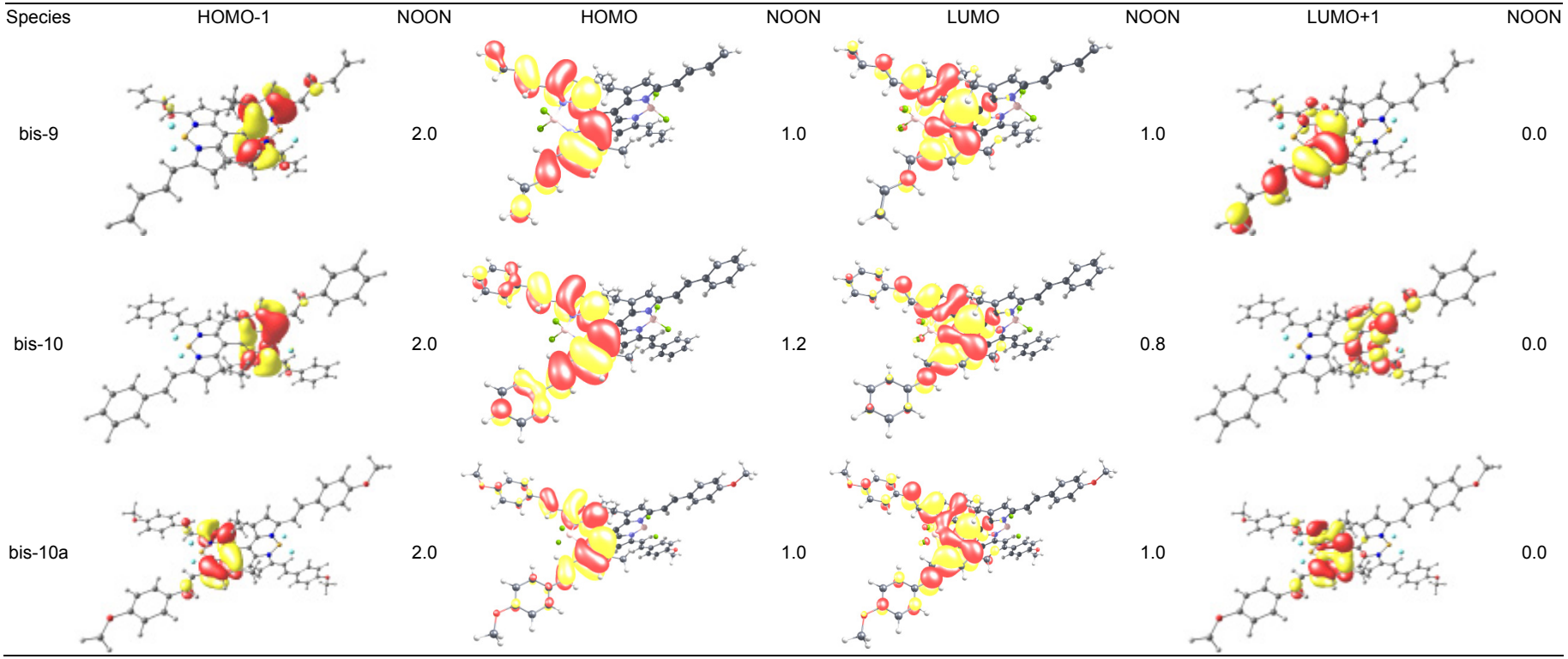


Figure S1. Top: BODIPY HOMO and LUMO. Bottom: Selected natural orbitals and occupation numbers of S_1 states of dimers **2** and **3**. SOMO designations for the S_1 state refer to frontier MOs of S_0. Surfaces are plotted at 0.275 a.u.



Calculations were done at CAS(6,6)/CEP-31G//(U)B3LYP/CEP-31G level.

Figure S2. Selected natural orbitals and occupation numbers for **bis-9**, **bis-10** and **bis-10a**.

TABLE S7. Natural Orbital Occupation Numbers (NOON) for **bis-1** Rotational Conformations

Angle	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2
20˚	1.94	1.91	1.07	0.93	0.08	0.05
25˚	1.94	1.90	1.01	0.99	0.08	0.05
27˚	1.94	1.90	1.01	0.99	0.09	0.05
28˚	1.94	1.90	1.01	0.99	0.09	0.05
29˚	1.99	1.43	1.04	0.97	0.57	0.00
30˚	1.95	1.38	1.02	0.98	0.62	0.04
40˚	1.96	1.29	1.03	0.97	0.71	0.04
50˚	1.96	1.18	1.07	0.93	0.82	0.04
60˚	1.96	1.13	1.10	0.90	0.87	0.04
70˚	1.96	1.13	1.08	0.91	0.88	0.04
80˚	1.96	1.13	1.04	0.96	0.87	0.04
90˚	1.96	1.13	1.00	1.00	0.87	0.04

TABLE S8. Natural Orbital Occupation Numbers (NOON) for **bis-9'** Rotational Conformations

Angle	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2
0˚	2.00	1.94	1.00	1.00	0.04	0.01
15˚	2.00	1.98	1.28	0.75	0.00	0.00
20˚	2.00	2.00	1.41	0.59	0.00	0.00
25˚	2.00	1.96	1.32	0.68	0.04	0.00
30˚	2.00	1.96	1.32	0.68	0.04	0.00
35˚	2.00	1.95	1.33	0.67	0.05	0.00
40˚	1.96	1.89	1.72	0.32	0.08	0.04
45˚	1.92	1.86	1.58	0.41	0.15	0.09
50˚	1.92	1.86	0.09	0.41	1.58	0.15
55˚	1.92	1.82	1.26	0.71	0.21	0.09
60˚	1.90	1.38	1.03	0.97	0.62	0.09
65˚	1.90	1.38	1.03	1.97	0.62	0.09
70˚	2.00	1.03	1.00	1.00	0.97	0.00
75˚	1.94	1.20	1.00	1.00	0.80	0.06
80˚	1.95	1.14	1.04	0.96	0.86	0.05
85˚	1.94	1.15	1.14	0.85	0.85	0.06
90˚	1.96	1.00	1.00	1.00	1.00	0.04

TABLE S9. Natural Orbital Occupation Numbers (NOON) for **bis-10'** Rotational Conformations

Angle	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2
0˚	2.00	1.94	1.00	1.00	0.04	0.01
30˚	1.96	1.95	1.05	0.95	0.05	0.04
40˚	1.95	1.93	1.03	0.97	0.07	0.05
50˚	1.95	1.93	1.08	0.92	0.06	0.04
60˚	1.95	1.93	1.08	0.92	0.06	0.04
63˚	1.92	1.06	1.00	1.00	0.94	0.08
65˚	1.92	1.06	1.00	1.00	0.94	0.08
70˚	1.92	1.06	1.00	1.00	0.94	0.08
80˚	1.92	1.06	1.00	1.00	0.94	0.08
90˚	2.00	1.07	1.00	1.00	0.93	0.00

TABLE S10. Relative Energies (eV) of S_2 and S_3 States for Selected Species at CAS(6,6)/CEP-31G level of theory

		S_2		S_3	
Species	**Binding Motif**	**ΔE_{rel} (eV)**	**NOON**	**ΔE_{rel} (eV)**	**NOON**
bis-4	8,8'	4.97	2.0 1.6 1.4 0.9 0.2 0.0		
bis-4'	8,2'	6.83	2.0 1.5 1.0 0.5 0.0 0.0		
bis-9	8,8'	3.92	2.0 1.0 1.0 1.0 1.0 0.0		
bis-9'	8,2'	3.41	2.0 2.0 1.0 1.0 0.0 0.0	4.84	2.0 1.0 1.0 1.0 1.0 0.0
bis-10	8,8'	2.16	2.0 1.5 1.0 0.5 0.0 0.0	3.47	2.0 1.0 1.0 1.0 1.0 0.0
bis-10'	8,2'	3.73	2.0 1.0 1.0 1.0 1.0 0.0		
bis-10a	8,8'	3.67	2.0 1.0 1.0 1.0 1.0 0.0		
bis-10a'	8,2'	3.24	2.0 1.6 1.0 1.0 0.4 0.0		*unconverged*

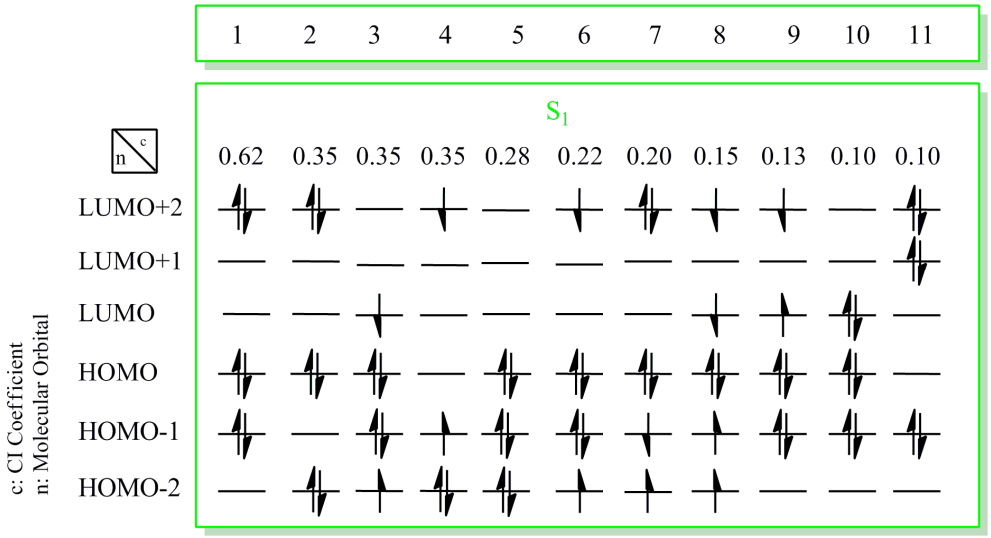


Figure S3. Details of the CAS(6,6) wave function for **bis-4** at S_2 state. Configurations with c-CSF smaller than 0.1 are omitted for clarity.

It is clearly visible from Figure S3 that DS configurations decrease with respect to S_1. In particular SS configurations such as 3, 4, and 6 became significant upon accessing S_2. At S_1 all configurations used to be of the DS type. The effect is also seen on NOONs. A transition from 1,1,1,1 (DS-TR) motif to 2,1,1,0 (SS) motif for π-truncated dimers and the reverse transition from SS to DS-TR for the π-extended dimers is envisioned on inspection of Table S10 and Figure S3. This also correlates with $^1O_2$ production, hence ISC performances of the dimers.

Table S11. Perturbation Corrected CASSCF Relative Energies (eV) for Selected Species at SA-CAS-MP2/ CEP-31G //CAS(6,6)/CEP-31G level of Theory

		S_1	S_2
Species	**Binding Motif**	**ΔE_{rel} (eV)**	
4	n/a	2.83	3.99
bis-4	8,8'	2.60	4.58
bis-4'	8,2'	2.85	4.68
9	n/a	1.32	3.98
bis-9	8,8'	1.97	3.07
bis-9'	8,2'	1.67	2.38

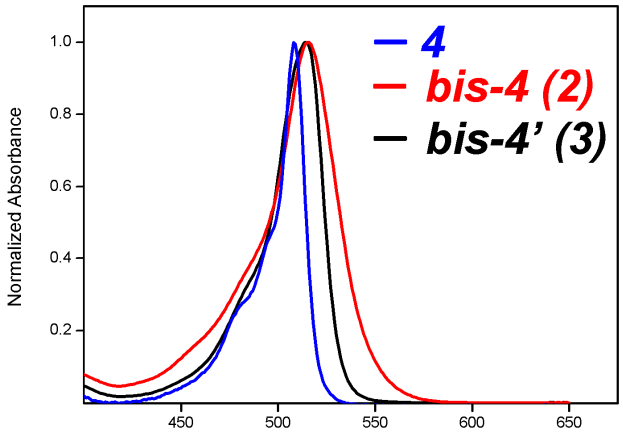


Figure S4. Comparison of the absorption spectra of tetramethyl BODIPY core (**4**) and the two dimers (**bis-4** and **bis-4'**) experimentally tested for $^1O_2$ production.

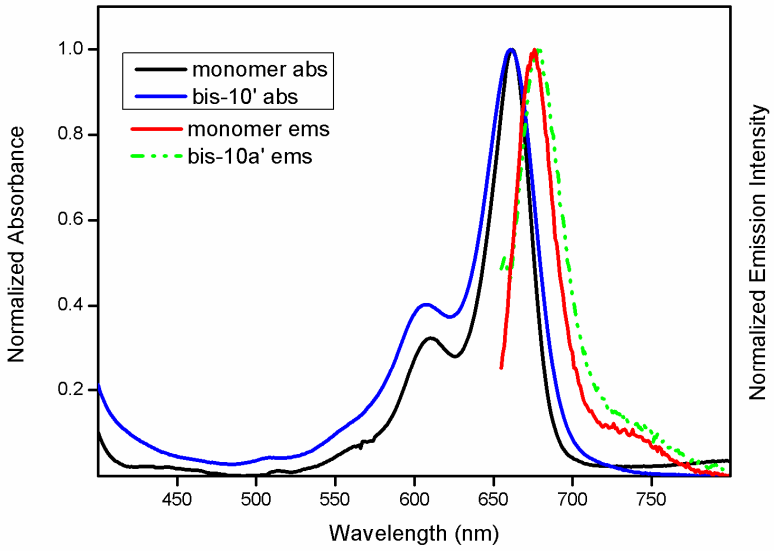


Figure S5. Comparison of the absorption and emission spectra of **10a'** and **bis-10a'**.

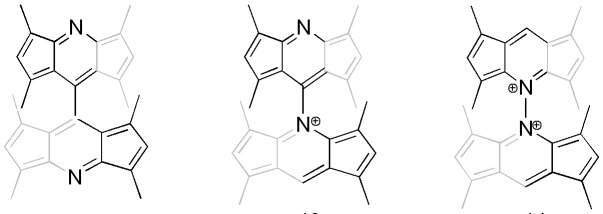
As explained in the accompanying manuscript only the π-truncated orthogonal dimers are expected to undergo ISC and produce $^1O_2$. On the other hand the π-extended dimers are expected to fluoresce. This is confirmed by uv-vis and singlet oxygen phosphorescence measurements on experimentally well characterized **4**, **bis-4**, **bis-4'**, **10a**, and **bis-10a'**. Figures S4 and S5 show the local character of the photophysics taking place and lend support on the VB type wave function that we predict and calculate for **bis-4** and **bis-4'**. The inefficient exchange mechanism for π-extended dimers is apparently explaining the near unity fluorescence quantum yield measured for **bis-10a'**. Absorptions resembling the monomers also suggest that the $^1O_2$ generator dimers should have a drastically different electronic structure than the valance excited **bis-10a'**.

TABLE S12. Selected Parameters for Modified BODIPY Cores **2**, **5**, **9** and **10** and Associated 8,8' Orthogonal bis-BODIPYs at Various Theoretical Levels[a,b]

Species	Basis set	MONOMER				DIMER						S_1
		E_H (eV)	E_L (eV)	ΔE_{H-L} (eV)	ΔE_{H-L} (nm)	E_{H-1} (eV)	E_H (eV)	E_L (eV)	E_{L+1} (eV)	$\Delta E_{L-(H-1)}$ (eV)	$\Delta E_{(L+1)-H}$ (eV)	
2	STO-3G	-3.52	-0.46	3.07	404	-3.57	-3.57	-0.67	-0.67	2.90	2.90	DS-TR
	6-31G(d,p)	-5.38	-2.42	2.96	419	-5.65	-5.56	-2.65	-2.65	3.00	2.92	
	6-311G(d,p)	-5.63	-2.68	2.95	421	-5.91	-5.80	-2.89	-2.89	3.02	2.91	
	cc-pVDZ	-5.58	-2.75	2.83	438	-5.93	-5.81	-2.89	-2.89	3.04	2.92	
5	STO-3G	-3.50	-0.62	2.87	431	-3.67	-3.64	-0.82	-0.79	2.85	2.84	DS-TR
	6-31G(d,p)	-5.24	-2.67	2.57	483	-5.49	-5.41	-2.89	-2.88	2.60	2.53	
	6-311G(d,p)	-5.49	-2.94	2.56	485	-5.75	-5.65	-3.14	-3.12	2.62	2.52	
	cc-pVDZ	-5.43	-2.99	2.43	510	-5.65	-5.56	-3.07	-3.04	2.59	2.52	
9	STO-3G	-3.00	-0.84	2.16	575	-3.48	-3.47	-0.94	-0.92	2.54	2.55	SS
	6-31G(d,p)	-4.97	-2.73	2.24	554	-5.16	-5.08	-2.89	-2.87	2.26	2.21	
	6-311G(d,p)	-5.22	-2.99	2.23	556	-5.43	-5.34	-3.14	-3.14	2.29	2.20	
	cc-pVDZ	-5.15	-3.04	2.12	586	-5.33	-5.24	-3.08	-3.04	2.25	2.20	
10	STO-3G	-3.22	-0.68	2.55	487	-3.43	-3.41	-0.91	-0.88	2.52	2.53	SS
	6-31G(d,p)	-4.88	-2.68	2.20	563	-5.05	-4.97	-2.81	-2.79	2.23	2.18	
	6-311G(d,p)	-5.13	-2.94	2.20	565	-5.31	-5.22	-3.06	-3.05	2.25	2.17	
	cc-pVDZ	-5.07	-2.98	2.08	595	-5.22	-5.13	-3.00	-2.97	2.22	2.17	

[a,b]MO energies were calculated with B3LYP and S_1 characters were analyzed at CAS(6,6) level.

Scheme S4. Molecular Structure of bis-aza-s-indacenes



12 13 14

TABLE S13. Orbital Energies and Nature of S_1 State for **12**, **13** and **14**

Species	E_{H-1} (eV)	E_H (eV)	E_L (eV)	E_{L+1} (eV)	$\Delta E_{L-(H-1)}$ (eV)	$\Delta E_{(L+1)-H}$ (eV)	NOON	S_1	S_1-T_1 (eV)
12	-5.20	-5.13	-3.12	-3.07	2.08	2.06	1111	DS-TR	1.35 – 0.70
13	-8.17	-7.99	-6.92	-5.97	1.24	2.02	2110	SS	2.02 – 0.66
14	-11.67	-11.62	-9.86	-9.85	1.82	1.76	1111	DS-TR	0.74 – 0.37

TABLE S14. Photophysical Properties (λ ab and oscillator strength) of Compound **12**, **13** and **14** at TD-DFT/CEP-31G Level of Theory

Species	λ (nm)	*f*
12	575	0.27
13	588 - 662	0.24 – 0.18
14	691	0.15

Geometry optimized at UB3LYP/CEP-31G
λ_{ab} values in chloroform.
Excitations with oscillator strength below 0.1 were neglected.

Experimental Details

General:

^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ solvent with tetramethylsilane as internal standard (operating at 400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR). All spectra were recorded at 25^{o}C and coupling constants (*J* values) are given in Hz. Chemical shifts are given in parts per million (ppm). Absorption spectra were performed by using a UV-VIS-NIR absorption spectrophotometer and fluorescence measurements were conducted on a spectrofluometer in $CHCl_3$. The Fluorescence decay measurements were carried out with the time-resolved fluorometer. The instrument response function was measured with an aqueous Ludox solution. Singlet oxygen phosphorescence around 1270 nm were also determined by using fluoremeter . The decays were analyzed with a multiexponential fitting function by iterative reconvolution and chi-square minimization. Mass spectra were recorded with Q-TOF HRMS-ESI. Irradiation of Bodipy photosensitizer and Methylene Blue (MB) were accomplished by using 660 nm LED. Reactions were monitored by thin layer chromatography. Silica gel column chromatography was performed over silica gel (particle size: 0.040-0.063 mm, 230-400 mesh ASTM). All other reagents and solvents were purchased from suppliers and used without further purification.

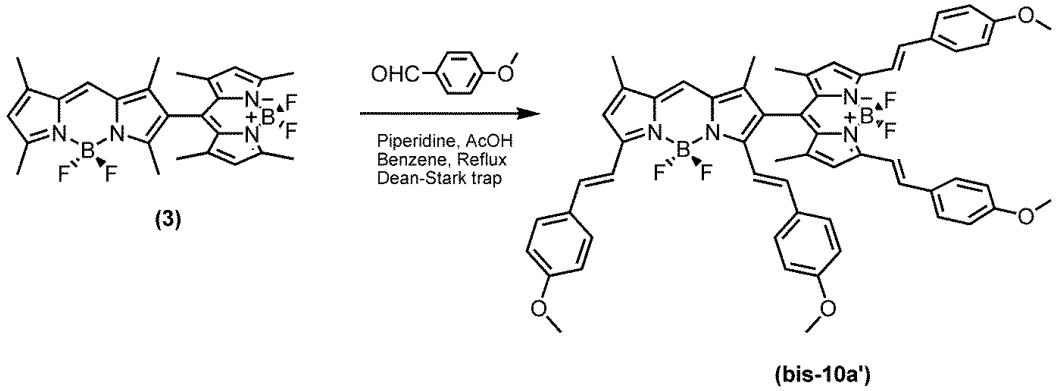


Figure S6. Reaction scheme for the synthesis of target compound.

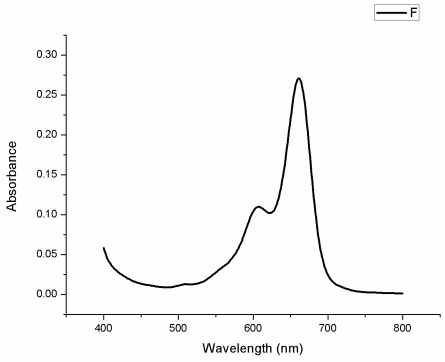


Figure S7. Absorption spectrum of **bis-10a'**.

TABLE S25. Photophysical Properties of the Synthesized BODIPY Compounds

Compound	λ_{abs}[a] / nm	ε_{max}/M^{-1} cm^{-1}	λ_{ems}[a] / nm	ϕ_f	τ[a] / ns	ϕ_Δ
2	515	20.3	588	0.31[a,c]	10.9	0.46
3	514	119.4	527	0.025[a,b]	2.5	0.51
bis-10a'	661	125.3	680	0.06[a,c]	2.2	0.06

[a] in $CHCl_3$
[b] with respect to Fluorescein in 0.1 M NaOH solution excited at 496 nm
[c] with respect to cresyl violet perchlorate in MeOH excited at 610 nm

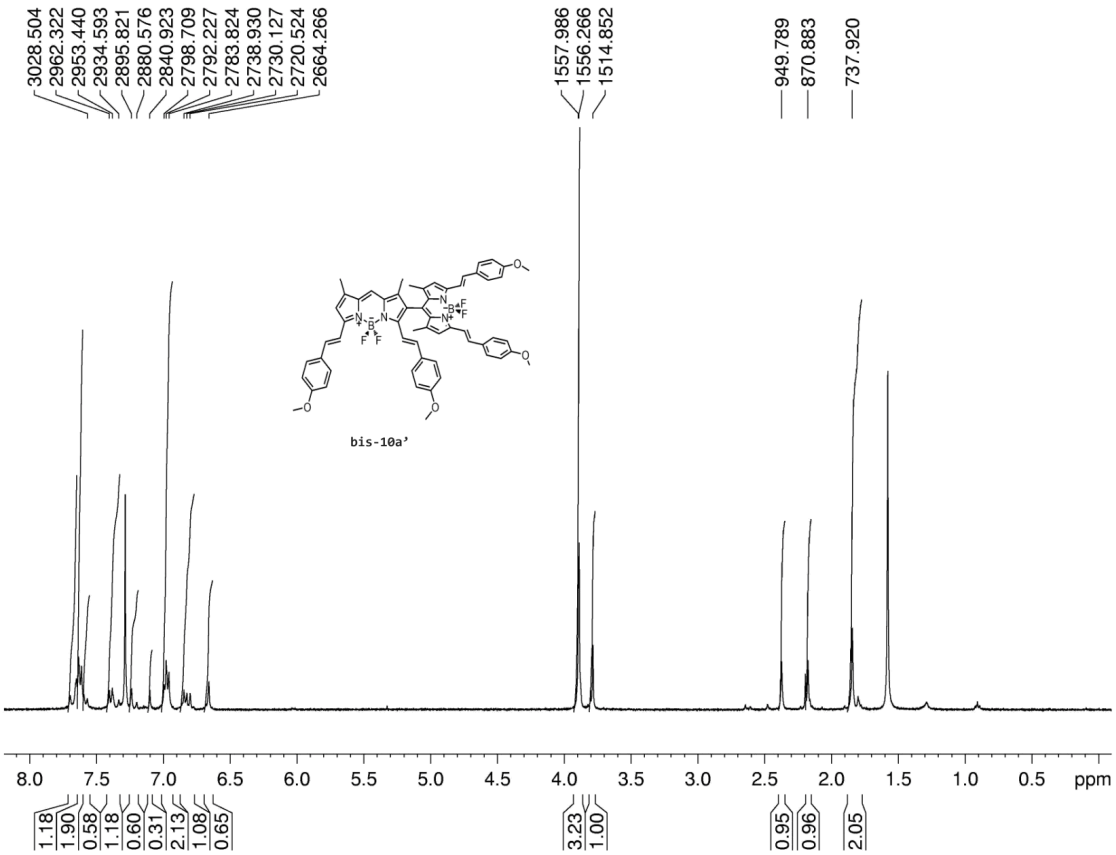


Figure S5. ^{1}H NMR spectrum of compound **bis-10a'**.

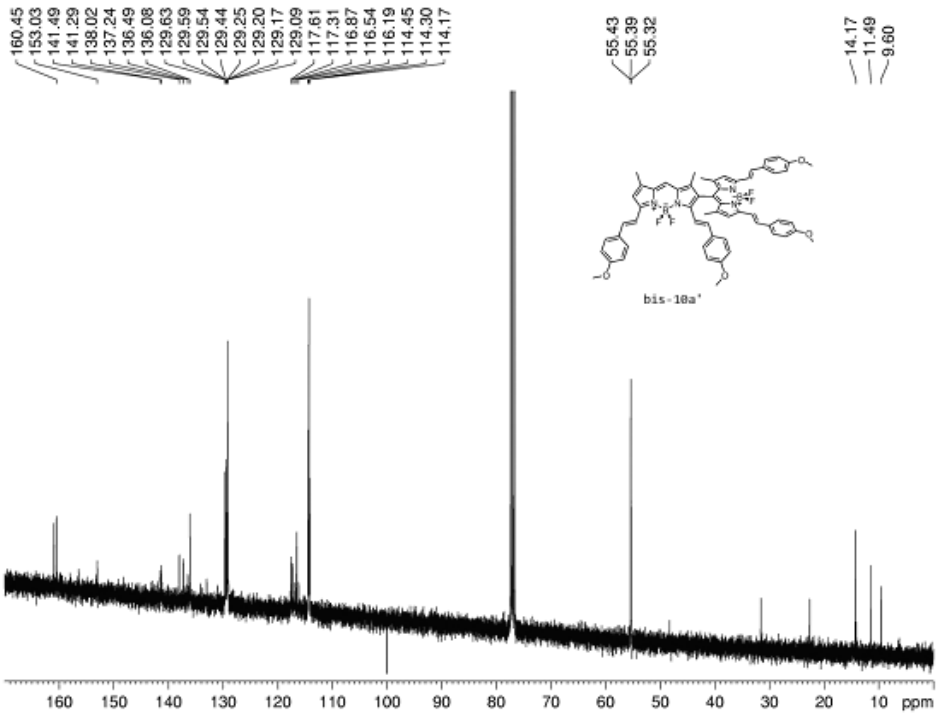


Figure S8. ^{13}C NMR spectrum of compound **bis-10a'**.

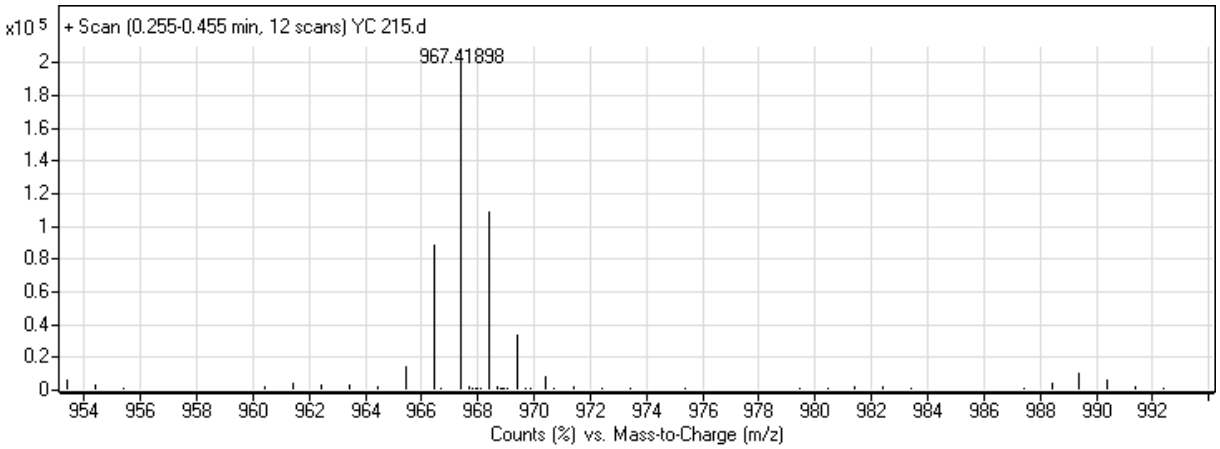


Figure S9. Mass Spectrum of compound **bis-10a'**.

TABLE S16. B3LYP Total Electronic Energies (Hartree) of Monomers

Species	E(AU) B3LYP/CEP-31G	
	S_0	T_1
1	-126.022485	-125.966593
4	-153.435349	-153.384208
4a	-180.821274	-180.771344
4b	-194.512337	-194.462405
4c	-208.201988	-208.152145
4l	-175.096100	-175.043043
5	-164.662562	-164.623186
5a	-178.366762	-178.327588
5b	-194.464452	-194.428780
5l	-186.311709	-186.272229
5al	-200.018520	-199.978750
6	-162.119418	-162.077000
7	-175.892691	-175.854796
8	-173.349346	-173.310027
9	-189.605322	-189.574141
9a	-203.307916	-203.276930
9b	-249.196554	-249.169248
9c	-283.854111	-283.822732
9d	-353.917424	-353.888808
9l	-211.256043	-211.224537
9al	-224.959339	-224.927452
10	-237.166640	-237.132942
10a	-282.734538	-282.701282
10l	-258.817780	-258.782802
11	-472.718854	-472.684544

TABLE S17. B3LYP Total Electronic Energies (Hartree) of Dimers

Binding Motif	Species	E (AU) B3LYP/CEP-31G
8,8'	**bis-1**	-250.843864
8,2'	**bis-1**	-250.851339
8,8'	**2**	-305.665073
8,2'	**3**	-305.669947
8,8'	**bis-4a**	-360.435303
8,8'	**bis-4b**	-387.817403
8,8'	**bis-4c**	-415.193290
8,8'	**bis-4l**	-348.979785
8,8'	**bis-5**	-328.119141
8,2'	**bis-5**	-328.123353
8,8'	**bis-5a**	-355.528267
8,2'	**bis-5a**	-355.532857
8,8'	**bis-5b**	-387.717851
8,2'	**bis-5b**	-387.722952
8,8'	**bis-5l**	-371.411534
8,8'	**bis-5al**	-398.823041
8,8'	**bis-6**	-323.031692
8,2'	**bis-6**	-323.053159
8,8'	**bis-7**	-350.572208
8,2'	**bis-7**	-350.577739
8,8'	**bis-8**	-345.485056
8,2'	**bis-8**	-345.492020
8,8'	**bis-9**	-378.005573
8,2'	**bis-9**	-378.010485
8,8'	**bis-9a**	-405.411320
8,2'	**bis-9a**	-405.416445
8,8'	**bis-9b**	-497.178830
8,2'	**bis-9b**	-497.183147
8,8'	**bis-9c**	-566.501292
8,2'	**bis-9c**	-566.505229
8,8'	**bis-9d**	-706.616575
8,2'	**bis-9d**	-706.622322
8,8'	**bis-9l**	-421.301143
8,8'	**bis-9al**	-448.706394
8,8'	**bis-10**	-473.127741
8,2'	**bis-10**	-473.133090
8,8'	**bis-10a**	−564.264074
8,2'	**bis-10a**	-564.269850
8,8'	**bis-10l**	-516.421375
8,8'	**bis-11**	-944.228075
8,2'	**bis-11**	-944.231831

TABLE S18. CASSCF(6,6)/CEP-31G Total Electronic Energies (Hartree) of bis-BODIPYs in S_0, S_1, and T_1 States

Description	Species	E(AU) S_0	E(AU) T_1	E(AU) S_1
8,8'	**bis-1**	-245.187491	-245.113113	-245.054439
8,2'	**bis-1**	-245.165844	-245.070063	-245.067823
8,8'	**2**	-298.319915	-298.253988	-298.184341
8,2'	**3**	-298.327829	-298.241579	-298.174839
8,8'	**bis-4a**	-351.406344	-351.322448	-351.262916
8,8'	**bis-4b**	-377.935881	-377.873617	-377.809108
8,8'	**bis-4c**	-404.474631	-404.412530	-404.348034
8,8'	**bis-4l**	-340.740764	-340.682714	-340.623049
8,8'	**bis-5**	-320.100839	-320.041414	-319.962210
8,2'	**bis-5**	-320.107354	-320.028877	-319.967286
8,8'	**bis-5a**	-346.669658	-346.610263	-346.547224
8,2'	**bis-5a**	-346.659665	-346.597743	-346.537128
8,8'	**bis-5b**	-378.201659	-378.143934	-378.066277
8,2'	**bis-5b**	-378.200454	-378.133138	-378.071416
8,8'	**bis-5l**	-362.492550	-362.440972	-362.387492
8,8'	**bis-5al**	-389.065558	-389.013793	-388.960314
8,8'	**bis-6**	-315.184637	-315.123704	-315.058576
8,2'	**bis-6**	-315.193963	-315.131163	-315.068701
8,8'	**bis-7**	-341.849512	-341.800437	-341.749982
8,2'	**bis-7**	-341.872756	-341.814510	-341.755811
8,8'	**bis-8**	-336.934949	-336.890120	-336.829467
8,2'	**bis-8**	-336.959105	-336.899302	-336.837976
8,8'	**bis-9**	-368.484856	-368.429425	-368.356860
8,2'	**bis-9**	-368.464872	-368.406055	-368.348048
8,8'	**bis-9a**	-395.036033	-394.982332	-394.919559
8,2'	**bis-9a**	-395.030030	-394.971149	-394.913652
8,8'	**bis-9b**	-484.653656	-484.599503	-484.536940
8,2'	**bis-9b**	-484.643819	-484.588773	-484.531356
8,8'	**bis-9c**	-554.455779	-554.400558	-554.3317559
8,2'	**bis-9c**	-554.434146	-554.375820	-554.316508
8,8'	**bis-9d**	-690.367736	-690.316992	-690.250444
8,2'	**bis-9d**	-690.365426	-690.309755	-690.251380
8,8'	**bis-9l**	-410.901102	-410.845403	-410.789331
8,8'	**bis-9al**	-437.476697	-437.421839	-437.358766
8,8'	**bis-10**	-460.779856	-460.723102	-460.659872
8,2'	**bis-10**	-460.771477	-460.712413	-460.655132
8,8'	**bis-10a**	-549.893447	-549.836478	-549.792114
8,2'	**bis-10a**	-549.886539	-549.828097	-549.771006
8,8'	**bis-10l**	-503.203224	-503.146468	-503.101630
8,8'	**bis-11**	-925.550832	-925.494492	-925.456623
8,2'	**bis-11**	-925.555659	-925.499151	-925.463085

TABLE S19. B3LYP and CASSCF Total Electronic Energies (Hartree) of **12**, **13** and **14**

Species	E (AU) B3LYP/CEP-31G	S_0 CAS(4,4)/CEP-31G	T_1 CAS(4,4)/CEP-31G	S_1 CAS(4,4)/CEP-31G
12	-205.690134	-199.631069	-199.605480	-199.581319
13	-206.075012	-199.973763	-199.949666	-199.899521
14	-206.317080	-200.253813	-200.240182	-200.226494

Complete reference 45

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A., Gaussian03, Revision C.02., Gaussian Inc., Wallingford: 2004.

B3LYP/CEP-31G CARTESIAN COORDINATES

Species 1, Monomer, Electronic state S_0

	x(Å)	y(Å)	z(Å)
N	-1.258310000	0.288986000	0.035297000
C	-1.233662000	-1.131405000	0.002101000
C	-0.000972000	-1.827697000	-0.041284000
C	1.232090000	-1.130827000	-0.052240000
N	1.257490000	0.289604000	-0.020309000
B	-0.000268000	1.215917000	0.025010000
C	2.597924000	-1.601183000	-0.091235000
C	3.431947000	-0.455464000	-0.082334000
C	2.564557000	0.690615000	-0.038219000
C	-2.599641000	-1.602459000	0.022792000
C	-3.433043000	-0.457138000	0.068541000
C	-2.565127000	0.689345000	0.074831000
H	-0.001280000	-2.918603000	-0.065888000
F	-0.025773000	2.073582000	-1.127224000
F	0.025548000	2.030025000	1.208199000
H	2.903992000	-2.643815000	-0.121141000
H	4.516877000	-0.426942000	-0.103911000
H	2.822810000	1.746088000	-0.019524000
H	-2.906248000	-2.645231000	0.006118000
H	-4.517896000	-0.429179000	0.094300000
H	-2.822788000	1.744694000	0.105006000

Species 2, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
N	-1.260651000	0.290057000	0.030481000
C	-1.230780000	-1.133515000	0.030557000
C	-0.000003000	-1.825577000	0.000032000
C	1.230775000	-1.133518000	-0.030541000
N	1.260647000	0.290054000	-0.030560000
B	-0.000002000	1.200879000	-0.000070000
C	2.595635000	-1.620847000	-0.064720000
C	3.422729000	-0.469136000	-0.084095000
C	2.574648000	0.696393000	-0.062529000
C	-2.595640000	-1.620841000	0.064768000
C	-3.422734000	-0.469128000	0.084063000
C	-2.574652000	0.696399000	0.062423000
H	-0.000003000	-2.916690000	0.000070000
F	-0.028143000	2.054064000	-1.169253000
F	0.028140000	2.054143000	1.169055000
H	4.508049000	-0.446955000	-0.110183000
H	-4.508054000	-0.446944000	0.110148000
C	3.028562000	-3.079006000	-0.079071000
H	2.647952000	-3.625331000	0.802555000
H	2.659464000	-3.603201000	-0.979162000
H	4.127377000	-3.154023000	-0.073401000
C	2.986019000	2.153668000	-0.070849000
H	2.607541000	2.668854000	0.827351000
H	4.082273000	2.239695000	-0.103463000
H	2.554118000	2.673966000	-0.941486000
C	-3.028570000	-3.078999000	0.079198000
H	-2.648124000	-3.625321000	-0.802502000
H	-2.659307000	-3.603199000	0.979217000
H	-4.127386000	-3.154012000	0.073728000
C	-2.986023000	2.153675000	0.070648000
H	-2.607538000	2.668803000	-0.827582000
H	-4.082277000	2.239704000	0.103250000
H	-2.554127000	2.674028000	0.941256000

Species 4a, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.426473000	-1.747125000	0.126999000
C	0.808570000	-1.133789000	0.434317000
C	-1.545175000	-0.984500000	-0.276569000

N	0.953712000	0.276332000	0.346651000
B	-0.172632000	1.255258000	-0.082915000
N	-1.451607000	0.428436000	-0.386382000
C	-2.890500000	-1.380891000	-0.634678000
C	-3.597843000	-0.187651000	-0.961142000
C	-2.674269000	0.912712000	-0.794287000
C	2.072829000	-1.696056000	0.859487000
C	2.973380000	-0.604279000	1.026152000
C	2.244777000	0.601163000	0.697994000
F	0.235548000	2.000469000	-1.257821000
F	-0.436881000	2.213080000	0.973073000
C	2.364267000	-3.173119000	1.073590000
C	-3.427171000	-2.803686000	-0.646061000
C	2.741207000	2.031907000	0.708408000
C	-2.924749000	2.390926000	-1.008108000
C	-5.059916000	-0.074689000	-1.373529000
C	-6.015685000	0.186280000	-0.164081000
C	4.438489000	-0.681293000	1.436028000
C	5.410200000	-0.753902000	0.213382000
H	-0.518123000	-2.831146000	0.202837000
H	2.982545000	-3.586318000	0.255002000
H	2.919194000	-3.336364000	2.013983000
H	1.437864000	-3.767699000	1.123246000
H	-2.613939000	-3.545784000	-0.599741000
H	-4.098209000	-2.989855000	0.213080000
H	-4.010414000	-3.001024000	-1.562492000
H	3.767082000	2.086438000	1.101087000
H	2.724985000	2.453818000	-0.310652000
H	2.081830000	2.665813000	1.322537000
H	-3.931541000	2.561293000	-1.416685000
H	-2.826551000	2.940881000	-0.056967000
H	-2.175822000	2.814762000	-1.696029000
H	-5.184018000	0.737680000	-2.111333000
H	-5.371176000	-1.005293000	-1.880612000
H	-7.065435000	0.259681000	-0.501094000
H	-5.946789000	-0.629648000	0.577062000
H	4.705278000	0.193173000	2.055565000
H	4.595727000	-1.571470000	2.070775000
H	6.461324000	-0.811013000	0.549263000
H	5.197215000	-1.641557000	-0.408296000
H	-5.752121000	1.127063000	0.350568000
H	5.301585000	0.137174000	-0.429727000

Species 4b, Monomer , Electronic state S_0

	x(Å)	**y(Å)**	**z(Å)**
C	-0.000095000	1.639457000	0.000037000
C	-1.220810000	0.947247000	0.163436000
C	1.220702000	0.947420000	-0.163499000
N	-1.248012000	-0.472810000	0.169544000
B	0.000078000	-1.380844000	0.000026000
N	1.248036000	-0.472652000	-0.169860000
C	2.573477000	1.429363000	-0.343127000
C	3.408010000	0.280144000	-0.459147000
C	2.551889000	-0.879532000	-0.343767000
C	-2.573623000	1.429042000	0.343189000
C	-3.408046000	0.279724000	0.459084000
C	-2.551812000	-0.879855000	0.343468000
F	-0.160277000	-2.237816000	-1.158685000
F	0.160617000	-2.237275000	1.159127000
C	-3.001795000	2.887371000	0.389828000
C	3.001566000	2.887723000	-0.389656000
C	-2.938934000	-2.343100000	0.393001000
C	2.939220000	-2.342721000	-0.393397000
C	4.920226000	0.262347000	-0.625205000
C	5.693121000	0.178211000	0.733808000
C	7.234399000	0.167947000	0.529884000
C	-4.920250000	0.261769000	0.625228000

C	-5.693256000	0.178743000	-0.733783000
C	-7.234517000	0.168211000	-0.529731000
H	-0.000167000	2.729995000	0.000158000
H	-3.506163000	3.190791000	-0.546434000
H	-3.713245000	3.066166000	1.214919000
H	-2.141286000	3.559738000	0.537030000
H	3.507879000	3.190484000	0.545763000
H	3.711334000	3.067073000	-1.216092000
H	2.140773000	3.560200000	-0.534634000
H	-4.003271000	-2.456783000	0.645860000
H	-2.749446000	-2.826369000	-0.580411000
H	-2.327987000	-2.879997000	1.135916000
H	4.003361000	-2.456247000	-0.647170000
H	2.750720000	-2.825836000	0.580290000
H	2.327723000	-2.879862000	-1.135666000
H	5.226147000	-0.590293000	-1.258776000
H	5.245272000	1.175550000	-1.157103000
H	5.401138000	1.033641000	1.371381000
H	5.378246000	-0.734039000	1.274191000
H	7.767646000	0.108784000	1.494748000
H	7.546674000	-0.697712000	-0.082906000
H	7.571659000	1.084748000	0.011519000
H	-5.226098000	-0.591416000	1.258095000
H	-5.245279000	1.174505000	1.157947000
H	-5.401399000	1.034725000	-1.370671000
H	-5.378368000	-0.733036000	-1.274956000
H	-7.767842000	0.109789000	-1.494597000
H	-7.546678000	-0.697967000	0.082385000
H	-7.571802000	1.084567000	-0.010598000

Species 4c, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.000049000	1.614069000	-0.000230000
C	1.203801000	0.922013000	-0.260633000
C	-1.203878000	0.921963000	0.260230000
N	1.230952000	-0.498078000	-0.267687000
B	0.000073000	-1.406162000	-0.000005000
N	-1.230914000	-0.498141000	0.267270000
C	-2.537752000	1.403912000	0.547744000
C	-3.360858000	0.254817000	0.727568000
C	-2.517254000	-0.905039000	0.543146000
C	2.537679000	1.404101000	-0.547988000
C	3.360903000	0.255080000	-0.727692000
C	2.517339000	-0.904868000	-0.543411000
C	-4.855836000	0.240029000	1.009686000
C	-5.727688000	0.202947000	-0.289743000
C	-7.254678000	0.197864000	0.010082000
C	-8.114268000	0.169310000	-1.286482000
C	4.855907000	0.240223000	-1.009652000
C	5.727636000	0.203098000	0.289849000
C	7.254652000	0.197754000	-0.009836000
C	8.114123000	0.169177000	1.286806000
F	0.251556000	-2.262632000	1.142719000
F	-0.251245000	-2.263224000	-1.142319000
H	-0.000039000	2.704638000	-0.000275000
H	-5.118527000	-0.630325000	1.637982000
H	-5.130954000	1.138659000	1.592239000
H	-5.475131000	1.075105000	-0.923062000
H	-5.462779000	-0.695334000	-0.880042000
H	-7.501337000	-0.680181000	0.638186000
H	-7.514017000	1.094059000	0.607222000
H	-9.194235000	0.165044000	-1.054292000
H	-7.906045000	1.052947000	-1.917575000
H	-7.892669000	-0.731921000	-1.887197000
H	5.118587000	-0.630144000	-1.637935000
H	5.131147000	1.138831000	-1.592177000
H	5.475146000	1.075365000	0.923047000

H	5.462533000	-0.695080000	0.880218000
H	7.501235000	-0.680385000	-0.637842000
H	7.514188000	1.093855000	-0.607029000
H	9.194110000	0.164719000	1.054709000
H	7.905989000	1.052898000	1.917810000
H	7.892326000	-0.731969000	1.887575000
C	-2.961499000	2.861930000	0.630201000
H	-3.535995000	3.166978000	-0.264168000
H	-3.608468000	3.037899000	1.507392000
H	-2.092792000	3.534723000	0.713171000
C	2.961128000	2.862230000	-0.629931000
H	3.614732000	3.036960000	-1.502386000
H	2.092625000	3.534292000	-0.720897000
H	3.528407000	3.169414000	0.268334000
C	2.901223000	-2.367741000	-0.619645000
H	2.823779000	-2.840571000	0.374328000
H	2.213859000	-2.914352000	-1.284186000
H	3.931570000	-2.481519000	-0.987365000
C	-2.901006000	-2.367946000	0.619420000
H	-2.213774000	-2.914419000	1.284220000
H	-3.931439000	-2.481789000	0.986879000
H	-2.823210000	-2.840874000	-0.374473000

Species 4I, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
N	-1.261849000	0.287141000	0.000041000
C	-1.231328000	-1.134443000	0.000130000
C	-0.000003000	-1.826491000	0.000009000
C	1.231322000	-1.134443000	-0.000138000
N	1.261843000	0.287140000	-0.000107000
B	-0.000002000	1.202284000	-0.000050000
C	2.591199000	-1.632307000	-0.000298000
C	3.413377000	-0.473043000	-0.000428000
C	2.572669000	0.704546000	-0.000283000
C	-2.591205000	-1.632306000	0.000346000
C	-3.413382000	-0.473041000	0.000345000
C	-2.572674000	0.704547000	0.000174000
H	-0.000003000	-2.916524000	0.000042000
F	-0.000077000	2.048325000	-1.169822000
F	0.000073000	2.048370000	1.169690000
C	3.025052000	-3.085962000	-0.000360000
H	3.641975000	-3.311488000	0.887198000
H	2.161670000	-3.769459000	-0.000216000
H	3.641682000	-3.311494000	-0.888118000
C	2.966822000	2.164124000	-0.000273000
H	2.551392000	2.672660000	0.885014000
H	4.060127000	2.268589000	-0.000582000
H	2.550840000	2.672845000	-0.885187000
C	-3.025058000	-3.085961000	0.000492000
H	-3.641880000	-3.311569000	-0.887116000
H	-2.161677000	-3.769458000	0.000508000
H	-3.641790000	-3.311411000	0.888201000
C	-2.966827000	2.164125000	0.000068000
H	-2.551372000	2.672610000	-0.885237000
H	-4.060131000	2.268590000	0.000340000
H	-2.550869000	2.672896000	0.884964000
I	-5.532533000	-0.472365000	0.000588000
I	5.532527000	-0.472367000	-0.000749000

Species 5, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.659871000	-1.374129000	0.000000000
C	-1.336253000	-1.222754000	1.230561000
N	-2.719120000	-0.913098000	1.264717000
B	-3.605711000	-0.713474000	0.000000000
N	-2.719120000	-0.913098000	-1.264717000
C	-1.336253000	-1.222754000	-1.230561000

C	-3.112256000	-0.825286000	-2.588612000
C	-1.962881000	-1.082790000	-3.429131000
C	-0.851503000	-1.331550000	-2.595273000
C	-0.851503000	-1.331550000	2.595273000
C	-1.962881000	-1.082790000	3.429131000
C	-3.112256000	-0.825286000	2.588612000
C	0.575182000	-1.651579000	-3.013541000
C	-4.497749000	-0.515140000	-2.979536000
C	0.575182000	-1.651579000	3.013541000
C	-4.497749000	-0.515140000	2.979536000
F	-4.696016000	-1.663963000	0.000000000
F	-4.183371000	0.612554000	0.000000000
C	-4.914747000	-0.420966000	-4.284029000
C	-4.914747000	-0.420966000	4.284029000
H	-1.964607000	-1.082655000	-4.514124000
H	-1.964607000	-1.082655000	4.514124000
H	0.660610000	-1.665915000	-4.111435000
H	1.288846000	-0.901061000	-2.628844000
H	0.896462000	-2.639248000	-2.636776000
H	-5.209911000	-0.356476000	-2.169179000
H	0.660610000	-1.665915000	4.111435000
H	0.896462000	-2.639248000	2.636776000
H	1.288846000	-0.901061000	2.628844000
H	-5.209911000	-0.356476000	2.169179000
H	-4.240587000	-0.571043000	-5.132524000
H	-4.240587000	-0.571043000	5.132524000
H	-5.957217000	-0.187697000	-4.518299000
H	-5.957217000	-0.187697000	4.518299000
H	0.404357000	-1.612362000	0.000000000

Species 5a, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.669530000	-1.378356000	0.000409000
C	-1.344113000	-1.216729000	1.230551000
N	-2.727128000	-0.902942000	1.264644000
B	-3.613557000	-0.710936000	-0.000112000
N	-2.730600000	-0.920236000	-1.264559000
C	-1.347462000	-1.233439000	-1.229971000
C	-3.127069000	-0.839715000	-2.588827000
C	-1.977672000	-1.106211000	-3.428554000
C	-0.866216000	-1.352264000	-2.594120000
C	-0.859126000	-1.316933000	2.594868000
C	-1.968354000	-1.059730000	3.428910000
C	-3.120036000	-0.804641000	2.588776000
C	0.559006000	-1.678553000	-3.013158000
C	-4.510117000	-0.529063000	-2.976926000
C	0.567256000	-1.637452000	3.014413000
C	-4.502016000	-0.488683000	2.976384000
F	-4.708742000	-1.658796000	0.007846000
F	-4.192776000	0.616541000	-0.008371000
C	-4.937967000	-0.439901000	-4.280447000
C	-4.926698000	-0.383439000	4.279743000
H	-1.978757000	-1.113821000	-4.513749000
H	-1.966462000	-1.052485000	4.514106000
H	0.641907000	-1.703102000	-4.111206000
H	1.275053000	-0.925866000	-2.636978000
H	0.879886000	-2.663187000	-2.628012000
H	-5.221278000	-0.363655000	-2.166302000
H	0.653386000	-1.646045000	4.112453000
H	0.886763000	-2.627686000	2.642706000
H	1.282368000	-0.890529000	2.625203000
H	-5.215026000	-0.332674000	2.165520000
H	-4.227857000	-0.605189000	-5.100362000
H	-4.214755000	-0.539306000	5.099914000
H	0.394047000	-1.619362000	0.000600000
C	-6.370295000	-0.118687000	-4.676208000
H	-6.413921000	0.798212000	-5.295164000

H	-6.805535000	-0.934870000	-5.284603000
H	-7.006025000	0.030332000	-3.789173000
C	-6.357865000	-0.056377000	4.674953000

Species 5b, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-2.461444000	-1.482738000	-0.008326000
C	-2.545269000	-0.075101000	-0.104324000
C	-1.212528000	-2.136453000	0.091693000
N	-1.376069000	0.719737000	-0.102781000
B	0.073606000	0.157405000	-0.000425000
N	-0.008095000	-1.395856000	0.098526000
C	-0.892373000	-3.551073000	0.198986000
C	0.514109000	-3.630391000	0.268965000
C	1.046517000	-2.285930000	0.205327000
C	-3.703744000	0.796870000	-0.214333000
C	-3.199326000	2.112720000	-0.277118000
C	-1.755330000	2.047250000	-0.206827000
C	-5.156926000	0.352155000	-0.252502000
C	-1.893943000	-4.694316000	0.226871000
C	-0.774727000	3.135958000	-0.233023000
C	-1.134791000	4.464055000	-0.337106000
C	-0.156075000	5.531374000	-0.361942000
C	2.441468000	-1.838070000	0.240164000
C	3.504536000	-2.711524000	0.346196000
C	4.879207000	-2.256700000	0.379631000
F	0.733876000	0.695004000	1.163782000
F	0.838287000	0.541194000	-1.161600000
H	-3.376895000	-2.074912000	-0.011438000
H	1.099664000	-4.539895000	0.355639000
H	-3.788734000	3.019807000	-0.363089000
H	-5.433685000	-0.205395000	0.659873000
H	-5.824821000	1.223761000	-0.330246000
H	-5.356286000	-0.304423000	-1.118070000
H	-2.495182000	-4.727748000	-0.699119000
H	-1.374325000	-5.659723000	0.325890000
H	-2.593913000	-4.598557000	1.075834000
H	0.279760000	2.866843000	-0.166406000
H	-2.179698000	4.775795000	-0.406155000
H	2.628718000	-0.765728000	0.178624000
H	3.360048000	-3.792628000	0.410288000
N	6.023539000	-1.915381000	0.409893000
N	0.624669000	6.435155000	-0.385207000
H	-6.792193000	-0.864712000	5.294365000
H	-6.399364000	0.868056000	5.282755000
H	-6.995607000	0.082284000	3.787685000

Species 5c, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-2.472102000	-1.721742000	0.000065000
C	-2.559148000	-0.310815000	0.000392000
C	-1.220637000	-2.378990000	-0.000289000
N	-1.391881000	0.483386000	0.000362000
N	-0.017985000	-1.639339000	-0.000327000
B	0.064119000	-0.080127000	-0.000006000
C	-0.901216000	-3.799654000	-0.000657000
C	0.505961000	-3.881964000	-0.000925000
C	1.037131000	-2.534803000	-0.000711000
C	-3.724404000	0.562320000	0.000786000
C	-3.223245000	1.879837000	0.000984000
C	-1.776764000	1.812814000	0.000718000
C	-5.177043000	0.115098000	0.000958000
C	-1.904183000	-4.941669000	-0.000673000
C	-0.799960000	2.903490000	0.000786000
C	-1.182687000	4.221323000	0.001113000
C	2.432222000	-2.090367000	-0.000851000
C	3.477714000	-2.979239000	-0.001223000

F	0.768163000	0.375059000	1.168212000
F	0.767771000	0.375565000	-1.168261000
H	-3.387334000	-2.314061000	0.000085000
H	1.093922000	-4.793791000	-0.001242000
H	-3.814395000	2.789609000	0.001285000
H	-5.412866000	-0.492899000	0.892240000
H	-5.848400000	0.987141000	0.001066000
H	-5.413097000	-0.492862000	-0.890286000
H	-2.556180000	-4.907238000	-0.891383000
H	-1.383637000	-5.911312000	-0.001770000
H	-2.554729000	-4.908494000	0.891152000
H	0.263609000	2.660523000	0.000570000
H	-2.196297000	4.613519000	0.001348000
H	2.646147000	-1.020587000	-0.000649000
H	3.420407000	-4.064563000	-0.001455000
N	4.863876000	-2.506101000	-0.001356000
O	5.773920000	-3.434208000	-0.001773000
O	5.114362000	-1.236945000	-0.001157000
N	-0.183354000	5.292116000	0.001179000

Species 5I, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.641295000	-1.378372000	0.000000000
C	-1.317245000	-1.227148000	1.229798000
N	-2.694817000	-0.918961000	1.272115000
B	-3.581995000	-0.720160000	0.000000000
N	-2.694817000	-0.918961000	-1.272115000
C	-1.317245000	-1.227148000	-1.229798000
C	-3.097355000	-0.828493000	-2.599512000
C	-1.922441000	-1.091574000	-3.425110000
C	-0.810796000	-1.340678000	-2.581282000
C	-0.810796000	-1.340678000	2.581282000
C	-1.922441000	-1.091574000	3.425110000
C	-3.097355000	-0.828493000	2.599512000
C	0.626827000	-1.663067000	-2.948827000
C	-4.502836000	-0.513585000	-2.911535000
C	0.626827000	-1.663067000	2.948827000
C	-4.502836000	-0.513585000	2.911535000
F	-4.664947000	-1.675048000	0.000000000
F	-4.153884000	0.605527000	0.000000000
C	-5.075525000	-0.384410000	-4.153483000
C	-5.075525000	-0.384410000	4.153483000
H	0.755752000	-1.684253000	-4.040299000
H	1.322094000	-0.908935000	-2.539484000
H	0.928564000	-2.648780000	-2.552434000
H	-5.137745000	-0.372217000	-2.037074000
H	0.755752000	-1.684253000	4.040299000
H	0.928564000	-2.648780000	2.552434000
H	1.322094000	-0.908935000	2.539484000
H	-5.137745000	-0.372217000	2.037074000
H	-4.534982000	-0.504663000	-5.091185000
H	-4.534982000	-0.504663000	5.091185000
H	-6.141532000	-0.145822000	-4.223026000
H	-6.141532000	-0.145822000	4.223026000
H	0.422335000	-1.616410000	0.000000000
I	-1.789586000	-1.121431000	5.545864000
I	-1.789586000	-1.121431000	-5.545864000

Species 5aI, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.612963000	-1.373262000	-0.000144000
C	-1.288161000	-1.219345000	1.230223000
N	-2.669686000	-0.921324000	1.270952000
B	-3.555983000	-0.727831000	0.000030000
N	-2.673784000	-0.939315000	-1.270873000
C	-1.292132000	-1.236775000	-1.230382000
C	-3.084838000	-0.860807000	-2.598370000

C	-1.911270000	-1.121284000	-3.423395000
C	-0.794096000	-1.355522000	-2.583586000
C	-0.785763000	-1.318928000	2.583361000
C	-1.900226000	-1.072787000	3.423365000
C	-3.076457000	-0.824003000	2.598519000
C	0.633665000	-1.669389000	-2.990308000
C	-4.490393000	-0.561158000	-2.908340000
C	0.643300000	-1.627079000	2.989879000
C	-4.481016000	-0.519974000	2.908749000
F	-4.648054000	-1.676569000	0.008508000
F	-4.126382000	0.600414000	-0.008453000
C	-5.062778000	-0.411689000	-4.150559000
C	-5.049325000	-0.352616000	4.150557000
H	1.052353000	-0.861161000	-3.615049000
H	1.285869000	-1.796096000	-2.112430000
H	0.678868000	-2.596703000	-3.587847000
H	-5.133086000	-0.447318000	-2.034827000
H	1.063710000	-0.810493000	3.602469000
H	0.690538000	-2.546314000	3.599628000
H	1.292848000	-1.765403000	2.111785000
H	-5.126578000	-0.418757000	2.035798000
H	-4.466239000	-0.511671000	-5.059848000
H	-4.449784000	-0.439414000	5.059224000
H	0.451961000	-1.601945000	-0.000243000
I	-1.735434000	-1.106313000	5.541626000
I	-1.753272000	-1.184678000	-5.541491000
C	-6.538850000	-0.098797000	-4.337119000
H	-6.671432000	0.850330000	-4.891076000
H	-7.034552000	-0.887481000	-4.935114000
H	-7.058984000	-0.014419000	-3.370065000

Species 6, Monomer , Electronic state S_0

	x(Å)	**y(Å)**	**z(Å)**
C	0.000045000	1.934680000	-0.000056000
C	-1.231821000	1.241340000	-0.000044000
C	1.231935000	1.241267000	-0.000015000
N	-1.260247000	-0.174181000	-0.000010000
B	0.000138000	-1.108247000	0.000048000
N	1.260311000	-0.174205000	0.000032000
C	2.596347000	1.740307000	0.000004000
C	3.432341000	0.601252000	-0.000063000
C	2.582727000	-0.569293000	0.000052000
C	-2.596269000	1.740401000	0.000003000
C	-3.432275000	0.601409000	-0.000110000
C	-2.582602000	-0.569215000	-0.000012000
C	-3.001480000	-1.941333000	-0.000025000
C	-3.384207000	-3.130270000	-0.000040000
C	3.001282000	-1.941518000	0.000004000
C	3.383704000	-3.130546000	-0.000041000
C	-3.015499000	3.202338000	0.000078000
C	3.015634000	3.202228000	-0.000015000
F	0.000021000	-1.929443000	-1.173930000
F	-0.000019000	-1.929340000	1.174101000
H	0.000038000	3.025278000	-0.000071000
H	4.516834000	0.576118000	-0.000123000
H	-4.516766000	0.576272000	-0.000188000
H	-3.688031000	-4.156539000	-0.000052000
H	3.687156000	-4.156925000	-0.000076000
H	-2.634963000	3.733102000	-0.890904000
H	-4.113269000	3.287602000	-0.000497000
H	-2.635937000	3.732718000	0.891711000
H	2.635621000	3.732823000	0.891295000
H	4.113404000	3.287450000	-0.000046000
H	2.635572000	3.732810000	-0.891311000

C	-6.524795000	-0.037082000	4.337434000
H	-7.048109000	0.033321000	3.370977000
H	-7.018482000	-0.817059000	4.948376000
H	-6.655612000	0.919942000	4.878061000

Species 7, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.939691000	-1.604746000	-0.085514000
C	-1.761273000	-1.536144000	1.061068000
N	-3.106389000	-1.117124000	0.963733000
B	-3.803934000	-0.699872000	-0.363118000
N	-2.774859000	-0.830584000	-1.522913000
C	-1.438460000	-1.257131000	-1.360172000
C	-2.985915000	-0.558522000	-2.868211000
C	-1.768254000	-0.812229000	-3.590494000
C	-0.787040000	-1.250700000	-2.663340000
C	-1.469465000	-1.840358000	2.455678000
C	-2.669860000	-1.591749000	3.171143000
C	-3.666282000	-1.146775000	2.234180000
C	-4.287159000	-0.089010000	-3.376447000
C	-5.068168000	-0.764445000	2.480183000
F	-4.948945000	-1.546921000	-0.613377000
F	-4.280983000	0.662002000	-0.269792000
C	-4.529425000	0.190743000	-4.697721000
C	-5.652246000	-0.780423000	3.721682000
H	-1.639707000	-0.685368000	-4.659433000
H	-2.826034000	-1.711119000	4.237263000
H	-5.082465000	0.033808000	-2.640860000
H	-5.649424000	-0.456496000	1.610705000
H	-3.766476000	0.084221000	-5.474572000
H	-5.113390000	-1.080759000	4.625213000
H	-5.515375000	0.536584000	-5.020332000
H	-6.697982000	-0.486362000	3.847156000
C	-0.160782000	-2.310343000	2.951576000
H	0.629370000	-2.431087000	2.203016000
C	0.132247000	-2.601850000	4.258654000
H	-0.607745000	-2.504242000	5.058251000
H	1.129088000	-2.946292000	4.548653000
C	0.618713000	-1.636950000	-2.896003000
H	1.191627000	-1.945427000	-2.015166000
C	1.248339000	-1.637620000	-4.113732000
H	0.737768000	-1.341676000	-5.034714000
H	2.296045000	-1.938175000	-4.205455000
H	0.094806000	-1.930852000	0.014831000

Species 8, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-1.029298000	-1.579178000	-0.090639000
C	-1.847296000	-1.493052000	1.058857000
N	-3.177581000	-1.034839000	0.960697000
B	-3.890151000	-0.584190000	-0.360474000
N	-2.843325000	-0.745337000	-1.515687000
C	-1.520321000	-1.209857000	-1.363580000
C	-3.041474000	-0.462125000	-2.857063000
C	-1.838615000	-0.743085000	-3.592300000
C	-0.868566000	-1.215599000	-2.667205000
C	-1.559427000	-1.813943000	2.451127000
C	-2.751710000	-1.533942000	3.172324000
C	-3.728324000	-1.057007000	2.231505000
F	-5.028877000	-1.416184000	-0.611434000
F	-4.296757000	0.785363000	-0.255249000
H	-1.729879000	-0.606137000	-4.662128000
H	-2.930900000	-1.646391000	4.235507000
C	-0.265698000	-2.324280000	2.945892000
H	0.522078000	-2.466737000	2.198802000
C	0.014315000	-2.627785000	4.253195000
H	-0.724308000	-2.509944000	5.051135000

H	0.999652000	-3.002966000	4.544238000
C	0.524520000	-1.639898000	-2.908565000
H	1.093390000	-1.971911000	-2.033818000
C	1.145930000	-1.647757000	-4.130592000
H	0.638528000	-1.329685000	-5.045761000
H	2.184090000	-1.977184000	-4.230874000
C	-5.076643000	-0.654197000	2.512779000
C	-6.246161000	-0.309610000	2.782152000
H	-7.252906000	-0.008097000	2.985204000
C	-4.280913000	0.034997000	-3.382419000
C	-5.349255000	0.467172000	-3.862985000
H	-6.276634000	0.837370000	-4.248470000
H	-0.004436000	-1.935689000	0.006016000

Species 9, Monomer, Electronic state S_0

x(Å)	y(Å)	z(Å)
C	5.033714000	-3.637081000	-0.037798000
N	5.482335000	-2.293891000	-0.052191000
B	4.541288000	-1.055482000	-0.037273000
N	3.068755000	-1.552539000	-0.004937000
C	2.681942000	-2.914512000	0.008256000
C	3.654815000	-3.940754000	-0.008035000
C	1.920563000	-0.772720000	0.015899000
C	0.770570000	-1.650721000	0.043114000
C	1.231795000	-2.985433000	0.038596000
C	6.192916000	-4.513547000	-0.058500000
C	7.324058000	-3.672538000	-0.085225000
C	6.868419000	-2.296017000	-0.081044000
C	6.161143000	-6.033960000	-0.052015000
C	7.654336000	-1.065308000	-0.102104000
C	0.395171000	-4.255885000	0.060752000
C	1.965751000	0.687713000	0.009403000
F	4.770613000	-0.238195000	-1.211068000
F	4.818890000	-0.229603000	1.119985000
C	9.037524000	-1.033427000	-0.130948000
C	0.842218000	1.494949000	0.029677000
H	3.337942000	-4.983588000	0.002508000
H	8.360694000	-3.993012000	-0.105550000
H	7.184256000	-6.441206000	-0.071754000
H	5.659000000	-6.425095000	0.851049000
H	5.621913000	-6.431919000	-0.930377000
H	7.100180000	-0.125104000	-0.094211000
H	-0.276114000	-4.303192000	-0.814979000
H	1.023328000	-5.160822000	0.051209000
H	-0.239307000	-4.296404000	0.963836000
H	2.953574000	1.151231000	-0.012889000
H	9.614414000	-1.965542000	-0.139394000
H	-0.159993000	1.051302000	0.052193000
C	9.806277000	0.218329000	-0.151752000
H	9.231264000	1.151769000	-0.143338000
C	11.181315000	0.261628000	-0.180601000
H	11.782183000	-0.654330000	-0.189627000
H	11.724075000	1.211106000	-0.195568000
C	0.913787000	2.962456000	0.022604000
H	1.915172000	3.408331000	0.000069000
C	-0.196764000	3.774630000	0.042627000
H	-1.209619000	3.357812000	0.065292000
H	-0.109036000	4.864864000	0.036654000
H	-0.265518000	-1.328279000	0.06338000

Species 9a, Monomer , Electronic state S_0

x(Å)	y(Å)	z(Å)
C	5.038336000	-3.621642000	-0.033562000
N	5.487336000	-2.278178000	-0.050951000
B	4.546007000	-1.040432000	-0.037147000
N	3.073617000	-1.536789000	-0.003201000
C	2.686967000	-2.899214000	0.012988000

C	3.659627000	-3.925649000	-0.002048000
C	1.925247000	-0.756113000	0.017207000
C	0.775482000	-1.635297000	0.047022000
C	1.237176000	-2.969759000	0.044161000
C	6.197400000	-4.497704000	-0.053999000
C	7.328795000	-3.657244000	-0.082690000
C	6.874026000	-2.279789000	-0.080767000
C	6.165331000	-6.018231000	-0.045080000
C	7.659982000	-1.050531000	-0.104644000
C	0.400821000	-4.240529000	0.068916000
C	1.969625000	0.703221000	0.008005000
F	4.775011000	-0.223311000	-1.212302000
F	4.824739000	-0.211567000	1.118843000
C	9.044157000	-1.022338000	-0.133819000
C	0.843222000	1.507956000	0.028748000
H	3.342857000	-4.968495000	0.010611000
H	8.365217000	-3.978540000	-0.103225000
H	7.188422000	-6.425847000	-0.065146000
H	5.663846000	-6.408008000	0.859027000
H	5.625049000	-6.417667000	-0.922216000
H	7.107172000	-0.109759000	-0.098542000
H	-0.270760000	-4.290163000	-0.806596000
H	1.029624000	-5.145106000	0.060878000
H	-0.233430000	-4.280032000	0.972330000
H	2.956609000	1.167926000	-0.016532000
H	9.613830000	-1.959541000	-0.140082000
H	-0.155800000	1.055967000	0.053740000
C	9.822038000	0.221133000	-0.157134000
H	9.258147000	1.162002000	-0.150940000
C	11.199695000	0.257045000	-0.186607000
H	11.751971000	-0.692783000	-0.193456000
C	0.902324000	2.973866000	0.019729000
H	1.898555000	3.432351000	-0.005148000
C	-0.214697000	3.781169000	0.039794000
H	-1.206411000	3.308746000	0.063477000
H	-0.260858000	-1.313534000	0.067494000
C	12.026843000	1.533386000	-0.212113000
H	12.705360000	1.586112000	0.661241000
H	12.667130000	1.575346000	-1.114491000
H	11.383173000	2.428249000	-0.203737000
C	-0.177767000	5.301909000	0.030037000
H	-0.675793000	5.718536000	0.926884000
H	0.858381000	5.677372000	0.004918000
H	-0.714987000	5.708045000	-0.848864000

Species 9b, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	5.021195000	-3.719613000	-0.340990000
N	5.499787000	-2.395366000	-0.243633000
B	4.597159000	-1.141293000	-0.061405000
N	3.114292000	-1.609205000	-0.008367000
C	2.693942000	-2.952642000	-0.111531000
C	3.635691000	-3.994576000	-0.275757000
C	1.987622000	-0.813372000	0.144177000
C	0.815035000	-1.665800000	0.138919000
C	1.240782000	-2.999502000	-0.019548000
C	6.155437000	-4.619188000	-0.504074000
C	7.305080000	-3.804668000	-0.501043000
C	6.883970000	-2.427013000	-0.338699000
C	6.082405000	-6.130588000	-0.646455000
C	7.693141000	-1.218533000	-0.274613000
C	0.382439000	-4.252065000	-0.084889000
C	2.073253000	0.633552000	0.279698000
F	4.792767000	-0.219825000	-1.157175000
F	4.946614000	-0.445167000	1.155711000
C	9.079310000	-1.214484000	-0.366379000
C	0.966644000	1.459129000	0.433769000

H	3.288505000	-5.024889000	-0.353208000
H	8.330762000	-4.144141000	-0.602324000
H	7.091341000	-6.556172000	-0.756997000
H	5.613302000	-6.597555000	0.237686000
H	5.492099000	-6.425046000	-1.532243000
H	7.163254000	-0.272469000	-0.147094000
H	0.515167000	-4.783306000	-1.044048000
H	0.635573000	-4.958221000	0.725700000
H	-0.683046000	-3.994300000	0.013052000
H	3.071084000	1.076135000	0.256622000
H	9.634668000	-2.147285000	-0.494298000
H	-0.043525000	1.042278000	0.460168000
C	9.835045000	0.023027000	-0.295913000
H	9.281275000	0.957266000	-0.167965000
C	11.228111000	0.104581000	-0.380575000
C	1.112649000	2.897578000	0.564471000
H	2.122417000	3.316527000	0.538276000
C	0.047538000	3.789259000	0.722255000
C	-1.334641000	3.331223000	0.769381000
N	-2.459481000	2.934574000	0.805434000
C	11.909302000	1.386566000	-0.300796000
N	12.462108000	2.441965000	-0.234592000
C	12.056137000	-1.081862000	-0.551340000
N	12.715532000	-2.066509000	-0.691217000
C	0.280164000	5.219069000	0.846347000
N	0.478066000	6.391430000	0.947589000
H	-0.211522000	-1.328937000	0.240042000

Species 9c, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	5.030022000	-3.645885000	-0.045586000
N	5.477988000	-2.303046000	-0.057701000
B	4.538534000	-1.064542000	-0.037842000
N	3.066733000	-1.561008000	-0.005239000
C	2.678312000	-2.921967000	0.005593000
C	3.650746000	-3.948789000	-0.014368000
C	1.919245000	-0.781238000	0.018845000
C	0.768029000	-1.655996000	0.045807000
C	1.227694000	-2.991603000	0.037878000
C	6.189578000	-4.522595000	-0.070090000
C	7.320687000	-3.680977000	-0.096793000
C	6.863476000	-2.306061000	-0.088790000
C	6.158732000	-6.042771000	-0.066972000
C	7.644032000	-1.071631000	-0.108292000
C	0.389051000	-4.260376000	0.058541000
C	1.972276000	0.679166000	0.015215000
F	4.767285000	-0.242536000	-1.208435000
F	4.818358000	-0.241227000	1.120662000
C	9.025950000	-1.038718000	-0.138993000
C	0.851125000	1.487554000	0.038965000
H	3.333212000	-4.991375000	-0.005582000
H	8.357183000	-4.001808000	-0.119558000
H	7.181819000	-6.449291000	-0.089215000
H	5.658336000	-6.435800000	0.836074000
H	5.618466000	-6.438652000	-0.945464000
H	7.085015000	-0.134525000	-0.097629000
H	-0.283456000	-4.303765000	-0.816217000
H	1.014951000	-5.166679000	0.046325000
H	-0.244276000	-4.300681000	0.962211000
H	2.962807000	1.136449000	-0.007775000
H	9.609532000	-1.963224000	-0.150265000
H	-0.152724000	1.054899000	0.062199000
C	9.768104000	0.224728000	-0.157830000
H	9.224791000	1.171618000	-0.147673000
C	11.128652000	0.292305000	-0.187882000
C	0.952538000	2.949616000	0.034238000
H	1.935695000	3.423747000	0.011420000

C	-0.131722000	3.774393000	0.057143000
F	11.861164000	1.463267000	-0.206263000
F	11.983178000	-0.798555000	-0.204563000
F	-0.074714000	5.154701000	0.053551000
F	-1.453115000	3.357476000	0.087440000
H	-0.267896000	-1.333088000	0.068157000

Species 9d, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	1.230949000	3.377873000	0.005622000
N	1.261277000	1.968618000	-0.012565000
B	-0.000007000	1.055474000	-0.014867000
N	-1.261281000	1.968628000	-0.012594000
C	-1.230945000	3.377883000	0.005610000
C	0.000006000	4.074525000	0.014881000
C	-2.589220000	1.565681000	-0.018807000
C	-3.432799000	2.745312000	-0.004465000
C	-2.600126000	3.880890000	0.010346000
C	2.600136000	3.880871000	0.010359000
C	3.432800000	2.745287000	-0.004456000
C	2.589212000	1.565662000	-0.018780000
C	3.013687000	5.342904000	0.027176000
C	2.974151000	0.162944000	-0.038719000
C	-3.013667000	5.342927000	0.027126000
C	-2.974169000	0.162967000	-0.038777000
F	-0.000019000	0.202304000	1.147714000
F	0.000002000	0.206959000	-1.181766000
C	4.298152000	-0.264894000	-0.031372000
C	-4.298172000	-0.264865000	-0.031372000
H	0.000012000	5.164388000	0.028618000
H	4.517847000	2.745011000	-0.009065000
H	4.110351000	5.432610000	0.019212000
H	2.623569000	5.883192000	-0.853406000
H	2.638585000	5.858168000	0.929102000
H	2.169309000	-0.574863000	-0.063071000
H	-4.110329000	5.432635000	0.019179000
H	-2.638538000	5.858232000	0.929016000
H	-2.623569000	5.883173000	-0.853495000
H	-2.169331000	-0.574842000	-0.063207000
H	5.126186000	0.441666000	-0.023779000
H	-5.126199000	0.441701000	-0.023682000
C	4.590528000	-1.684530000	-0.049397000
H	3.745781000	-2.378981000	-0.078106000
C	5.835533000	-2.293491000	-0.011272000
C	-4.590548000	-1.684500000	-0.049433000
H	-3.745797000	-2.378943000	-0.078212000
C	-5.835545000	-2.293483000	-0.011269000
N	5.925416000	-3.767418000	-0.082791000
O	6.984799000	-4.290698000	-0.593567000
O	4.894409000	-4.438197000	0.325986000
N	7.113752000	-1.578052000	0.113173000
O	7.192880000	-0.399352000	-0.428172000
O	8.059644000	-2.128134000	0.789694000
N	-5.925387000	-3.767416000	-0.082822000
O	-6.984753000	-4.290721000	-0.593605000
O	-4.894359000	-4.438173000	0.325937000
N	-7.113773000	-1.578076000	0.113222000
O	-7.192910000	-0.399340000	-0.428040000
O	-8.059668000	-2.128220000	0.789690000
H	-4.517846000	2.745042000	-0.009065000

Species 9I, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	5.013131000	-3.723446000	-0.035750000
N	5.467830000	-2.387949000	-0.050751000
B	4.520468000	-1.147522000	-0.036860000
N	3.040948000	-1.642178000	-0.004467000

C	2.662580000	-3.002211000	0.009100000
C	3.634955000	-4.027582000	-0.006342000
C	1.893676000	-0.848637000	0.015623000
C	0.750825000	-1.755471000	0.042821000
C	1.217901000	-3.092460000	0.038904000
C	6.153435000	-4.616930000	-0.055162000
C	7.294048000	-3.778312000	-0.082002000
C	6.860989000	-2.381299000	-0.079255000
C	6.069427000	-6.133082000	-0.046938000
C	7.577163000	-1.108107000	-0.099359000
C	0.400143000	-4.370563000	0.060982000
C	2.017429000	0.607126000	0.006934000
F	4.748044000	-0.336014000	-1.212436000
F	4.795702000	-0.325733000	1.121254000
C	8.945455000	-0.895949000	-0.128342000
C	1.000695000	1.547096000	0.023719000
H	3.319195000	-5.070072000	0.004554000
H	7.073191000	-6.580970000	-0.065208000
H	5.550929000	-6.498750000	0.857072000
H	5.515050000	-6.506436000	-0.926179000
H	6.934690000	-0.226455000	-0.089922000
H	-0.272356000	-4.423740000	-0.812985000
H	1.044480000	-5.263125000	0.051487000
H	-0.235961000	-4.416356000	0.962191000
H	3.043290000	0.977560000	-0.015593000
H	9.654282000	-1.725432000	-0.139460000
H	-0.050148000	1.253352000	0.046423000
C	9.513298000	0.459799000	-0.145923000
H	8.804145000	1.295889000	-0.134966000
C	10.866752000	0.706908000	-0.174915000
H	11.596253000	-0.110085000	-0.186328000
H	11.262668000	1.726442000	-0.187633000
C	1.284608000	2.989391000	0.011791000
H	2.339302000	3.288040000	-0.010972000
C	0.298768000	3.949323000	0.027795000
H	-0.762168000	3.677885000	0.050570000
H	0.538291000	5.016522000	0.018374000
I	-1.322297000	-1.293396000	0.083237000
I	9.280489000	-4.536758000	-0.119161000

Species 9aI, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	5.002684000	-3.755469000	-0.032256000
N	5.458612000	-2.420070000	-0.049398000
B	4.512013000	-1.179696000	-0.035628000
N	3.032428000	-1.672611000	-0.001319000
C	2.653206000	-3.032733000	0.014312000
C	3.624498000	-4.059132000	-0.000929000
C	1.885611000	-0.876922000	0.018942000
C	0.742836000	-1.784587000	0.048481000
C	1.208753000	-3.121778000	0.045831000
C	6.142187000	-4.649553000	-0.051893000
C	7.283124000	-3.811808000	-0.081061000
C	6.852595000	-2.413474000	-0.079454000
C	6.056645000	-6.165705000	-0.041763000
C	7.568934000	-1.142254000	-0.101879000
C	0.390341000	-4.399571000	0.070382000
C	2.010286000	0.577162000	0.008237000
F	4.739440000	-0.367817000	-1.212269000
F	4.789463000	-0.355572000	1.121588000
C	8.938792000	-0.932650000	-0.132196000
C	0.992242000	1.517440000	0.025323000
H	3.308082000	-5.101383000	0.011605000
H	7.059877000	-6.614903000	-0.061308000
H	5.539195000	-6.529781000	0.863546000
H	5.500097000	-6.539493000	-0.919500000
H	6.927762000	-0.259856000	-0.093223000

H	-0.282846000	-4.454197000	-0.803049000
H	1.034780000	-5.292105000	0.061725000
H	-0.245169000	-4.444206000	0.972143000
H	3.035990000	0.947390000	-0.016196000
H	9.641896000	-1.767665000	-0.142408000
H	-0.057334000	1.217501000	0.049924000
C	9.514154000	0.416828000	-0.152059000
H	8.813213000	1.260581000	-0.141924000
C	10.870964000	0.660317000	-0.182243000
H	11.559932000	-0.195247000	-0.192013000
C	1.268570000	2.958357000	0.011386000
H	2.321163000	3.266268000	-0.013305000
C	0.279479000	3.918762000	0.027785000
H	-0.769782000	3.594417000	0.052541000
C	11.494962000	2.046728000	-0.203274000
H	12.158825000	2.197073000	0.669938000
H	12.121177000	2.187088000	-1.105477000
H	10.723924000	2.834292000	-0.191351000
C	0.536517000	5.417372000	0.014043000
H	0.102324000	5.903383000	0.909081000
H	1.615887000	5.639342000	-0.010793000
H	0.063441000	5.893775000	-0.866331000
I	-1.331438000	-1.322734000	0.090297000
I	9.269301000	-4.574033000	-0.11980700

Species 10, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	3.841320000	0.000096000	0.000000000
C	3.145692000	-0.000071000	1.229817000
N	1.729721000	-0.000139000	1.262883000
B	0.823564000	0.002098000	0.000000000
N	1.729721000	-0.000139000	-1.262883000
C	3.145692000	-0.000071000	-1.229817000
C	1.322433000	-0.000392000	-2.589445000
C	2.503891000	-0.000782000	-3.429475000
C	3.640894000	-0.000594000	-2.595382000
C	3.640894000	-0.000594000	2.595382000
C	2.503891000	-0.000782000	3.429475000
C	1.322433000	-0.000392000	2.589445000
C	5.103117000	-0.001305000	-3.013392000
C	-0.086988000	-0.000437000	-2.969594000
C	5.103117000	-0.001305000	3.013392000
C	-0.086988000	-0.000437000	2.969594000
F	-0.043396000	-1.160389000	0.000000000
F	-0.037288000	1.169053000	0.000000000
C	-0.520032000	-0.000106000	-4.280776000
C	-0.520032000	-0.000106000	4.280776000
C	-1.928693000	-0.000227000	-4.736013000
C	-1.928693000	-0.000227000	4.736013000
C	-3.044754000	-0.000684000	-3.831130000
C	-4.370788000	-0.000819000	-4.328045000
C	-4.617596000	-0.000504000	-5.733198000
C	-3.521815000	-0.000041000	-6.640849000
C	-2.191641000	0.000098000	-6.146201000
C	-2.191641000	0.000098000	6.146201000
C	-3.521815000	-0.000041000	6.640849000
C	-4.617596000	-0.000504000	5.733198000
C	-4.370788000	-0.000819000	4.328045000
C	-3.044754000	-0.000684000	3.831130000
H	2.506350000	-0.001210000	-4.514645000
H	2.506350000	-0.001210000	4.514645000
H	5.190469000	0.003075000	-4.111320000
H	5.635472000	0.886954000	-2.628352000
H	5.632354000	-0.894656000	-2.635803000
H	-0.804697000	-0.000918000	-2.150337000
H	5.190469000	0.003075000	4.111320000
H	5.632354000	-0.894656000	2.635803000

H	5.635472000	0.886954000	2.628352000
H	-0.804697000	-0.000918000	2.150337000
H	0.225576000	0.000344000	-5.083767000
H	0.225576000	0.000344000	5.083767000
H	-2.876001000	-0.000915000	-2.753007000
H	-5.209588000	-0.001161000	-3.627489000
H	-3.701656000	0.000210000	-7.718701000
H	-1.350541000	0.000458000	-6.845491000
H	-1.350541000	0.000458000	6.845491000
H	-3.701656000	0.000210000	7.718701000
H	-5.209588000	-0.001161000	3.627489000
H	-2.876001000	-0.000915000	2.753007000
H	-5.643698000	-0.000611000	6.109590000
H	-5.643698000	-0.000611000	-6.109590000
H	4.931602000	0.000150000	0.000000000

Species 10a, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	4.621743000	-0.000022000	0.000000000
C	3.925678000	-0.000094000	1.229684000
N	2.509460000	0.000012000	1.262670000
B	1.604183000	0.002319000	0.000000000
N	2.509460000	0.000012000	-1.262670000
C	3.925678000	-0.000094000	-1.229684000
C	2.101022000	-0.000319000	-2.589541000
C	3.283133000	-0.000558000	-3.429423000
C	4.420084000	-0.000828000	-2.595272000
C	4.420084000	-0.000828000	2.595272000
C	3.283133000	-0.000558000	3.429423000
C	2.101022000	-0.000319000	2.589541000
C	5.882311000	-0.001933000	-3.013585000
C	0.692822000	-0.000317000	-2.969450000
C	5.882311000	-0.001933000	3.013585000
C	0.692822000	-0.000317000	2.969450000
F	0.735414000	-1.160273000	0.000000000
F	0.741677000	1.169474000	0.000000000
C	0.259250000	0.000095000	-4.281830000
C	0.259250000	0.000095000	4.281830000
C	-1.145228000	-0.000056000	-4.738421000
C	-1.145228000	-0.000056000	4.738421000
C	-2.268714000	-0.000790000	-3.836535000
C	-3.589840000	-0.000867000	-4.325684000
C	-3.831974000	-0.000223000	-5.734886000
C	-2.741119000	0.000490000	-6.652087000
C	-1.414986000	0.000550000	-6.144219000
C	-1.414986000	0.000550000	6.144219000
C	-2.741119000	0.000490000	6.652087000
C	-3.831974000	-0.000223000	5.734886000
C	-3.589840000	-0.000867000	4.325684000
C	-2.268714000	-0.000790000	3.836535000
O	-5.185327000	-0.000191000	-6.109625000
O	-5.185327000	-0.000191000	6.109625000
H	3.285796000	-0.000866000	-4.514667000
H	3.285796000	-0.000866000	4.514667000
H	5.969596000	0.002520000	-4.111627000
H	6.415240000	0.886049000	-2.628486000
H	6.411638000	-0.895366000	-2.636089000
H	-0.024983000	-0.000818000	-2.150282000
H	5.969596000	0.002520000	4.111627000
H	6.411638000	-0.895366000	2.636089000
H	6.415240000	0.886049000	2.628486000
H	-0.024983000	-0.000818000	2.150282000
H	1.006384000	0.000616000	-5.083587000
H	1.006384000	0.000616000	5.083587000
H	-2.104697000	-0.001366000	-2.757880000
H	-4.445601000	-0.001454000	-3.649525000
H	-2.905020000	0.001044000	-7.729622000

H	-0.577640000	0.001120000	-6.847759000
H	-0.577640000	0.001120000	6.847759000
H	-2.905020000	0.001044000	7.729622000
H	-4.445601000	-0.001454000	3.649525000
H	-2.104697000	-0.001366000	2.757880000
C	-5.513553000	-0.000827000	7.537077000
H	-5.116685000	-0.904386000	8.033682000
H	-5.119879000	0.904178000	8.033630000
H	-6.609664000	-0.002836000	7.579851000
C	-5.513553000	-0.000827000	-7.537077000
H	-5.116685000	-0.904386000	-8.033682000
H	-6.609664000	-0.002836000	-7.579851000
H	-5.119879000	0.904178000	-8.033630000
H	5.712024000	-0.000133000	0.000000000

Species 10I, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	3.057690000	-0.000023000	0.000000000
C	2.362907000	-0.000033000	1.229700000
N	0.951501000	-0.000048000	1.269276000
B	0.045903000	0.000027000	0.000000000
N	0.951501000	-0.000048000	-1.269276000
C	2.362907000	-0.000033000	-1.229700000
C	0.530852000	-0.000035000	-2.599836000
C	1.735446000	0.000008000	-3.424295000
C	2.874965000	0.000006000	-2.583727000
C	2.874965000	0.000006000	2.583727000
C	1.735446000	0.000008000	3.424295000
C	0.530852000	-0.000035000	2.599836000
C	4.337438000	0.000051000	-2.988557000
C	-0.897373000	-0.000029000	-2.904277000
C	4.337438000	0.000051000	2.988557000
C	-0.897373000	-0.000029000	2.904277000
F	-0.814484000	-1.165457000	0.000000000
F	-0.814352000	1.165519000	0.000000000
C	-1.482009000	-0.000085000	-4.155875000
C	-1.482009000	-0.000085000	4.155875000
C	-2.939937000	-0.000035000	-4.418201000
C	-2.939937000	-0.000035000	4.418201000
C	-3.931665000	0.000124000	-3.378730000
C	-5.310104000	0.000161000	-3.703712000
C	-5.732628000	0.000043000	-5.066283000
C	-4.761167000	-0.000116000	-6.106098000
C	-3.379369000	-0.000155000	-5.784017000
C	-3.379369000	-0.000155000	5.784017000
C	-4.761167000	-0.000116000	6.106098000
C	-5.732628000	0.000043000	5.066283000
C	-5.310104000	0.000161000	3.703712000
C	-3.931665000	0.000124000	3.378730000
H	4.577754000	0.887780000	-3.599363000
H	5.000308000	0.000257000	-2.109645000
H	4.577907000	-0.887820000	-3.599090000
H	-1.538825000	0.000034000	-2.025210000
H	4.577754000	0.887780000	3.599363000
H	4.577907000	-0.887820000	3.599090000
H	5.000308000	0.000257000	2.109645000
H	-1.538825000	0.000034000	2.025210000
H	-0.854678000	-0.000168000	-5.048110000
H	-0.854678000	-0.000168000	5.048110000
H	-3.629518000	0.000222000	-2.330193000
H	-6.053523000	0.000283000	-2.902736000
H	-5.076546000	-0.000208000	-7.152256000
H	-2.632937000	-0.000276000	-6.583296000
H	-2.632937000	-0.000276000	6.583296000
H	-5.076546000	-0.000208000	7.152256000
H	-6.053523000	0.000283000	2.902736000
H	-3.629518000	0.000222000	2.330193000

H	-6.798204000	0.000072000	5.309504000
H	-6.798204000	0.000072000	-5.309504000
H	4.146608000	-0.000023000	0.000000000
I	1.911175000	0.000009000	5.542506000
I	1.911175000	0.000009000	-5.542506000

Species 11, Monomer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	0.000003000	4.794746000	-0.000175000
C	1.230792000	4.100262000	-0.000201000
N	1.264207000	2.686993000	-0.000249000
B	-0.000002000	1.775886000	-0.000170000
N	-1.264216000	2.686992000	-0.000177000
C	-1.230789000	4.100259000	-0.000151000
C	-2.589575000	2.282900000	-0.000130000
C	-3.430559000	3.463516000	-0.000074000
C	-2.596673000	4.599891000	-0.000076000
C	2.596678000	4.599884000	-0.000173000
C	3.430556000	3.463505000	-0.000226000
C	2.589567000	2.282896000	-0.000262000
C	-3.012850000	6.062075000	0.000103000
C	-2.971447000	0.870062000	-0.000145000
C	3.012868000	6.062064000	0.000007000
C	2.971442000	0.870059000	-0.000351000
F	-0.000039000	0.928475000	-1.168138000
F	0.000034000	0.928592000	1.167868000
C	-4.297702000	0.481877000	0.000068000
C	4.297697000	0.481876000	0.000009000
C	-4.824893000	-0.895007000	0.000102000
C	4.824888000	-0.895010000	-0.000012000
C	-4.048344000	-2.099883000	-0.000187000
C	-4.635318000	-3.386121000	-0.000114000
C	-6.045901000	-3.525235000	0.000234000
C	-6.855780000	-2.362935000	0.000515000
C	-6.245238000	-1.090119000	0.000451000
C	6.245234000	-1.090116000	0.000762000
C	6.855779000	-2.362930000	0.000816000
C	6.045905000	-3.525232000	0.000074000
C	4.635322000	-3.386124000	-0.000724000
C	4.048343000	-2.099888000	-0.000770000
H	-4.515579000	3.469227000	-0.000070000
H	4.515577000	3.469206000	-0.000279000
H	-4.110238000	6.150400000	-0.001649000
H	-2.632552000	6.591096000	0.892111000
H	-2.629581000	6.592220000	-0.889947000
H	-2.165793000	0.139628000	-0.000326000
H	4.110256000	6.150378000	-0.001858000
H	2.629509000	6.592243000	-0.889984000
H	2.632671000	6.591059000	0.892073000
H	2.165788000	0.139627000	-0.000692000
H	-5.073759000	1.248574000	0.000272000
H	5.073753000	1.248574000	0.000420000
F	-2.658496000	-2.034791000	-0.000547000
F	-3.835241000	-4.519813000	-0.000398000
F	-6.625961000	-4.783947000	0.000293000
F	-8.239024000	-2.482858000	0.000874000
F	-7.083194000	0.029091000	0.000743000
F	7.083182000	0.029098000	0.001523000
F	8.239024000	-2.482849000	0.001619000
F	3.835253000	-4.519820000	-0.001476000
F	2.658494000	-2.034805000	-0.001629000
F	6.625968000	-4.783943000	0.000127000
H	-0.000001000	5.884973000	-0.000179000

Species 2, 8,2' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	4.515288000	-0.021710000	1.052163000

N	4.613167000	0.006135000	-0.369238000
B	3.395771000	0.025599000	-1.337848000
N	2.095828000	0.007257000	-0.485608000
C	2.056046000	-0.020401000	0.933921000
C	3.257277000	-0.034422000	1.685329000
C	0.802540000	0.016789000	-0.958459000
C	-0.100822000	-0.004908000	0.160225000
C	0.675482000	-0.028117000	1.353250000
C	5.859535000	-0.031691000	1.603525000
C	6.737643000	-0.009589000	0.493397000
C	5.943314000	0.013664000	-0.712347000
C	6.222814000	-0.060123000	3.079873000
C	0.155360000	-0.053417000	2.780553000
F	3.435788000	-1.126168000	-2.211902000
F	3.434565000	1.213700000	-2.162416000
C	-1.595429000	-0.002498000	0.084502000
C	-2.303408000	1.234799000	0.074778000
N	-3.729225000	1.253978000	0.031812000
B	-4.638518000	0.001675000	0.009066000
N	-3.732051000	-1.252873000	0.005945000
C	-2.306160000	-1.237750000	0.046871000
C	-4.163100000	-2.557873000	-0.029052000
C	-3.015965000	-3.422582000	-0.013567000
C	-1.847007000	-2.621114000	0.032756000
C	-1.841329000	2.617183000	0.095150000
C	-3.008488000	3.421985000	0.064509000
C	-4.157398000	2.560325000	0.026056000
C	-0.422426000	-3.157912000	0.052555000
C	-0.415833000	3.150504000	0.134347000
F	-5.507065000	-0.009453000	1.170865000
F	-5.483590000	0.014950000	-1.167873000
H	3.208287000	-0.055114000	2.774717000
H	7.823035000	-0.009497000	0.520565000
H	7.316585000	-0.059583000	3.206828000
H	5.819996000	0.819147000	3.613927000
H	5.825092000	-0.962297000	3.578390000
H	-0.481658000	-0.938306000	2.955744000
H	0.976062000	-0.073809000	3.514780000
H	-0.469056000	0.832810000	2.991293000
H	-3.052476000	-4.507537000	-0.037167000
H	-3.042700000	4.507267000	0.066488000
H	-0.441771000	-4.259388000	0.038794000
H	0.160672000	-2.817731000	-0.819171000
H	0.130429000	-2.835477000	0.950625000
H	-0.433312000	4.251869000	0.156693000
H	0.134967000	2.797705000	1.022188000
H	0.168221000	2.838403000	-0.747196000
C	6.423827000	0.042256000	-2.147478000
H	6.042331000	0.937224000	-2.665890000
H	7.523097000	0.043277000	-2.182085000
H	6.042851000	-0.831659000	-2.700989000
C	0.463058000	0.044790000	-2.433384000
H	0.878049000	-0.839856000	-2.944125000
H	-0.626743000	0.067425000	-2.575020000
H	0.912737000	0.926571000	-2.918514000
C	-5.619568000	2.952075000	-0.014032000
H	-6.161367000	2.522417000	0.844344000
H	-5.718547000	4.047630000	0.005068000
H	-6.102566000	2.558925000	-0.923520000
C	-5.626300000	-2.945341000	-0.073452000
H	-5.727308000	-4.040549000	-0.099003000
H	-6.160009000	-2.551243000	0.806952000
H	-6.116188000	-2.513265000	-0.961188000

Species 3, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	0.399432000	0.419545000	0.010293000

C	0.530907000	1.534712000	-0.860257000
C	1.453500000	0.046408000	0.886780000
N	2.670154000	0.791623000	0.902815000
N	1.733665000	2.302175000	-0.864143000
B	2.970481000	2.032158000	0.026848000
C	1.576463000	-1.030649000	1.862395000
C	2.867800000	-0.895728000	2.431836000
C	3.521543000	0.231621000	1.826110000
C	-0.375194000	2.119486000	-1.842142000
C	0.317239000	3.221749000	-2.403986000
C	1.612022000	3.313844000	-1.787563000
C	-0.877629000	-0.381283000	-0.000087000
C	-0.999475000	-1.489250000	-0.881225000
N	-2.202481000	-2.255925000	-0.905471000
B	-3.449435000	-1.992504000	-0.026826000
N	-3.158869000	-0.759267000	0.862645000
C	-1.941602000	-0.014878000	0.867262000
C	-2.070691000	-3.260079000	-1.835704000
C	-0.768771000	-3.163777000	-2.436161000
C	-0.082296000	-2.066604000	-1.857269000
C	-4.020706000	-0.206631000	1.780650000
C	-3.373263000	0.914777000	2.403918000
C	-2.075255000	1.053710000	1.850814000
F	-3.735769000	-3.149153000	0.797909000
F	-4.608077000	-1.748478000	-0.861388000
F	3.246700000	3.182256000	0.864055000
F	4.138832000	1.795285000	-0.796261000
H	3.301883000	-1.529927000	3.198708000
H	-0.056670000	3.891529000	-3.172325000
H	-0.386270000	-3.827358000	-3.205641000
H	-3.815705000	1.542576000	3.171287000
C	2.707504000	4.323669000	-2.056923000
H	2.968115000	4.870092000	-1.135845000
H	3.626477000	3.818417000	-2.396459000
H	2.381716000	5.040143000	-2.825282000
C	-1.781344000	1.682592000	-2.228904000
H	-2.181960000	2.363118000	-2.996488000
H	-1.798183000	0.659174000	-2.638828000
H	-2.470229000	1.694893000	-1.368515000
C	0.561975000	-2.102074000	2.237115000
H	0.271813000	-2.719756000	1.371458000
H	0.991186000	-2.767453000	3.002535000
H	-0.365156000	-1.666553000	2.645111000
C	4.909034000	0.769793000	2.104957000
H	5.394944000	0.174686000	2.892124000
H	5.527867000	0.740948000	1.193102000
H	4.860882000	1.824248000	2.422028000
C	-1.064660000	2.120979000	2.247370000
H	-1.502210000	2.778596000	3.014760000
H	-0.142156000	1.681071000	2.661081000
H	-0.764925000	2.747425000	1.391300000
C	-5.412184000	-0.745476000	2.037443000
H	-6.022906000	-0.697143000	1.120859000
H	-5.370159000	-1.805817000	2.334798000
H	-5.903257000	-0.163466000	2.831177000
C	1.328574000	-1.627815000	-2.224327000
H	2.007151000	-1.645723000	-1.355899000
H	1.738121000	-2.303737000	-2.991268000
H	1.350755000	-0.601916000	-2.627815000
C	-3.163695000	-4.266763000	-2.126017000
H	-2.829768000	-4.977049000	-2.896644000
H	-3.435078000	-4.820810000	-1.212636000
H	-4.078409000	-3.757925000	-2.471620000

Species 4a, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	0.250938000	0.378700000	0.010492000

C	0.404922000	1.502435000	-0.846255000
C	1.284477000	-0.008252000	0.906489000
N	2.497588000	0.734083000	0.958566000
N	1.611028000	2.257275000	-0.820952000
B	2.822756000	1.974622000	0.095911000
C	1.386665000	-1.095657000	1.870683000
C	2.667706000	-0.978370000	2.485786000
C	3.326828000	0.162458000	1.894871000
C	-0.477743000	2.107852000	-1.834665000
C	0.225846000	3.218715000	-2.385902000
C	1.512988000	3.280286000	-1.734485000
C	-1.028913000	-0.417004000	-0.034951000
C	-1.138505000	-1.510149000	-0.937305000
N	-2.340409000	-2.270143000	-0.992595000
B	-3.597938000	-2.016843000	-0.130761000
N	-3.321856000	-0.800389000	0.781761000
C	-2.106615000	-0.060813000	0.820857000
C	-2.197605000	-3.257825000	-1.938665000
C	-0.882964000	-3.168774000	-2.528857000
C	-0.211074000	-2.074290000	-1.909409000
C	-4.198283000	-0.261759000	1.694242000
C	-3.570888000	0.856523000	2.358264000
C	-2.257487000	0.989402000	1.819428000
F	-3.903180000	-3.186166000	0.673090000
F	-4.744761000	-1.760474000	-0.981685000
F	3.087361000	3.124297000	0.941447000
F	4.012632000	1.733922000	-0.698765000
C	2.630702000	4.278688000	-1.953228000
H	2.785427000	4.890116000	-1.048274000
H	3.582062000	3.759281000	-2.148348000
H	2.398970000	4.943665000	-2.797667000
C	-1.884341000	1.672113000	-2.222399000
H	-1.908321000	0.634568000	-2.592874000
H	-2.578974000	1.721502000	-1.367631000
H	-2.281645000	2.323651000	-3.015388000
C	0.349624000	-2.166846000	2.180135000
H	0.117376000	-2.780796000	1.294345000
H	0.717663000	-2.841301000	2.968085000
H	-0.602748000	-1.731906000	2.524161000
C	4.708322000	0.708020000	2.191211000
H	5.155129000	0.190149000	3.052148000
H	5.369804000	0.582247000	1.317364000
H	4.662957000	1.788535000	2.399051000
C	-1.231425000	2.033747000	2.238184000
H	-1.671238000	2.733034000	2.965539000
H	-0.347550000	1.572001000	2.709454000
H	-0.864717000	2.621681000	1.381880000
C	-5.590158000	-0.821008000	1.903525000
H	-6.162282000	-0.799735000	0.961725000
H	-5.539261000	-1.876774000	2.216376000
H	-6.130730000	-0.244917000	2.668041000
C	1.201530000	-1.608113000	-2.235405000
H	1.842697000	-1.571111000	-1.340617000
H	1.670928000	-2.290033000	-2.960698000
H	1.208325000	-0.596266000	-2.674612000
C	-3.304210000	-4.243441000	-2.251401000
H	-2.966252000	-4.987543000	-2.986762000
H	-3.634087000	-4.760500000	-1.336136000
H	-4.187264000	-3.718266000	-2.651835000
C	-0.352404000	-4.070246000	-3.636869000
H	0.741809000	-4.176662000	-3.540623000
H	-0.770232000	-5.086030000	-3.524762000
C	-0.686904000	-3.536215000	-5.067166000
H	-0.246215000	-2.536347000	-5.227180000
H	-1.778442000	-3.446969000	-5.210097000
H	-0.291830000	-4.216442000	-5.842884000
C	-4.205774000	1.699304000	3.457614000

H	-3.823697000	2.733357000	3.403155000
H	-5.295670000	1.766064000	3.295584000
C	-3.936125000	1.133360000	4.889406000
H	-2.852569000	1.091054000	5.098033000
H	-4.336021000	0.108834000	4.991278000
H	-4.411994000	1.767605000	5.658707000
C	3.270284000	-1.892467000	3.545559000
H	3.920671000	-1.306908000	4.218638000
H	2.468552000	-2.308294000	4.179514000
C	4.098037000	-3.069384000	2.935013000
H	4.932212000	-2.688043000	2.319759000
H	3.465702000	-3.700868000	2.286205000
H	4.520903000	-3.706884000	3.732071000
C	-0.276622000	4.200792000	-3.437160000
H	0.564862000	4.537404000	-4.067741000
H	-0.984083000	3.693446000	-4.115022000
C	-0.977574000	5.450817000	-2.813151000
H	-0.287223000	5.998894000	-2.147785000
H	-1.853956000	5.151313000	-2.211726000
H	-1.319860000	6.144234000	-3.602155000

Species 4b, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	0.751965000	-0.003570000	0.002942000
C	1.443377000	-0.745974000	0.998969000
C	1.458875000	0.731729000	-0.987119000
N	2.866322000	-0.758840000	1.018361000
N	2.881892000	0.728162000	-0.996528000
B	3.779289000	-0.023160000	0.012237000
C	1.009201000	1.563713000	-2.095110000
C	2.181895000	2.040893000	-2.751149000
C	3.320293000	1.505811000	-2.042412000
C	0.976438000	-1.569865000	2.105852000
C	2.138959000	-2.058642000	2.771440000
C	3.288370000	-1.539136000	2.069084000
C	2.251976000	2.978949000	-3.947788000
C	2.305810000	4.491334000	-3.547340000
C	2.383227000	5.421728000	-4.790609000
C	2.189020000	-2.991117000	3.973455000
C	2.217976000	-4.506853000	3.583224000
C	2.271730000	-5.429320000	4.833749000
F	4.629799000	-0.974439000	-0.678989000
F	4.644155000	0.913324000	0.705376000
C	-0.755409000	0.002722000	-0.003404000
C	-1.455286000	-0.993214000	-0.737728000
N	-2.878288000	-1.003567000	-0.746561000
B	-3.782865000	0.009973000	-0.010495000
N	-2.876839000	1.022548000	0.725325000
C	-1.453915000	1.003779000	0.725048000
C	-3.309162000	-2.056060000	-1.519772000
C	-2.165649000	-2.768109000	-2.039079000
C	-0.997602000	-2.107220000	-1.557131000
C	-3.306094000	2.080399000	1.491930000
C	-2.161463000	2.788201000	2.014770000
C	-0.994579000	2.118424000	1.542586000
C	-2.219021000	3.999469000	2.934801000
C	-2.252936000	3.624687000	4.454365000
C	-2.311663000	4.884428000	5.363844000
C	-2.224952000	-3.974213000	-2.965686000
C	-2.250205000	-3.591072000	-4.483307000
C	-2.312328000	-4.845456000	-5.399923000
C	-0.461245000	-1.881142000	2.499187000
C	-0.422227000	1.892408000	-2.496876000
C	-4.779101000	-2.348935000	-1.737948000
C	-4.775567000	2.382827000	1.700083000
C	4.755815000	-1.762688000	2.370374000
C	4.792271000	1.712283000	-2.333594000

C	0.436795000	-2.510882000	-1.870353000
C	0.440513000	2.516055000	1.860420000
F	-4.640736000	-0.675047000	0.938683000
F	-4.640357000	0.695969000	-0.958866000
H	3.140096000	2.743491000	-4.561629000
H	1.377054000	2.820097000	-4.603284000
H	1.411974000	4.738443000	-2.944582000
H	3.180757000	4.663175000	-2.892566000
H	2.418774000	6.485021000	-4.495982000
H	3.286653000	5.206192000	-5.390479000
H	1.503919000	5.280841000	-5.445954000
H	3.078978000	-2.767128000	4.588846000
H	1.314820000	-2.813100000	4.625012000
H	1.323158000	-4.742288000	2.977310000
H	3.093302000	-4.699026000	2.934662000
H	2.289879000	-6.495265000	4.547289000
H	3.175438000	-5.225289000	5.437179000
H	1.391314000	-5.267568000	5.482720000
H	-1.346048000	4.651786000	2.753535000
H	-3.109815000	4.609913000	2.700930000
H	-3.127894000	2.976669000	4.649982000
H	-1.358090000	3.022496000	4.699122000
H	-2.332471000	4.608781000	6.432581000
H	-1.431842000	5.533197000	5.198065000
H	-3.215755000	5.484290000	5.151131000
H	-1.356111000	-4.631914000	-2.783995000
H	-3.119919000	-4.581435000	-2.739329000
H	-3.120712000	-2.937120000	-4.679034000
H	-1.350936000	-2.992691000	-4.721064000
H	-2.327510000	-4.563830000	-6.467203000
H	-1.436772000	-5.500047000	-5.234427000
H	-3.220543000	-5.441425000	-5.193944000
H	-0.986235000	-2.450150000	1.713620000
H	-0.483160000	-2.484360000	3.419535000
H	-1.050069000	-0.967607000	2.678836000
H	-0.945963000	2.464834000	-1.712931000
H	-0.431326000	2.498604000	-3.415458000
H	-1.019876000	0.985871000	-2.682952000
H	-4.909336000	-3.255629000	-2.345881000
H	-5.295670000	-2.481155000	-0.773627000
H	-5.270937000	-1.502234000	-2.244710000
H	-5.284259000	1.524316000	2.168283000
H	-4.904215000	3.268888000	2.337983000
H	-5.276659000	2.556357000	0.733814000
H	4.878398000	-2.398268000	3.258979000
H	5.257933000	-2.240774000	1.513302000
H	5.268183000	-0.801566000	2.538719000
H	4.928242000	2.333317000	-3.230514000
H	5.290894000	2.199254000	-1.479386000
H	5.297593000	0.744359000	-2.482469000
H	1.022249000	-2.705078000	-0.957467000
H	0.451053000	-3.425403000	-2.482531000
H	0.970151000	-1.724710000	-2.430445000
H	1.025372000	2.721078000	0.949256000
H	0.456356000	3.422837000	2.483939000
H	0.973463000	1.722271000	2.409721000

Species 4c, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.033101000	-0.064334000	0.848986000
C	1.046698000	0.458704000	1.611847000
C	-1.133604000	-0.705983000	1.479885000
N	1.037001000	0.346929000	3.030155000
N	-1.168412000	-0.831498000	2.897105000
B	-0.081828000	-0.314172000	3.866025000
C	-2.340712000	-1.324282000	0.948972000
C	-3.078502000	-1.810064000	2.068190000

C	-2.321131000	-1.491319000	3.254777000
C	2.272782000	1.145042000	1.227989000
C	2.977994000	1.429009000	2.434338000
C	2.182298000	0.924002000	3.527654000
C	-4.394021000	-2.575111000	2.047377000
C	-4.193235000	-4.128001000	2.012119000
C	-5.528156000	-4.929578000	2.062573000
C	4.302825000	2.164905000	2.575788000
C	4.127186000	3.707939000	2.779547000
C	5.474657000	4.463216000	2.986963000
F	-0.648618000	0.648211000	4.793144000
F	0.454612000	-1.410752000	4.650097000
C	-0.004224000	0.056755000	-0.653298000
C	-0.587181000	1.194128000	-1.275775000
N	-0.556989000	1.324975000	-2.693136000
B	0.087580000	0.315037000	-3.669020000
N	0.663206000	-0.856713000	-2.841914000
C	0.615771000	-0.964245000	-1.424235000
C	-1.176159000	2.502256000	-3.041976000
C	-1.632852000	3.175141000	-1.849479000
C	-1.270142000	2.362588000	-0.736300000
C	1.312871000	-1.958238000	-3.348579000
C	1.704015000	-2.824805000	-2.262315000
C	1.273848000	-2.208948000	-1.050610000
C	2.477510000	-4.127345000	-2.409830000
C	4.029266000	-3.928192000	-2.337559000
C	4.831527000	-5.259962000	-2.443300000
C	-2.399730000	4.489742000	-1.824896000
C	-3.953200000	4.290855000	-1.852851000
C	-4.752127000	5.627210000	-1.791906000
C	2.738727000	1.508699000	-0.175325000
C	-2.759324000	-1.450390000	-0.509699000
C	-1.294632000	2.961512000	-4.480795000
C	1.533256000	-2.150496000	-4.834661000
C	2.481368000	0.973515000	5.011475000
C	-2.660777000	-1.801867000	4.697785000
C	-1.563898000	2.683749000	0.722956000
C	1.483849000	-2.771147000	0.348711000
F	1.139635000	0.958861000	-4.433155000
F	-0.898400000	-0.176537000	-4.614943000
H	-4.994897000	-2.318460000	2.938899000
H	-4.990852000	-2.264539000	1.173729000
H	-3.627120000	-4.400035000	1.100656000
H	-3.560202000	-4.419819000	2.871784000
H	-6.100833000	-4.626346000	2.960622000
H	-5.293357000	-6.002900000	2.190215000
H	4.871249000	1.759331000	3.432605000
H	4.922548000	1.982516000	1.682060000
H	3.591287000	4.130902000	1.908278000
H	3.475097000	3.874846000	3.658137000
H	6.019979000	4.006850000	3.835806000
H	5.255916000	5.506766000	3.281015000
H	2.178028000	-4.836625000	-1.617102000
H	2.214373000	-4.607742000	-3.367183000
H	4.345965000	-3.237615000	-3.142919000
H	4.273380000	-3.426143000	-1.382185000
H	5.893705000	-5.054993000	-2.213033000
H	4.473313000	-5.963699000	-1.666961000
H	-2.137076000	5.064239000	-0.918197000
H	-2.093934000	5.111595000	-2.682965000
H	-4.232667000	3.730607000	-2.766104000
H	-4.239787000	3.652388000	-0.995891000
H	-5.823336000	5.394851000	-1.644259000
H	-4.432027000	6.203256000	-0.901857000
H	2.015809000	2.162541000	-0.689791000
H	3.701943000	2.038873000	-0.133647000
H	2.868929000	0.617299000	-0.810501000

H	-2.029276000	-2.031139000	-1.097322000
H	-3.732340000	-1.958564000	-0.586502000
H	-2.850668000	-0.466814000	-0.998563000
H	-1.543382000	2.116908000	-5.139321000
H	-2.065686000	3.740015000	-4.577742000
H	-0.333360000	3.373492000	-4.835842000
H	2.102586000	-1.304763000	-5.253530000
H	2.078749000	-3.084459000	-5.030571000
H	0.568912000	-2.174192000	-5.367984000
H	3.441934000	1.474348000	5.198353000
H	1.682873000	1.510554000	5.549016000
H	2.514161000	-0.044166000	5.433836000
H	-3.688082000	-2.185184000	4.780614000
H	-1.965876000	-2.555982000	5.105105000
H	-2.554216000	-0.903163000	5.324710000
H	-2.254677000	1.951049000	1.173363000
H	-0.650774000	2.680775000	1.338906000
H	-2.027690000	3.678211000	0.808944000
H	2.124811000	-2.115428000	0.961456000
H	0.533624000	-2.886997000	0.894212000
H	1.967005000	-3.758573000	0.295667000
C	-4.597450000	6.511607000	-3.064022000
C	4.739453000	-5.939034000	-3.841364000
C	6.389630000	4.472102000	1.727674000
C	-6.417933000	-4.752673000	0.797151000
H	-5.223376000	7.419157000	-2.992846000
H	-3.553526000	6.840123000	-3.211564000
H	-4.909112000	5.957359000	-3.969158000
H	5.368383000	-6.846416000	-3.882881000
H	3.705534000	-6.241613000	-4.084243000
H	5.086143000	-5.251579000	-4.635647000
H	5.861665000	4.912069000	0.860876000
H	7.301883000	5.069306000	1.905339000
H	6.709823000	3.453475000	1.446647000
H	-7.320467000	-5.387035000	0.856687000
H	-6.754768000	-3.708126000	0.674849000
H	-5.864358000	-5.038799000	-0.116762000

Species 4I, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.003983000	-0.007967000	0.753669000
C	0.874135000	0.857477000	1.462386000
C	-0.882991000	-0.888012000	1.442882000
N	-0.896116000	-0.913478000	2.866819000
N	0.884851000	0.853713000	2.886604000
B	-0.008544000	-0.037079000	3.789373000
C	-1.860300000	-1.856646000	0.958564000
C	-2.427247000	-2.430807000	2.129943000
C	-1.818699000	-1.835434000	3.297966000
C	1.853855000	1.834175000	0.999791000
C	2.419989000	2.382989000	2.183685000
C	1.808595000	1.764736000	3.338174000
C	-0.001852000	0.007115000	-0.753675000
C	0.878127000	-0.858428000	-1.459965000
N	0.893012000	-0.854419000	-2.884144000
B	0.002846000	0.037121000	-3.789367000
N	-0.887328000	0.913449000	-2.869272000
C	-0.878475000	0.887635000	-1.445307000
C	1.817906000	-1.765533000	-3.333167000
C	2.425823000	-2.384078000	-2.176999000
C	1.856335000	-1.835355000	-0.994672000
C	-1.807997000	1.836123000	-3.302957000
C	-2.419848000	2.431419000	-2.136624000
C	-1.856778000	1.856621000	-0.963690000
F	-0.822306000	-0.786951000	-4.641601000
F	0.827449000	0.875299000	-4.627564000
F	-0.836215000	0.787648000	4.638472000

F	0.813083000	-0.875097000	4.630691000
C	2.069874000	2.008034000	4.807173000
H	1.143104000	2.320214000	5.315126000
H	2.403243000	1.078483000	5.296615000
H	2.836371000	2.783133000	4.937810000
C	2.213040000	2.205260000	-0.429790000
H	2.980664000	2.991942000	-0.430205000
H	2.609590000	1.341835000	-0.988275000
H	1.339343000	2.580420000	-0.986557000
C	-2.216068000	-2.198594000	-0.479102000
H	-1.340879000	-2.562347000	-1.041107000
H	-2.983684000	-2.985076000	-0.497629000
H	-2.610948000	-1.323863000	-1.020895000
C	-2.080351000	-2.110983000	4.761169000
H	-2.868072000	-2.867249000	4.874731000
H	-1.160681000	-2.464661000	5.255133000
H	-2.383134000	-1.185920000	5.277710000
C	-2.216823000	2.198297000	0.472975000
H	-2.984255000	2.985007000	0.489355000
H	-2.613613000	1.323548000	1.013334000
H	-1.343252000	2.561657000	1.037752000
C	-2.064215000	2.113085000	-4.766859000
H	-1.145452000	2.478097000	-5.254432000
H	-2.354103000	1.186491000	-5.287834000
H	-2.858892000	2.861686000	-4.882789000
C	2.211480000	-2.206507000	0.435900000
H	1.335701000	-2.579131000	0.991040000
H	2.977199000	-2.995041000	0.438449000
H	2.608992000	-1.343677000	0.994674000
C	2.083525000	-2.008540000	-4.801434000
H	2.851088000	-2.782938000	-4.929942000
H	1.158471000	-2.321572000	-5.311995000
H	2.417385000	-1.078661000	-5.289907000
I	-3.920768000	3.928698000	-2.203551000
I	3.925387000	3.874252000	2.279207000
I	-3.929301000	-3.927133000	2.192720000
I	3.931342000	-3.875477000	-2.268384000

Species 5, 8,2' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	4.753839000	-4.319200000	-0.920554000
N	4.922746000	-3.234084000	-1.818486000
B	3.765289000	-2.316510000	-2.313662000
N	2.438387000	-2.787603000	-1.648702000
C	2.337786000	-3.881582000	-0.759091000
C	3.483405000	-4.635612000	-0.402604000
C	1.174741000	-2.238813000	-1.819467000
C	0.238291000	-2.998234000	-1.020770000
C	0.958855000	-4.024533000	-0.356401000
C	6.050038000	-4.941972000	-0.697112000
C	6.975055000	-4.212256000	-1.470305000
C	6.259484000	-3.156851000	-2.159599000
C	6.321082000	-6.139667000	0.199283000
C	6.779270000	-2.133808000	-3.081735000
C	0.391969000	-5.067892000	0.591762000
C	0.966530000	-1.074785000	-2.697926000
F	3.656632000	-2.390377000	-3.753741000
F	4.040265000	-0.940238000	-1.964546000
C	-1.236605000	-2.789839000	-0.877410000
C	-1.737548000	-1.964932000	0.171059000
N	-3.135713000	-1.824834000	0.379689000
B	-4.232094000	-2.539171000	-0.449310000
N	-3.542385000	-3.363783000	-1.564550000
C	-2.137395000	-3.478333000	-1.740953000
C	-4.176432000	-4.120805000	-2.532902000
C	-3.170248000	-4.736109000	-3.361816000
C	-1.897793000	-4.349130000	-2.888145000

C	-1.050351000	-1.141347000	1.161805000
C	-2.060727000	-0.536654000	1.940690000
C	-3.343879000	-0.970149000	1.446830000
C	-0.571567000	-4.767698000	-3.506488000
C	-5.643138000	-4.223646000	-2.621828000
C	0.444046000	-0.919746000	1.346301000
C	-4.691268000	-0.620761000	1.928773000
F	-5.023673000	-3.404972000	0.401448000
F	-5.135251000	-1.566196000	-1.030173000
C	-6.291924000	-4.973008000	-3.571078000
C	-4.920230000	0.213271000	2.994366000
C	8.102012000	-2.038064000	-3.436100000
C	-0.238930000	-0.462236000	-2.940467000
H	3.380829000	-5.475777000	0.284406000
H	8.041008000	-4.400156000	-1.543303000
H	7.389649000	-6.404339000	0.176371000
H	6.047040000	-5.930134000	1.248741000
H	5.746162000	-7.025923000	-0.123642000
H	6.054072000	-1.428813000	-3.488748000
H	-0.394117000	-5.666863000	0.099580000
H	1.171729000	-5.757553000	0.950821000
H	-0.076029000	-4.593298000	1.472159000
H	1.862789000	-0.687216000	-3.183158000
H	-3.361124000	-5.383103000	-4.211462000
H	-1.900448000	0.146370000	2.768165000
H	-0.756205000	-5.438973000	-4.360235000
H	0.000963000	-3.900217000	-3.874254000
H	0.074043000	-5.297014000	-2.786401000
H	-6.218923000	-3.664924000	-1.883912000
H	0.615372000	-0.237096000	2.193777000
H	0.982672000	-1.860253000	1.548701000
H	0.904684000	-0.471646000	0.450448000
H	-5.532450000	-1.060540000	1.392773000
H	-5.760131000	-5.550127000	-4.333328000
H	-4.111341000	0.679550000	3.564648000
H	8.867134000	-2.720789000	-3.055012000
H	-1.182075000	-0.784741000	-2.498100000
H	-7.384508000	-5.015029000	-3.594050000
H	-5.941759000	0.441386000	3.311383000
H	8.436977000	-1.258377000	-4.125787000
H	-0.281540000	0.400036000	-3.612602000

Species 5, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	0.753258000	-0.000020000	0.000286000
C	1.453782000	-0.906898000	-0.840152000
C	1.454131000	0.906707000	0.840635000
N	2.874569000	0.921354000	0.854443000
N	2.874202000	-0.922061000	-0.854072000
B	3.780688000	0.000292000	-0.000719000
C	0.982678000	1.921294000	1.780728000
C	2.139911000	2.514302000	2.329707000
C	3.300952000	1.887079000	1.748300000
C	0.981841000	-1.921442000	-1.779991000
C	2.138788000	-2.515145000	-2.328828000
C	3.300134000	-1.888069000	-1.747854000
C	-0.753244000	0.000142000	0.000281000
C	-1.454082000	-0.840167000	0.907070000
N	-2.874516000	-0.853863000	0.921900000
B	-3.780684000	-0.000372000	-0.000657000
N	-2.874233000	0.854465000	-0.921673000
C	-1.453804000	0.840450000	-0.906696000
C	-3.300841000	-1.747802000	1.887577000
C	-2.139762000	-2.328632000	2.515264000
C	-0.982567000	-1.780014000	1.921837000
C	-3.300242000	1.748567000	-1.887330000
C	-2.138951000	2.329709000	-2.514359000

C	-0.981952000	1.780163000	-1.921412000
F	-4.639771000	0.854561000	0.791524000
F	-4.636599000	-0.857124000	-0.794782000
F	4.636563000	0.794297000	-0.857540000
F	4.639817000	-0.792132000	0.854037000
C	-0.448323000	-2.304248000	-2.135007000
H	-0.440305000	-3.112784000	-2.882610000
H	-1.011830000	-2.658236000	-1.256378000
H	-1.010891000	-1.455617000	-2.557148000
C	-0.447262000	2.304536000	2.136193000
H	-1.009721000	1.456181000	2.559059000
H	-0.438749000	3.113430000	2.883402000
H	-1.011145000	2.658149000	1.257677000
C	0.448167000	2.134986000	-2.304560000
H	0.440054000	2.882200000	-3.113454000
H	1.010811000	2.557537000	-1.456177000
H	1.011658000	1.256213000	-2.658189000
C	0.447408000	-2.135099000	2.305293000
H	1.010505000	-1.256552000	2.660189000
H	0.438977000	-2.883111000	3.113447000
H	1.010606000	-2.556630000	1.456807000
C	4.725547000	-2.160269000	-1.998536000
H	5.445488000	-1.559987000	-1.442235000
C	5.167855000	-3.114098000	-2.880734000
H	4.487565000	-3.742608000	-3.462961000
C	4.726502000	2.158836000	1.998719000
H	5.446139000	1.558464000	1.442121000
C	5.169268000	3.112256000	2.881129000
H	4.489271000	3.740736000	3.463732000
C	-4.725697000	1.999486000	-2.159198000
H	-5.445564000	1.442316000	-1.559632000
C	-5.168059000	2.882926000	-3.111847000
H	-4.487775000	3.466137000	-3.739449000
C	-4.726379000	-1.998533000	2.159125000
H	-5.446049000	-1.442384000	1.558374000
C	-5.169090000	-2.880480000	3.112998000
H	-4.489050000	-3.462435000	3.742031000
H	-6.239009000	3.032676000	-3.274727000
H	-6.240102000	-3.030222000	3.275476000
H	6.240291000	3.274887000	3.030634000
H	6.238803000	-3.277018000	-3.030468000
H	2.153375000	-3.311453000	-3.065424000
H	2.154883000	3.310403000	3.066520000
H	-2.153614000	3.066543000	-3.310445000
H	-2.154687000	-3.065254000	3.311543000

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	x(Å)	**y(Å)**	**z(Å)**
C	-4.682027000	-0.000428000	-1.724962000
N	-4.915684000	-0.000151000	-0.325148000
B	-3.791270000	0.000188000	0.751052000
N	-2.412286000	-0.000111000	0.031045000
C	-2.246992000	-0.000411000	-1.374228000
C	-3.369862000	-0.000560000	-2.237548000
C	-1.156790000	0.000012000	0.625496000
C	-0.159470000	-0.000229000	-0.424192000
C	-0.834256000	-0.000504000	-1.671292000
C	-5.966103000	-0.000547000	-2.407176000
C	-6.949798000	-0.000331000	-1.397653000
C	-6.281871000	-0.000086000	-0.110321000
C	-6.175589000	-0.000869000	-3.913222000
C	-6.862729000	0.000202000	1.238604000
C	-0.195572000	-0.000881000	-3.049905000
C	-1.011561000	0.000345000	2.087774000
F	-3.916036000	-1.166455000	1.600742000
F	-3.915931000	1.167446000	1.599905000

C	1.328977000	-0.000125000	-0.271630000
C	2.037340000	1.235172000	-0.224117000
N	3.455906000	1.256622000	-0.130455000
B	4.357599000	0.000075000	-0.071704000
N	3.456050000	-1.256594000	-0.130148000
C	2.037484000	-1.235321000	-0.223799000
C	3.883302000	-2.572386000	-0.096747000
C	2.723011000	-3.427109000	-0.165333000
C	1.569101000	-2.617319000	-0.242890000
C	1.568810000	2.617116000	-0.243575000
C	2.722634000	3.427049000	-0.166213000
C	3.883015000	2.572472000	-0.097375000
C	0.140903000	-3.139510000	-0.311052000
C	5.304199000	-2.938975000	-0.006253000
C	0.140569000	3.139169000	-0.311891000
C	5.303871000	2.939240000	-0.006934000
F	5.298656000	-0.000008000	-1.175368000
F	5.137278000	0.000271000	1.152890000
C	5.757554000	-4.236401000	0.017477000
C	5.757081000	4.236725000	0.016368000
C	-8.214707000	0.000331000	1.489326000
C	0.178308000	0.000334000	2.780171000
H	-3.218011000	-0.000770000	-3.317028000
H	-8.024300000	-0.000349000	-1.549065000
H	-7.250366000	-0.000624000	-4.153460000
H	-5.723560000	0.889657000	-4.385620000
H	-5.724073000	-0.891901000	-4.385161000
H	-6.160173000	0.000310000	2.073002000
H	0.447949000	-0.887328000	-3.189714000
H	-0.952941000	0.000096000	-3.849353000
H	0.449846000	0.884238000	-3.189294000
H	-1.944672000	0.000612000	2.653136000
H	2.735227000	-4.512109000	-0.153768000
H	2.734727000	4.512053000	-0.154917000
H	0.148532000	-4.241269000	-0.301930000
H	-0.463377000	-2.795819000	0.544434000
H	-0.379339000	-2.807335000	-1.224786000
H	6.022132000	-2.119402000	0.043255000
H	0.148118000	4.240931000	-0.303216000
H	-0.379692000	2.806585000	-1.225464000
H	-0.463644000	2.795783000	0.543766000
H	6.021888000	2.119761000	0.042887000
H	5.040738000	5.066174000	-0.034881000
H	-8.924485000	0.000209000	0.652642000
H	1.133532000	0.000038000	2.248701000
C	7.227193000	4.613200000	0.110167000
H	7.866558000	3.717500000	0.157294000
H	7.537643000	5.218216000	-0.763518000
H	7.421746000	5.228950000	1.009445000
C	-8.811137000	0.000703000	2.887192000
H	-9.452925000	0.889171000	3.042714000
H	-9.453483000	-0.887305000	3.042977000
H	-8.024302000	0.000594000	3.657734000
C	0.252224000	0.000735000	4.297865000
H	0.804645000	0.887593000	4.662659000
H	-0.751407000	0.000984000	4.751628000
H	0.804449000	-0.886038000	4.663146000
C	7.227711000	-4.612684000	0.111363000
H	7.422303000	-5.228358000	1.010686000
H	7.538265000	-5.217732000	-0.762263000
H	7.866969000	-3.716907000	0.158451000
H	5.041295000	-5.065947000	-0.033408000

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	X(Å)	Y(Å)	Z(Å)
C	0.753287000	-0.000007000	-0.000105000
C	1.454599000	0.874716000	0.872963000

C	1.454704000	-0.874692000	-0.873141000
N	2.876375000	-0.889274000	-0.887663000
N	2.876264000	0.889394000	0.887577000
B	3.780845000	-0.000034000	0.000109000
C	0.984589000	-1.853217000	-1.849782000
C	2.141343000	-2.425779000	-2.421096000
C	3.304370000	-1.820935000	-1.817438000
C	0.984347000	1.853228000	1.849537000
C	2.141019000	2.425913000	2.420894000
C	3.304132000	1.821130000	1.817335000
C	-0.753286000	-0.000051000	-0.000101000
C	-1.454683000	0.873215000	-0.874566000
N	-2.876352000	0.887833000	-0.889092000
B	-3.780845000	-0.000190000	-0.000130000
N	-2.876287000	-0.887916000	0.889065000
C	-1.454620000	-0.873269000	0.874462000
C	-3.304319000	1.817801000	-1.820574000
C	-2.141271000	2.421634000	-2.425208000
C	-0.984537000	1.850096000	-1.852828000
C	-3.304184000	-1.817815000	1.820647000
C	-2.141090000	-2.421529000	2.425313000
C	-0.984399000	-1.850009000	1.852830000
F	-4.642319000	-0.825789000	-0.824571000
F	-4.642883000	0.825044000	0.824010000
F	4.642376000	-0.824175000	0.825895000
F	4.642825000	0.823944000	-0.825400000
C	-0.445751000	2.223054000	2.218845000
H	-0.437601000	3.002880000	2.996612000
H	-1.009080000	2.609484000	1.353878000
H	-1.008644000	1.358918000	2.607799000
C	-0.445447000	-2.223151000	-2.219218000
H	-1.008377000	-1.359060000	-2.608208000
H	-0.437166000	-3.002964000	-2.996998000
H	-1.008822000	-2.609646000	-1.354312000
C	0.445682000	-2.219346000	2.222692000
H	0.437495000	-2.996693000	3.002936000
H	1.008398000	-2.608877000	1.358696000
H	1.009214000	-1.354274000	2.608573000
C	0.445517000	2.219569000	-2.222660000
H	1.009138000	1.354560000	-2.608542000
H	0.437271000	2.996933000	-3.002887000
H	1.008175000	2.609143000	-1.358642000
C	4.727429000	2.080544000	2.075955000
H	5.446717000	1.500501000	1.496756000
C	5.181354000	2.999027000	2.992572000
H	4.463333000	3.586055000	3.578723000
C	4.727702000	-2.080224000	-2.075983000
H	5.446908000	-1.499915000	-1.496947000
C	5.181755000	-2.998867000	-2.992378000
H	4.463818000	-3.586163000	-3.578362000
C	-4.727488000	-2.076464000	2.079984000
H	-5.446757000	-1.497386000	1.499794000
C	-5.181442000	-2.992972000	2.998563000
H	-4.463439000	-3.578967000	3.585768000
C	-4.727642000	2.076423000	-2.079831000
H	-5.446868000	1.497290000	-1.499644000
C	-5.181670000	2.992994000	-2.998311000
H	-4.463715000	3.579079000	-3.585486000
H	2.153433000	3.194006000	3.187215000
H	2.153866000	-3.193803000	-3.187484000
H	-2.153530000	-3.188025000	3.193231000
H	-2.153770000	3.188235000	-3.193021000
C	-6.654579000	3.258283000	-3.264363000
H	-6.906925000	3.060821000	-4.324029000
H	-7.295490000	2.625470000	-2.630439000
H	-6.907161000	4.318284000	-3.069022000
C	-6.654323000	-3.258305000	3.264711000

H	-7.295303000	-2.625520000	2.630830000
H	-6.906870000	-4.318318000	3.069358000
H	-6.906614000	-3.060887000	4.324394000
C	6.654669000	-3.264957000	-3.257600000
H	7.295575000	-2.630913000	-2.624903000
H	6.907021000	-4.324586000	-3.059944000
H	6.907256000	-3.069811000	-4.317635000
C	6.654233000	3.265234000	3.257876000
H	6.906819000	3.069786000	4.317867000
H	7.295217000	2.631413000	2.625031000
H	6.906478000	4.324937000	3.060544000

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	x(Å)	y(Å)	z(Å)
C	-1.968599000	4.721313000	0.000000000
N	-0.579363000	4.994984000	0.000000000
B	0.534257000	3.905851000	0.000000000
N	-0.148759000	2.505303000	0.000000000
C	-1.542680000	2.296197000	0.000000000
C	-2.441389000	3.394966000	0.000000000
C	0.483299000	1.269009000	0.000000000
C	-0.531237000	0.238733000	0.000000000
C	-1.800241000	0.874085000	0.000000000
C	-2.693268000	5.986608000	0.000000000
C	-1.713921000	6.998401000	0.000000000
C	-0.408830000	6.366179000	0.000000000
C	-4.204117000	6.149270000	0.000000000
C	0.920580000	6.982698000	0.000000000
C	-3.158989000	0.194475000	0.000000000
C	1.946208000	1.177224000	0.000000000
F	1.369866000	4.051485000	1.166652000
F	1.369866000	4.051485000	-1.166652000
C	-0.335822000	-1.244431000	0.000000000
C	-0.269133000	-1.950518000	-1.237289000
N	-0.158875000	-3.363091000	-1.255720000
B	-0.179778000	-4.272869000	0.000000000
N	-0.158875000	-3.363091000	1.255720000
C	-0.269133000	-1.950518000	1.237289000
C	-0.100941000	-3.787535000	2.571001000
C	-0.167391000	-2.629999000	3.429257000
C	-0.272795000	-1.478164000	2.622074000
C	-0.272795000	-1.478164000	-2.622074000
C	-0.167391000	-2.629999000	-3.429257000
C	-0.100941000	-3.787535000	-2.571001000
C	-0.347163000	-0.051328000	3.145780000
C	0.003640000	-5.204524000	2.931951000
C	-0.347163000	-0.051328000	-3.145780000
C	0.003640000	-5.204524000	-2.931951000
F	-1.368543000	-5.093072000	0.000000000
F	0.963862000	-5.152836000	0.000000000
C	0.028767000	-5.638567000	4.241257000
C	0.028767000	-5.638567000	-4.241257000
C	1.107690000	8.349514000	0.000000000
C	2.668859000	0.000583000	0.000000000
H	-3.515568000	3.210716000	0.000000000
H	-1.898844000	8.067549000	0.000000000
H	-4.477616000	7.215322000	0.000000000
H	-4.660579000	5.683192000	-0.891112000
H	-4.660579000	5.683192000	0.891112000
H	1.784479000	6.317828000	0.000000000
H	-3.279809000	-0.453137000	0.885833000
H	-3.981006000	0.926485000	0.000000000
H	-3.279809000	-0.453137000	-0.885833000
H	2.488244000	2.123141000	0.000000000
H	-0.132776000	-2.639947000	4.513686000
H	-0.132776000	-2.639947000	-4.513686000
H	-0.334892000	-0.059975000	4.246607000

H	0.506095000	0.557250000	2.803971000
H	-1.265259000	0.463112000	2.817283000
H	0.065660000	-5.930391000	2.121301000
H	-0.334892000	-0.059975000	-4.246607000
H	-1.265259000	0.463112000	-2.817283000
H	0.506095000	0.557250000	-2.803971000
H	0.065660000	-5.930391000	-2.121301000
H	-0.028977000	-4.943810000	5.082510000
H	-0.028977000	-4.943810000	-5.082510000
H	0.267919000	9.048515000	0.000000000
H	2.199334000	-0.983049000	0.000000000
C	0.130522000	-7.040973000	4.588797000
N	0.211746000	-8.188280000	4.910765000
C	0.130522000	-7.040973000	-4.588797000
N	0.211746000	-8.188280000	-4.910765000
C	4.117821000	0.006241000	0.000000000
N	5.311631000	-0.021262000	0.000000000
C	2.426169000	8.948880000	0.000000000
N	3.498035000	9.475441000	0.000000000

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	x(Å)	y(Å)	z(Å)
C	-0.752903000	0.001138000	-0.000044000
C	-1.452950000	-0.874965000	-0.875043000
C	-1.454353000	0.877512000	0.873583000
N	-2.871051000	0.889887000	0.885635000
N	-2.869648000	-0.888198000	-0.888497000
B	-3.779539000	-0.005179000	0.003871000
C	-0.982160000	1.859104000	1.851273000
C	-2.139587000	2.430312000	2.420307000
C	-3.298911000	1.821994000	1.814292000
C	-0.979137000	-1.853960000	-1.854616000
C	-2.135660000	-2.424532000	-2.426102000
C	-3.295972000	-1.818604000	-1.819561000
C	0.752907000	0.001341000	0.000717000
C	1.454067000	0.877467000	-0.873396000
N	2.870763000	0.890076000	-0.885689000
B	3.779527000	-0.006199000	-0.005437000
N	2.869948000	-0.886923000	0.889518000
C	1.453246000	-0.874036000	0.876207000
C	3.298296000	1.822257000	-1.814423000
C	2.138766000	2.430571000	-2.420048000
C	0.981532000	1.859279000	-1.850701000
C	3.296601000	-1.816739000	1.821008000
C	2.136502000	-2.422586000	2.428044000
C	0.979781000	-1.852694000	1.856272000
F	4.644589000	0.810228000	0.812084000
F	4.614848000	-0.838673000	-0.838250000
F	-4.618670000	-0.835179000	0.835196000
F	-4.640861000	0.812546000	-0.816429000
C	0.450176000	-2.223710000	-2.225143000
H	0.441515000	-2.998735000	-3.006545000
H	1.014237000	-1.359245000	-2.611367000
H	1.011832000	-2.618240000	-1.362783000
C	0.446572000	2.231193000	2.221726000
H	1.006846000	2.628405000	1.359656000
H	0.436685000	3.004899000	3.004423000
H	1.012581000	1.367213000	2.606150000
C	-0.449402000	-2.223218000	2.226526000
H	-0.440469000	-3.000678000	3.005503000
H	-1.012873000	-1.359742000	2.615844000
H	-1.011795000	-2.614851000	1.363337000
C	-0.447332000	2.232141000	-2.219859000
H	-1.006794000	2.629183000	-1.357168000
H	-0.437742000	3.006254000	-3.002157000
H	-1.013993000	1.368585000	-2.604232000
C	-4.716823000	-2.073434000	-2.074449000

H	-5.445427000	-1.497749000	-1.503852000
C	-5.152464000	-3.001736000	-2.997302000
H	-4.456815000	-3.600175000	-3.590326000
C	-4.720182000	2.075952000	2.067753000
H	-5.447858000	1.503395000	1.492839000
C	-5.157324000	3.000686000	2.993470000
H	-4.462637000	3.596043000	3.590711000
C	4.717553000	-2.071311000	2.075695000
H	5.445972000	-1.495379000	1.505110000
C	5.153472000	-2.999100000	2.998928000
H	4.457992000	-3.597352000	3.592337000
C	4.719481000	2.076348000	-2.068229000
H	5.447335000	1.505327000	-1.492016000
C	5.156329000	2.999212000	-2.995948000
H	4.461459000	3.592709000	-3.594825000
H	-2.147212000	-3.190786000	-3.194216000
H	-2.152382000	3.198840000	3.186129000
H	2.148326000	-3.188792000	3.196201000
H	2.151301000	3.199577000	-3.185394000
C	6.563342000	3.242691000	-3.238050000
N	7.714437000	3.468453000	-3.462477000
C	6.560240000	-3.241745000	3.243273000
N	7.711113000	-3.466481000	3.469856000
C	-6.564411000	3.244091000	3.235211000
N	-7.715574000	3.469803000	3.459343000
C	-6.559165000	-3.245060000	-3.241365000
N	-7.709979000	-3.470511000	-3.467544000

Species 5c, 8,2' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-2.293239000	4.788358000	0.000000000
N	-0.915550000	5.109493000	0.000000000
B	0.238935000	4.059216000	0.000000000
N	-0.400003000	2.634266000	0.000000000
C	-1.783718000	2.378423000	0.000000000
C	-2.719685000	3.446878000	0.000000000
C	0.272036000	1.420444000	0.000000000
C	-0.706868000	0.355999000	0.000000000
C	-1.996517000	0.947819000	0.000000000
C	-3.064673000	6.027969000	0.000000000
C	-2.121381000	7.072440000	0.000000000
C	-0.795045000	6.484695000	0.000000000
C	-4.580007000	6.136282000	0.000000000
C	0.511390000	7.148128000	0.000000000
C	-3.332324000	0.224142000	0.000000000
C	1.736214000	1.377451000	0.000000000
F	1.058228000	4.229745000	1.168805000
F	1.058228000	4.229745000	-1.168805000
C	-0.464031000	-1.120445000	0.000000000
C	-0.380120000	-1.824521000	-1.238063000
N	-0.245359000	-3.232995000	-1.256069000
B	-0.313033000	-4.146623000	0.000000000
N	-0.245359000	-3.232995000	1.256069000
C	-0.380120000	-1.824521000	1.238063000
C	-0.167413000	-3.653004000	2.570818000
C	-0.243090000	-2.495679000	3.429728000
C	-0.377583000	-1.347659000	2.623229000
C	-0.377583000	-1.347659000	-2.623229000
C	-0.243090000	-2.495679000	-3.429728000
C	-0.167413000	-3.653004000	-2.570818000
C	-0.470246000	0.078441000	3.145449000
C	-0.040340000	-5.066578000	2.934229000
C	-0.470246000	0.078441000	-3.145449000
C	-0.040340000	-5.066578000	-2.934229000
F	-1.551306000	-4.884080000	0.000000000
F	0.777566000	-5.080825000	0.000000000
C	-0.017215000	-5.477087000	4.242464000

C	-0.017215000	-5.477087000	-4.242464000
C	0.629834000	8.513851000	0.000000000
C	2.480866000	0.225618000	0.000000000
H	-3.786879000	3.225697000	0.000000000
H	-2.341697000	8.134694000	0.000000000
H	-4.891039000	7.191723000	0.000000000
H	-5.019120000	5.654318000	-0.891264000
H	-5.019120000	5.654318000	0.891264000
H	1.414596000	6.536410000	0.000000000
H	-3.431967000	-0.426946000	0.885771000
H	-4.178160000	0.928317000	0.000000000
H	-3.431967000	-0.426946000	-0.885771000
H	2.271151000	2.328595000	0.000000000
H	-0.192889000	-2.504882000	4.513407000
H	-0.192889000	-2.504882000	-4.513407000
H	-0.453257000	0.071005000	4.245970000
H	0.373371000	0.699097000	2.801273000
H	-1.397351000	0.578830000	2.820745000
H	0.041874000	-5.811035000	2.141505000
H	-0.453257000	0.071005000	-4.245970000
H	-1.397351000	0.578830000	-2.820745000
H	0.373371000	0.699097000	-2.801273000
H	0.041874000	-5.811035000	-2.141505000
H	-0.087391000	-4.855858000	5.131616000
H	-0.087391000	-4.855858000	-5.131616000
H	-0.171875000	9.248044000	0.000000000
H	2.136100000	-0.803079000	0.000000000
N	1.953055000	9.149904000	0.000000000
O	1.948900000	10.448117000	0.000000000
O	3.018416000	8.418114000	0.000000000
N	3.950069000	0.306646000	0.000000000
O	4.532461000	1.460996000	0.000000000
O	4.571626000	-0.831977000	0.000000000
N	0.109479000	-6.898606000	4.579124000
O	0.113133000	-7.175251000	5.848455000
O	0.205644000	-7.779169000	3.637254000
N	0.109479000	-6.898606000	-4.579124000
O	0.113133000	-7.175251000	-5.848455000
O	0.205644000	-7.779169000	-3.637254000

Species 5c, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	0.752932000	0.000008000	-0.000002000
C	1.452808000	-0.835958000	-0.914046000
C	1.452793000	0.836142000	0.913908000
N	2.867497000	0.848361000	0.927056000
N	2.867510000	-0.848067000	-0.927285000
B	3.781128000	-0.000553000	0.000531000
C	0.976632000	1.771544000	1.936533000
C	2.132880000	2.315947000	2.531836000
C	3.292613000	1.736244000	1.897886000
C	0.976642000	-1.771090000	-1.936909000
C	2.132891000	-2.315356000	-2.532339000
C	3.292626000	-1.735724000	-1.898326000
C	-0.752945000	-0.000033000	-0.000018000
C	-1.452816000	-0.914123000	0.835922000
N	-2.867516000	-0.927429000	0.847953000
B	-3.781160000	-0.000134000	-0.000052000
N	-2.867497000	0.927228000	-0.848152000
C	-1.452808000	0.913975000	-0.836014000
C	-3.292639000	-1.898407000	1.735702000
C	-2.132909000	-2.532232000	2.315519000
C	-0.976653000	-1.936857000	1.771196000
C	-3.292612000	1.898250000	-1.735798000
C	-2.132860000	2.532170000	-2.315540000
C	-0.976623000	1.936748000	-1.771264000
F	-4.620261000	0.788528000	0.862231000

F	-4.620270000	-0.788693000	-0.862413000
F	4.621575000	0.860933000	-0.787602000
F	4.618971000	-0.863436000	0.789953000
C	-0.452600000	-2.124051000	-2.323011000
H	-0.443949000	-2.866134000	-3.135413000
H	-1.015179000	-2.554037000	-1.478434000
H	-1.015429000	-1.244208000	-2.674837000
C	-0.452605000	2.124598000	2.322571000
H	-1.015324000	1.244865000	2.674866000
H	-0.443942000	2.867051000	3.134634000
H	-1.015302000	2.554136000	1.477854000
C	0.452628000	2.322773000	-2.124266000
H	0.443989000	3.134675000	-2.866896000
H	1.015261000	2.675290000	-1.244564000
H	1.015390000	1.477980000	-2.553578000
C	0.452573000	-2.322863000	2.124334000
H	1.015182000	-1.478147000	2.554006000
H	0.443872000	-3.134975000	2.866732000
H	1.015414000	-2.675066000	1.244650000
C	4.712930000	-1.978658000	-2.164316000
H	5.461797000	-1.443471000	-1.579261000
C	5.127612000	-2.860271000	-3.128829000
H	4.506173000	-3.462164000	-3.787030000
C	4.712918000	1.979309000	2.163757000
H	5.461784000	1.444843000	1.578042000
C	5.127602000	2.860304000	3.128834000
H	4.506164000	3.461380000	3.787781000
C	-4.712908000	2.164367000	-1.978642000
H	-5.461798000	1.579298000	-1.443502000
C	-5.127563000	3.128946000	-2.860196000
H	-4.506106000	3.787139000	-3.462078000
C	-4.712939000	-2.164521000	1.978500000
H	-5.461819000	-1.579688000	1.443086000
C	-5.127638000	-3.128846000	2.860314000
H	-4.506215000	-3.786762000	3.462534000
H	2.145880000	-3.047186000	-3.333095000
H	2.145871000	3.048065000	3.332329000
H	-2.145857000	3.332862000	-3.047439000
H	-2.145893000	-3.332875000	3.047473000
N	-6.557395000	-3.373210000	3.083044000
O	-7.437417000	-2.675200000	2.443082000
O	-6.838116000	-4.308200000	3.939087000
N	-6.557305000	3.373341000	-3.082974000
O	-6.837977000	4.309245000	-3.938034000
O	-7.437360000	2.674650000	-2.443798000
N	6.557352000	3.083377000	3.372919000
O	6.838051000	3.937298000	4.309854000
O	7.437390000	2.445708000	2.672834000
N	6.557362000	-3.083122000	-3.373117000
O	7.437397000	-2.444024000	-2.674332000
O	6.838061000	-3.938575000	-4.308653000

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	x(Å)	y(Å)	z(Å)
C	-0.753726000	0.025345000	0.024877000
C	-1.455112000	0.933094000	-0.816576000
C	-1.453544000	-0.849065000	0.902457000
N	-2.869237000	-0.837039000	0.951506000
N	-2.871042000	0.982135000	-0.797891000
B	-3.773771000	0.071100000	0.076271000
C	-0.967282000	-1.847508000	1.847415000
C	-2.129972000	-2.411576000	2.435279000
C	-3.313440000	-1.780761000	1.870129000
C	-0.972411000	1.912215000	-1.783617000
C	-2.136815000	2.520901000	-2.321110000
C	-3.317903000	1.933578000	-1.706315000
C	0.751687000	-0.013069000	-0.017023000

C	1.498593000	0.844139000	0.838173000
N	2.915049000	0.832170000	0.807921000
B	3.771436000	-0.087708000	-0.101913000
N	2.820910000	-0.965321000	-0.959750000
C	1.406017000	-0.905979000	-0.910748000
C	3.410285000	1.741761000	1.733583000
C	2.261281000	2.363070000	2.374507000
C	1.066913000	1.819324000	1.832494000
C	3.216902000	-1.900511000	-1.907525000
C	2.003653000	-2.464536000	-2.480203000
C	0.870558000	-1.859943000	-1.875326000
F	4.629618000	-0.927283000	0.706322000
F	4.619121000	0.712341000	-0.960723000
F	-4.631046000	-0.734557000	-0.761484000
F	-4.623467000	0.886287000	0.924431000
C	0.468531000	2.237904000	-2.143575000
H	0.497392000	2.986830000	-2.946936000
H	1.020988000	2.644808000	-1.281183000
H	1.014687000	1.346497000	-2.489258000
C	0.475095000	-2.213513000	2.159698000
H	1.049871000	-1.342364000	2.511414000
H	0.509130000	-2.981757000	2.944357000
H	0.995088000	-2.610977000	1.273359000
C	-0.588276000	-2.165991000	-2.175479000
H	-0.660864000	-2.907971000	-2.982559000
H	-1.108753000	-2.572641000	-1.293496000
H	-1.137645000	-1.265453000	-2.491549000
C	-0.355258000	2.196981000	2.215662000
H	-0.928584000	1.324306000	2.565802000
H	-0.343331000	2.941664000	3.023392000
H	-0.906011000	2.629137000	1.364643000
I	1.865353000	-4.011330000	-3.934153000
I	-2.077545000	4.101164000	-3.743950000
I	-2.063248000	-3.899878000	3.953943000
I	2.285080000	3.911404000	3.832720000
C	-4.760076000	2.175395000	-1.863383000
H	-5.384618000	1.728451000	-1.089447000
C	-5.385587000	2.871859000	-2.871720000
H	-4.811474000	3.313914000	-3.688770000
C	-4.755834000	-1.951809000	2.100518000
H	-5.383195000	-1.185953000	1.644082000
C	-5.381463000	-2.958848000	2.798918000
H	-4.807250000	-3.767264000	3.256025000
C	4.648219000	-2.152340000	-2.133081000
H	5.310853000	-1.726992000	-1.378833000
C	5.221111000	-2.833812000	-3.182062000
H	4.606255000	-3.253068000	-3.981263000
C	4.862968000	1.923059000	1.877255000
H	5.458561000	1.488854000	1.073487000
C	5.528368000	2.547696000	2.906655000
H	4.982701000	2.970359000	3.753165000
C	-6.894448000	3.047742000	-2.928162000
H	-7.303498000	2.620130000	-3.863377000
H	-7.390328000	2.559708000	-2.074551000
H	-7.163921000	4.121407000	-2.925357000
C	-6.891700000	-3.023110000	2.959262000
H	-7.172469000	-3.014915000	4.030001000
H	-7.387538000	-2.175703000	2.460533000
H	-7.290754000	-3.963599000	2.533671000
C	6.723884000	-3.023436000	-3.309884000
H	7.262823000	-2.557891000	-2.469943000
H	6.981444000	-4.099580000	-3.340567000
H	7.095108000	-2.580989000	-4.253944000
C	7.043401000	2.665248000	2.947566000
H	7.508600000	2.201683000	2.063588000
H	7.352671000	3.727165000	2.992313000
H	7.449250000	2.177481000	3.854283000

Species 5I, 8,8' Dimer , Electronic state S_0

	x (Å)	y(Å)	z(Å)
C	-0.125336000	-0.828480000	-0.217516000
C	-1.330820000	-1.019865000	-0.948533000
C	0.374046000	-1.837361000	0.652736000
N	-0.318106000	-3.063090000	0.800929000
N	-2.065729000	-2.222568000	-0.817479000
B	-1.643983000	-3.421622000	0.075425000
C	1.563208000	-1.872957000	1.496735000
C	1.545269000	-3.146204000	2.124677000
C	0.370172000	-3.882931000	1.686178000
C	-2.029396000	-0.151142000	-1.889282000
C	-3.181845000	-0.876039000	-2.291643000
C	-3.196840000	-2.167388000	-1.622042000
C	0.637199000	0.461632000	-0.368504000
C	0.286613000	1.580314000	0.437680000
N	0.984433000	2.804950000	0.307315000
B	2.155603000	3.052114000	-0.682835000
N	2.435652000	1.739288000	-1.464284000
C	1.697329000	0.540698000	-1.314232000
C	0.453100000	3.740062000	1.186296000
C	-0.622366000	3.081464000	1.911291000
C	-0.739610000	1.739732000	1.462049000
C	3.408725000	1.568002000	-2.440159000
C	3.287425000	0.203665000	-2.929615000
C	2.228494000	-0.449129000	-2.245128000
F	3.340093000	3.456057000	0.045392000
F	1.814016000	4.111821000	-1.601758000
F	-1.462841000	-4.604114000	-0.734573000
F	-2.678177000	-3.701648000	1.048035000
C	-1.630026000	1.240838000	-2.352250000
H	-2.274964000	1.561926000	-3.181801000
H	-1.731230000	1.982376000	-1.542247000
H	-0.586534000	1.274983000	-2.698838000
C	2.612557000	-0.788948000	1.683936000
H	2.159562000	0.184654000	1.923201000
H	3.290752000	-1.059753000	2.504778000
H	3.222442000	-0.652901000	0.775241000
C	1.766695000	-1.882666000	-2.453259000
H	2.271295000	-2.317987000	-3.326845000
H	1.999396000	-2.515987000	-1.581027000
H	0.681055000	-1.943583000	-2.621615000
C	-1.736011000	0.705007000	1.959858000
H	-1.246965000	-0.243276000	2.227549000
H	-2.257527000	1.082659000	2.850116000
H	-2.498613000	0.477148000	1.196206000
I	4.495693000	-0.757443000	-4.389726000
I	-4.623842000	-0.104232000	-3.648569000
I	3.034030000	-3.782793000	3.501278000
I	-1.851163000	3.906924000	3.435873000
C	-4.123936000	-3.313091000	-1.652660000
H	-3.860573000	-4.127673000	-0.979412000
C	-5.250919000	-3.456881000	-2.424589000
H	-5.605919000	-2.712579000	-3.135399000
C	-0.162688000	-5.220133000	2.003840000
H	-1.134819000	-5.437238000	1.563323000
C	0.428653000	-6.194283000	2.770492000
H	1.401437000	-6.090693000	3.248284000
C	4.314670000	2.683129000	-2.770695000
H	4.232330000	3.546212000	-2.111210000
C	5.218688000	2.743531000	-3.802881000
H	5.370979000	1.947227000	-4.529659000
C	1.022051000	5.099197000	1.235121000
H	1.912311000	5.240306000	0.623684000
C	0.551964000	6.175897000	1.946578000
H	-0.334578000	6.152584000	2.578173000

H	5.824078000	3.647346000	-3.923825000
H	1.086302000	7.128694000	1.877985000
H	-0.095251000	-7.144485000	2.914257000
H	-5.838863000	-4.375714000	-2.334428000

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	x(Å)	y(Å)	z(Å)
C	4.669219000	-0.126668000	0.713014000
N	4.707602000	0.119778000	-0.681612000
B	3.445452000	0.283794000	-1.581891000
N	2.184894000	0.121050000	-0.678405000
C	2.223665000	-0.126127000	0.711758000
C	3.449915000	-0.249253000	1.405419000
C	0.867270000	0.192814000	-1.083051000
C	0.014503000	-0.010260000	0.054022000
C	0.860983000	-0.211965000	1.187364000
C	6.040918000	-0.212374000	1.189932000
C	6.877393000	-0.012973000	0.056863000
C	6.024912000	0.189271000	-1.084616000
F	3.441997000	-0.716994000	-2.620044000
F	3.443645000	1.586760000	-2.201197000
C	-1.480072000	-0.008122000	0.046430000
C	-2.187077000	1.222691000	0.190899000
N	-3.604410000	1.241779000	0.162921000
B	-4.536906000	0.004356000	-0.020199000
N	-3.607663000	-1.242847000	-0.144473000
C	-2.190132000	-1.234496000	-0.118178000
C	-4.030559000	-2.543733000	-0.316510000
C	-2.880583000	-3.408222000	-0.403557000
C	-1.722021000	-2.609119000	-0.282020000
C	-1.715398000	2.591755000	0.387672000
C	-2.871871000	3.399068000	0.469294000
C	-4.023944000	2.544820000	0.327072000
C	-0.295143000	-3.137736000	-0.313300000
C	-0.287402000	3.105996000	0.503378000
F	-5.399971000	-0.134705000	1.116071000
F	-5.321177000	0.152496000	-1.212739000
H	3.450641000	-0.440269000	2.478594000
H	7.961395000	-0.011551000	0.042170000
H	-2.922523000	-4.483537000	-0.538951000
H	-2.910993000	4.473137000	0.615054000
H	-0.307769000	-4.223349000	-0.498631000
H	0.307016000	-2.664939000	-1.106138000
H	0.225769000	-2.961862000	0.642598000
H	-0.300366000	4.191136000	0.691157000
H	0.256404000	2.622032000	1.330982000
H	0.294095000	2.930553000	-0.416891000
C	6.433435000	0.439370000	-2.520249000
H	6.009194000	1.389373000	-2.883723000
H	7.529099000	0.474785000	-2.604003000
H	6.044510000	-0.356350000	-3.176659000
C	0.462042000	0.442365000	-2.519455000
H	0.826111000	-0.369792000	-3.170396000
H	-0.631522000	0.509997000	-2.604547000
H	0.916386000	1.373696000	-2.894185000
C	6.417292000	-0.454787000	2.556950000
C	6.693188000	-0.668298000	3.759917000
H	6.950986000	-0.849671000	4.782845000
C	0.478629000	-0.456940000	2.549946000
C	0.162130000	-0.672479000	3.742514000
H	-0.133770000	-0.854625000	4.755149000
C	-5.410091000	-2.928659000	-0.394489000
C	-6.601857000	-3.294545000	-0.466822000
H	-7.631541000	-3.580355000	-0.526310000
C	-5.402392000	2.940938000	0.345779000
C	-6.593155000	3.316580000	0.365142000
H	-7.622041000	3.611043000	0.377791000

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	x(Å)	y(Å)	z(Å)
C	0.752641000	-0.000037000	-0.000077000
C	1.453383000	-0.876764000	-0.874106000
C	1.453270000	0.876742000	0.873983000
N	2.871434000	0.886557000	0.883692000
N	2.871555000	-0.886443000	-0.883755000
B	3.803673000	0.000055000	0.000036000
C	0.980148000	1.856649000	1.850945000
C	2.138092000	2.430072000	2.422533000
C	3.290924000	1.817085000	1.811356000
C	0.980406000	-1.856678000	-1.851145000
C	2.138434000	-2.430013000	-2.422647000
C	3.291176000	-1.816979000	-1.811353000
C	-0.752640000	-0.000065000	-0.000097000
C	-1.453310000	-0.874627000	0.876149000
N	-2.871476000	-0.884428000	0.885797000
B	-3.803672000	-0.000077000	-0.000059000
N	-2.871511000	0.884350000	-0.885876000
C	-1.453341000	0.874560000	-0.876262000
C	-3.291018000	-1.812642000	1.815752000
C	-2.138221000	-2.424100000	2.428524000
C	-0.980244000	-1.852103000	1.855577000
C	-3.291080000	1.812648000	-1.815741000
C	-2.138302000	2.424149000	-2.428500000
C	-0.980307000	1.852099000	-1.855643000
F	-4.625620000	0.831090000	0.829777000
F	-4.625462000	-0.831383000	-0.829977000
F	4.625612000	0.829287000	-0.831777000
F	4.625473000	-0.829178000	0.831981000
C	-0.449159000	-2.227748000	-2.221329000
H	-0.439280000	-3.006788000	-2.999072000
H	-1.012143000	-2.616995000	-1.357464000
H	-1.012405000	-1.364654000	-2.611901000
C	-0.449483000	2.227605000	2.220990000
H	-1.012690000	1.364467000	2.611526000
H	-0.439744000	3.006663000	2.998718000
H	-1.012419000	2.616784000	1.357062000
C	0.449282000	2.222286000	-2.226620000
H	0.439453000	2.998387000	-3.007296000
H	1.011706000	2.615063000	-1.363966000
H	1.013055000	1.357952000	-2.613624000
C	0.449361000	-2.222250000	2.226530000
H	1.013169000	-1.357876000	2.613390000
H	0.439567000	-2.998256000	3.007302000
H	1.011731000	-2.615145000	1.363891000
H	2.177710000	-3.197606000	-3.187902000
H	2.177255000	3.197678000	3.187782000
H	-2.177532000	3.189857000	-3.195644000
H	-2.177428000	-3.189736000	3.195741000
C	4.669804000	2.095776000	2.089119000
C	5.862602000	2.357402000	2.349773000
C	4.670100000	-2.095615000	-2.088958000
C	5.862999000	-2.357201000	-2.349187000
H	6.892954000	-2.564048000	-2.554959000
H	6.892496000	2.564243000	2.555855000
C	-4.669989000	2.090651000	-2.094053000
C	-5.862895000	2.351474000	-2.355010000
C	-4.669914000	-2.090590000	2.094183000
C	-5.862724000	-2.351522000	2.355475000
H	-6.892629000	-2.557807000	2.562057000
H	-6.892838000	2.557749000	-2.561419000

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	x(Å)	y(Å)	z(Å)
C	4.572991000	-4.385313000	0.340103000

N	5.090939000	-3.089953000	0.561844000
B	4.230951000	-1.794766000	0.609666000
N	2.742457000	-2.178973000	0.352834000
C	2.289883000	-3.495373000	0.137159000
C	3.193989000	-4.584295000	0.131156000
C	1.649675000	-1.318938000	0.304851000
C	0.463188000	-2.100593000	0.051588000
C	0.851013000	-3.471175000	-0.055483000
C	5.676442000	-5.339104000	0.375960000
C	6.845689000	-4.575720000	0.622295000
C	6.464093000	-3.191844000	0.733536000
C	7.310983000	-2.012627000	0.983694000
C	1.828772000	0.129983000	0.500387000
F	4.686647000	-0.859679000	-0.393257000
F	4.364544000	-1.159471000	1.900859000
C	-0.933254000	-1.579751000	-0.077264000
C	-1.769112000	-1.493946000	1.078090000
N	-3.118823000	-1.076198000	0.957081000
B	-3.825232000	-0.716627000	-0.368433000
N	-2.788042000	-0.799458000	-1.509815000
C	-1.441638000	-1.219192000	-1.362960000
C	-3.032141000	-0.520958000	-2.846455000
C	-1.830793000	-0.754451000	-3.588732000
C	-0.820197000	-1.189458000	-2.692194000
C	-1.516928000	-1.774260000	2.496377000
C	-2.737434000	-1.512670000	3.171508000
C	-3.710147000	-1.086913000	2.211526000
C	-4.347240000	-0.062796000	-3.330031000
C	-5.117701000	-0.704181000	2.424835000
F	-4.919937000	-1.635175000	-0.618525000
F	-4.392775000	0.614539000	-0.294881000
C	-4.618879000	0.196323000	-4.649553000
C	-5.725461000	-0.714679000	3.654716000
C	8.669134000	-2.080497000	1.167207000
C	0.836628000	1.078590000	0.467735000
H	2.818382000	-5.592109000	-0.038313000
H	7.858519000	-4.951548000	0.711915000
H	6.805481000	-1.047414000	1.018619000
H	2.853877000	0.451092000	0.685771000
H	-1.717661000	-0.599650000	-4.655158000
H	-2.909294000	-1.594330000	4.238186000
H	-5.125915000	0.070967000	-2.579442000
H	-5.681689000	-0.398501000	1.543878000
H	-3.873515000	0.077937000	-5.441572000
H	-5.204477000	-1.010715000	4.570046000
H	9.223791000	-3.023156000	1.142201000
H	-0.214925000	0.854979000	0.288340000
H	-5.612178000	0.536404000	-4.955345000
H	-6.773197000	-0.419262000	3.758580000
H	9.250449000	-1.172429000	1.349042000
H	1.093082000	2.130088000	0.627759000
C	-0.256634000	-2.219126000	3.134559000
H	0.640035000	-2.243549000	2.521559000
C	-0.144950000	-2.584298000	4.451317000
H	-0.996815000	-2.598689000	5.137255000
H	0.823251000	-2.881644000	4.864029000
C	5.527419000	-6.795197000	0.183823000
H	4.512435000	-7.161796000	-0.001333000
C	6.551324000	-7.705911000	0.219994000
H	7.589059000	-7.411072000	0.400754000
H	6.361257000	-8.772152000	0.067735000
C	0.059495000	-4.690977000	-0.304736000
H	0.637805000	-5.620726000	-0.333512000
C	-1.294202000	-4.791054000	-0.500093000
H	-1.969614000	-3.936361000	-0.492834000
H	-1.748436000	-5.771117000	-0.675042000
C	0.576786000	-1.517021000	-3.058580000

H	1.275261000	-1.723130000	-2.252364000
C	1.048750000	-1.559952000	-4.345053000
H	0.414530000	-1.372817000	-5.216257000
H	2.099693000	-1.789060000	-4.542961000

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	x(Å)	y(Å)	z(Å)
C	0.753242000	-0.000061000	0.000008000
C	1.454521000	0.876946000	0.875825000
C	1.454321000	-0.877298000	-0.875997000
N	2.872083000	-0.886786000	-0.884755000
N	2.872364000	0.886253000	0.884505000
B	3.776543000	-0.000408000	-0.000211000
C	0.994696000	-1.863736000	-1.860714000
C	2.167951000	-2.428802000	-2.423978000
C	3.310458000	-1.818563000	-1.814422000
C	0.995182000	1.863619000	1.860688000
C	2.168525000	2.428497000	2.423646000
C	3.310910000	1.817994000	1.813888000
C	-0.753213000	-0.000053000	0.000016000
C	-1.454378000	0.877512000	-0.875479000
N	-2.872189000	0.887119000	-0.883996000
B	-3.776507000	-0.000145000	-0.000157000
N	-2.872237000	-0.887251000	0.883908000
C	-1.454409000	-0.877665000	0.875418000
C	-3.310636000	1.819579000	-1.812841000
C	-2.168191000	2.430098000	-2.422327000
C	-0.994896000	1.864609000	-1.859704000
C	-3.310709000	-1.819497000	1.812953000
C	-2.168283000	-2.429970000	2.422523000
C	-0.994971000	-1.864543000	1.859904000
F	-4.636320000	-0.823599000	-0.826671000
F	-4.636439000	0.823308000	0.826365000
F	4.636327000	-0.824548000	0.825695000
F	4.636423000	0.823734000	-0.825991000
H	2.207116000	3.194342000	3.189030000
H	2.206187000	-3.194646000	-3.189385000
H	-2.206732000	-3.196317000	3.187415000
H	-2.206598000	3.196162000	-3.187503000
C	0.397258000	-2.221139000	2.217087000
H	1.203790000	-1.701819000	1.707515000
C	0.738288000	-3.164860000	3.150762000
H	-0.002796000	-3.738962000	3.714165000
H	1.789705000	-3.376283000	3.364064000
C	0.397338000	2.221280000	-2.216790000
H	1.203854000	1.699249000	-1.709966000
C	0.738401000	3.168032000	-3.147379000
H	-0.002645000	3.745237000	-3.707651000
H	1.789824000	3.379043000	-3.361063000
C	-4.741192000	2.071303000	-2.062891000
H	-5.451914000	1.486179000	-1.479703000
C	-5.197922000	2.987906000	-2.975776000
H	-4.527461000	3.600226000	-3.585920000
H	-6.271094000	3.136586000	-3.123540000
C	-4.741276000	-2.071272000	2.062897000
H	-5.451970000	-1.486182000	1.479643000
C	-5.198026000	-2.987891000	2.975759000
H	-4.527565000	-3.600067000	3.586048000
H	-6.271196000	-3.136699000	3.123393000
C	4.741001000	-2.069901000	-2.064907000
H	5.451749000	-1.485238000	-1.481282000
C	5.197728000	-2.985757000	-2.978543000
H	4.527261000	-3.597611000	-3.589149000
H	6.270900000	-3.134316000	-3.126431000
C	4.741466000	2.069342000	2.064298000
H	5.452190000	1.484537000	1.480797000
C	5.198191000	2.985357000	2.977781000

H	4.527729000	3.597337000	3.588263000
H	6.271360000	3.133912000	3.125677000
C	-0.397044000	2.220327000	2.217788000
H	-1.203574000	1.699371000	1.709895000
C	-0.738013000	3.166024000	3.149483000
H	0.003135000	3.742004000	3.710885000
H	-1.789402000	3.377323000	3.363031000
C	-0.397569000	-2.220295000	-2.217780000
H	-1.204051000	-1.699759000	-1.709349000
C	-0.738757000	-3.165291000	-3.150114000
H	0.002210000	-3.740786000	-3.712240000
H	-1.790215000	-3.376424000	-3.363508000

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	x(Å)	y(Å)	z(Å)
C	4.586656000	-4.381635000	0.343919000
N	5.074119000	-3.074336000	0.558120000
B	4.203904000	-1.773025000	0.590444000
N	2.721230000	-2.218032000	0.339370000
C	2.284497000	-3.539429000	0.129521000
C	3.210907000	-4.610911000	0.131822000
C	1.614977000	-1.389534000	0.285583000
C	0.435121000	-2.173263000	0.037187000
C	0.842422000	-3.538521000	-0.064254000
C	5.707131000	-5.316259000	0.390247000
C	6.863244000	-4.529235000	0.636252000
C	6.444492000	-3.156389000	0.734567000
F	4.622892000	-0.875198000	-0.442208000
F	4.310993000	-1.142502000	1.870891000
C	-0.946837000	-1.617672000	-0.084389000
C	-1.772383000	-1.506524000	1.077541000
N	-3.104101000	-1.044058000	0.958739000
B	-3.825327000	-0.635020000	-0.357762000
N	-2.773446000	-0.758259000	-1.497473000
C	-1.443342000	-1.221471000	-1.365222000
C	-3.006042000	-0.461757000	-2.827964000
C	-1.821619000	-0.723304000	-3.587031000
C	-0.822353000	-1.200318000	-2.696290000
C	-1.521681000	-1.805049000	2.493699000
C	-2.732255000	-1.508940000	3.176491000
C	-3.684608000	-1.046731000	2.213740000
F	-4.924607000	-1.528218000	-0.609518000
F	-4.305916000	0.710817000	-0.266224000
H	2.856715000	-5.627550000	-0.032250000
H	7.889518000	-4.863183000	0.737163000
H	-1.728607000	-0.553195000	-4.653054000
H	-2.925103000	-1.583844000	4.240065000
C	-0.275118000	-2.290729000	3.128151000
H	0.624558000	-2.325852000	2.519974000
C	-0.179722000	-2.679051000	4.439888000
H	-1.035964000	-2.684467000	5.120195000
H	0.779321000	-3.003652000	4.853357000
C	5.590656000	-6.776467000	0.209334000
H	4.585670000	-7.168670000	0.022866000
C	6.636700000	-7.661266000	0.258002000
H	7.666031000	-7.339967000	0.440827000
H	6.472735000	-8.732930000	0.114027000
C	0.062008000	-4.765430000	-0.308797000
H	0.643739000	-5.693124000	-0.334848000
C	-1.291952000	-4.864540000	-0.503077000
H	-1.964748000	-4.006842000	-0.496973000
H	-1.749840000	-5.843050000	-0.675547000
C	0.561562000	-1.566683000	-3.073925000
H	1.267068000	-1.775991000	-2.274573000
C	1.013833000	-1.638717000	-4.366494000
H	0.370279000	-1.452124000	-5.230740000
H	2.057128000	-1.891593000	-4.575352000

C	-5.038336000	-0.640582000	2.461600000
C	-6.211072000	-0.296269000	2.715747000
H	-7.220227000	0.006971000	2.903296000
C	-4.260567000	0.028563000	-3.322775000
C	-5.337262000	0.454540000	-3.789376000
H	-6.272140000	0.820733000	-4.160097000
C	7.275492000	-2.012455000	0.976225000
C	8.014064000	-1.028226000	1.187064000
H	8.627259000	-0.169209000	1.366790000
C	1.679784000	0.029297000	0.455946000
C	1.709467000	1.268648000	0.601000000
H	1.744272000	2.331473000	0.726399000

Species 8, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	0.752451000	-0.000078000	-0.000037000
C	1.454345000	0.878519000	0.875982000
C	1.454485000	-0.878610000	-0.875997000
N	2.869589000	-0.883502000	-0.880189000
N	2.869458000	0.883472000	0.880261000
B	3.800090000	0.000047000	0.000040000
C	0.992402000	-1.866149000	-1.860311000
C	2.167246000	-2.432771000	-2.424176000
C	3.301074000	-1.814924000	-1.808038000
C	0.992137000	1.865971000	1.860279000
C	2.166910000	2.432683000	2.424225000
C	3.300816000	1.814970000	1.808124000
C	-0.752447000	-0.000102000	-0.000087000
C	-1.454396000	0.877346000	-0.877210000
N	-2.869498000	0.882271000	-0.881466000
B	-3.800097000	-0.000018000	-0.000059000
N	-2.869533000	-0.882301000	0.881389000
C	-1.454429000	-0.877445000	0.877115000
C	-3.300913000	1.812543000	-1.810513000
C	-2.167040000	2.429489000	-2.427461000
C	-0.992239000	1.863538000	-1.862829000
C	-3.300976000	-1.812439000	1.810564000
C	-2.167121000	-2.429370000	2.427556000
C	-0.992303000	-1.863522000	1.862853000
F	-4.624359000	-0.830064000	-0.830990000
F	-4.624551000	0.829931000	0.830715000
F	4.624528000	-0.828779000	0.832007000
F	4.624429000	0.828959000	-0.831939000
H	2.229162000	3.198403000	3.188136000
H	2.229601000	-3.198497000	-3.188071000
H	-2.229438000	-3.194118000	3.192434000
H	-2.229336000	3.194180000	-3.192397000
C	0.398458000	-2.221514000	2.221792000
H	1.207934000	-1.705160000	1.713693000
C	0.733974000	-3.165565000	3.157730000
H	-0.010341000	-3.736571000	3.719686000
H	1.784354000	-3.379337000	3.373464000
C	0.398534000	2.221571000	-2.221682000
H	1.207996000	1.704857000	-1.713932000
C	0.734071000	3.165984000	-3.157248000
H	-0.010231000	3.737455000	-3.718751000
H	1.784455000	3.379693000	-3.373025000
C	-0.398653000	2.224436000	2.218627000
H	-1.208089000	1.706855000	1.711710000
C	-0.734247000	3.170315000	3.152691000
H	0.010017000	3.742745000	3.713264000
H	-1.784644000	3.384280000	3.368146000
C	-0.398342000	-2.224748000	-2.218719000
H	-1.207841000	-1.707106000	-1.711970000
C	-0.733803000	-3.170805000	-3.152645000
H	0.010547000	-3.743310000	-3.713031000
H	-1.784168000	-3.384855000	-3.368175000

C	-4.684828000	2.079735000	-2.077005000
C	-5.879098000	2.336791000	-2.333764000
C	-4.684899000	-2.079593000	2.077057000
C	-5.879272000	-2.336762000	2.333216000
H	-6.911403000	-2.537838000	2.533669000
H	-6.911224000	2.537773000	-2.534336000
C	4.685010000	-2.082399000	-2.074149000
C	5.879300000	-2.339881000	-2.330386000
C	4.684714000	2.082580000	2.074287000
C	5.879008000	2.340179000	2.330393000
H	6.911461000	-2.541051000	-2.530589000
H	6.911109000	2.541589000	2.530664000

Species 9, 8,2' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	5.078839000	-3.665084000	-0.064010000
N	5.512934000	-2.316471000	-0.046010000
B	4.558972000	-1.088689000	-0.009669000
N	3.090487000	-1.599020000	-0.024616000
C	2.721597000	-2.962672000	-0.041185000
C	3.705168000	-3.982082000	-0.060247000
C	1.934341000	-0.825599000	-0.011394000
C	0.793092000	-1.720408000	-0.019454000
C	1.279087000	-3.050815000	-0.037611000
C	6.249488000	-4.528993000	-0.086226000
C	7.369986000	-3.675560000	-0.080958000
C	6.898495000	-2.303046000	-0.055377000
C	6.233976000	-6.049213000	-0.110923000
C	7.671713000	-1.065021000	-0.039550000
C	0.448197000	-4.323302000	-0.051290000
C	1.997569000	0.633425000	0.005333000
F	4.805734000	-0.231075000	-1.150677000
F	4.805104000	-0.302683000	1.181896000
C	-0.656669000	-1.352547000	-0.012649000
C	-1.349240000	-1.212069000	1.225359000
N	-2.737755000	-0.918333000	1.250499000
B	-3.622736000	-0.709234000	-0.000484000
N	-2.743623000	-0.897327000	-1.258909000
C	-1.354881000	-1.190681000	-1.245009000
C	-3.166123000	-0.788941000	-2.574725000
C	-2.027841000	-1.011980000	-3.434616000
C	-0.895948000	-1.259898000	-2.630246000
C	-0.884044000	-1.305084000	2.607082000
C	-2.012097000	-1.069945000	3.420689000
C	-3.154170000	-0.831858000	2.569875000
C	0.508431000	-1.517596000	-3.157361000
C	-4.550698000	-0.494142000	-2.935265000
C	0.522640000	-1.572509000	3.123037000
C	-4.537004000	-0.542566000	2.941386000
F	-4.727997000	-1.648454000	-0.005703000
F	-4.201203000	0.623188000	0.012023000
C	-4.998875000	-0.379243000	-4.239227000
C	-4.979426000	-0.448153000	4.248946000
C	9.055055000	-1.020738000	-0.046771000
C	0.910978000	1.492861000	0.026027000
H	3.396430000	-5.027249000	-0.073337000
H	8.410380000	-3.983763000	-0.093810000
H	7.261377000	-6.445385000	-0.121663000
H	5.720841000	-6.463444000	0.775373000
H	5.713493000	-6.434332000	-1.006056000
H	7.108639000	-0.130383000	-0.021123000
H	-0.217980000	-4.354691000	-0.931339000
H	1.082386000	-5.223311000	-0.072089000
H	-0.201228000	-4.384373000	0.839747000
H	2.999635000	1.065765000	-0.000664000
H	-2.039746000	-0.986555000	-4.519377000
H	-2.019067000	-1.062628000	4.505765000

H	0.500399000	-1.494839000	-4.258798000
H	1.223495000	-0.755455000	-2.806560000
H	0.900016000	-2.497352000	-2.837340000
H	-5.258250000	-0.360433000	-2.115548000
H	0.519219000	-1.572221000	4.224726000
H	0.913644000	-2.545181000	2.781465000
H	1.235843000	-0.802866000	2.785029000
H	-5.248222000	-0.395797000	2.127081000
H	-4.305816000	-0.510376000	-5.078314000
H	-4.282823000	-0.592567000	5.082901000
H	9.639904000	-1.947684000	-0.065680000
H	-0.112219000	1.111219000	0.033008000
C	-6.375918000	-0.154414000	4.598458000
H	-7.073383000	-0.008664000	3.765153000
C	-6.828083000	-0.057728000	5.894448000
H	-6.154645000	-0.197878000	6.747063000
H	-7.875241000	0.163027000	6.120497000
C	-6.396868000	-0.080490000	-4.578220000
H	-7.090883000	0.052187000	-3.739865000
C	-6.854533000	0.036028000	-5.870654000
H	-6.184681000	-0.090684000	-6.728190000
H	-7.902688000	0.259903000	-6.088868000
C	9.812917000	0.237399000	-0.029978000
H	9.230501000	1.165940000	-0.010848000
C	11.187862000	0.290868000	-0.037105000
H	11.795731000	-0.620272000	-0.056141000
H	11.723717000	1.244206000	-0.023962000
C	1.064639000	2.953778000	0.040391000
H	2.088256000	3.346888000	0.034305000
C	-0.006255000	3.817533000	0.060361000
H	-1.037504000	3.448953000	0.066494000
H	0.134791000	4.902285000	0.070506000

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	x(Å)	y(Å)	z(Å)
C	0.753008000	-0.000002000	-0.000060000
C	1.456381000	-0.871238000	0.876281000
C	1.456448000	0.871191000	-0.876390000
N	2.875711000	0.884811000	-0.890121000
N	2.875645000	-0.884927000	0.890049000
B	3.780754000	0.000033000	0.000089000
C	0.985725000	1.846916000	-1.857843000
C	2.141251000	2.416899000	-2.431269000
C	3.305553000	1.814136000	-1.824885000
C	0.985584000	-1.846973000	1.857691000
C	2.141068000	-2.417021000	2.431136000
C	3.305416000	-1.814292000	1.824806000
C	-0.753008000	0.000040000	-0.000070000
C	-1.456395000	0.876383000	0.871151000
N	-2.875659000	0.890151000	0.884819000
B	-3.780754000	-0.000119000	0.000155000
N	-2.875697000	-0.890005000	-0.884933000
C	-1.456434000	-0.876275000	-0.871290000
C	-3.305445000	1.824943000	1.814142000
C	-2.141107000	2.431304000	2.416859000
C	-0.985614000	1.857819000	1.846868000
C	-3.305524000	-1.824721000	-1.814314000
C	-2.141212000	-2.431054000	-2.417109000
C	-0.985695000	-1.857686000	-1.847049000
F	-4.643871000	0.821613000	-0.826385000
F	-4.643102000	-0.822230000	0.827114000
F	4.643693000	-0.826629000	-0.821706000
F	4.643280000	0.826879000	0.822129000
C	-0.444873000	-2.214764000	2.227664000
H	-0.437475000	-2.991254000	3.008678000
H	-1.007694000	-1.349001000	2.612970000
H	-1.007724000	-2.605072000	1.364167000

C	-0.444705000	2.214756000	-2.227872000
H	-1.007559000	2.605126000	-1.364403000
H	-0.437249000	2.991216000	-3.008915000
H	-1.007555000	1.349003000	-2.613158000
C	0.444741000	-2.227692000	-2.214889000
H	0.437298000	-3.008690000	-2.991394000
H	1.007601000	-1.364200000	-2.605200000
H	1.007577000	-2.613029000	-1.349150000
C	0.444837000	2.227799000	2.214676000
H	1.007646000	2.613168000	1.348933000
H	0.437426000	3.008768000	2.991211000
H	1.007708000	1.364291000	2.604931000
C	4.718924000	-2.073208000	2.085203000
H	5.443526000	-1.498145000	1.506844000
C	5.173863000	-2.994668000	3.011915000
H	4.463991000	-3.583601000	3.604204000
C	4.719082000	2.072993000	-2.085234000
H	5.443640000	1.497807000	-1.506941000
C	5.174092000	2.994522000	-3.011842000
H	4.464265000	3.583576000	-3.604066000
C	6.601237000	-3.239617000	3.258235000
H	7.313273000	-2.651848000	2.667112000
C	7.063948000	-4.153318000	4.177124000
H	6.376511000	-4.754698000	4.781941000
C	6.601484000	3.239399000	-3.258124000
H	7.313475000	2.651514000	-2.667061000
C	7.064266000	4.153171000	-4.176907000
H	6.376876000	4.754667000	-4.781663000
H	8.134154000	-4.312398000	4.337092000
H	8.134485000	4.312195000	-4.336848000
C	-4.719048000	-2.085067000	-2.073197000
H	-5.443616000	-1.506625000	-1.498173000
C	-5.174043000	-3.011820000	-2.994588000
H	-4.464207000	-3.604195000	-3.583478000
C	-4.718957000	2.085335000	2.073039000
H	-5.443550000	1.507044000	1.497895000
C	-5.173912000	3.011982000	2.994557000
H	-4.464049000	3.604208000	3.583566000
C	-6.601432000	-3.258081000	-3.239509000
H	-7.313432000	-2.666876000	-2.651779000
C	-7.064199000	-4.177012000	-4.153139000
H	-6.376799000	-4.781910000	-4.754480000
C	-6.601289000	3.258303000	3.239482000
H	-7.313316000	2.667237000	2.651644000
C	-7.064015000	4.177124000	4.153244000
H	-6.376587000	4.781882000	4.754695000
H	-8.134415000	-4.336934000	-4.312201000
H	-8.134223000	4.337094000	4.312305000
H	-2.152900000	3.200824000	3.181774000
H	-2.153038000	-3.200480000	-3.182118000
H	2.153089000	3.181825000	-3.200778000
H	2.152848000	-3.181986000	3.200607000

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	x(Å)	y(Å)	z(Å)
C	5.082402000	-3.657771000	-0.053215000
N	5.511733000	-2.307392000	-0.041327000
B	4.552942000	-1.083622000	-0.015561000
N	3.086696000	-1.598829000	-0.022342000
C	2.722831000	-2.964480000	-0.033430000
C	3.709529000	-3.980249000	-0.048377000
C	1.927392000	-0.828824000	-0.011503000
C	0.789256000	-1.729425000	-0.015528000
C	1.280506000	-3.057316000	-0.028818000
C	6.255833000	-4.516832000	-0.070715000
C	7.373726000	-3.659643000	-0.069061000
C	6.898100000	-2.288124000	-0.050304000

C	6.245864000	-6.037393000	-0.088044000
C	7.666193000	-1.048252000	-0.040654000
C	0.454258000	-4.332987000	-0.036885000
C	1.983993000	0.628962000	-0.000004000
F	4.794676000	-0.235667000	-1.166191000
F	4.799450000	-0.282358000	1.167050000
C	-0.661012000	-1.363772000	-0.009274000
C	-1.353295000	-1.218168000	1.228147000
N	-2.740803000	-0.917077000	1.253364000
B	-3.620908000	-0.692539000	0.002230000
N	-2.747250000	-0.901973000	-1.256010000
C	-1.359548000	-1.202885000	-1.241400000
C	-3.170339000	-0.796294000	-2.572551000
C	-2.032829000	-1.029729000	-3.431435000
C	-0.902019000	-1.279990000	-2.626176000
C	-0.888797000	-1.312158000	2.609511000
C	-2.015369000	-1.070887000	3.423468000
C	-3.157128000	-0.826781000	2.573211000
C	0.500918000	-1.547188000	-3.152630000
C	-4.551902000	-0.493305000	-2.933723000
C	0.516805000	-1.586062000	3.125288000
C	-4.536780000	-0.527566000	2.944686000
F	-4.748780000	-1.605645000	-0.000337000
F	-4.170990000	0.653822000	0.011753000
C	-4.996699000	-0.376052000	-4.239527000
C	-4.975193000	-0.424103000	4.253803000
C	9.050380000	-1.000542000	-0.049673000
C	0.890124000	1.481327000	0.015575000
H	3.404715000	-5.026615000	-0.057108000
H	8.415089000	-3.964870000	-0.079717000
H	7.274848000	-6.429953000	-0.094931000
H	5.732430000	-6.449478000	0.799181000
H	5.728402000	-6.428998000	-0.982230000
H	7.100187000	-0.115532000	-0.025599000
H	-0.215953000	-4.368035000	-0.913794000
H	1.091955000	-5.230594000	-0.059381000
H	-0.191058000	-4.395364000	0.857170000
H	2.983404000	1.066979000	-0.005211000
H	-2.044520000	-1.009880000	-4.516369000
H	-2.021571000	-1.063824000	4.508607000
H	0.492746000	-1.528593000	-4.254308000
H	1.220110000	-0.787774000	-2.804394000
H	0.887794000	-2.527555000	-2.828801000
H	-5.259275000	-0.355147000	-2.114850000
H	0.514091000	-1.582986000	4.227141000
H	0.902654000	-2.561517000	2.785795000
H	1.233976000	-0.821438000	2.784325000
H	-5.248268000	-0.380742000	2.130890000
H	-4.297985000	-0.513243000	-5.073647000
H	-4.272549000	-0.570051000	5.083121000
H	9.633020000	-1.929607000	-0.065323000
H	-0.128168000	1.085871000	0.021507000
C	-6.364882000	-0.119813000	4.612449000
H	-7.070925000	0.028107000	3.785945000
C	-6.811675000	-0.013290000	5.912027000
H	-6.094257000	-0.163637000	6.730532000
C	-6.388019000	-0.068167000	-4.588582000
H	-7.090333000	0.071209000	-3.757433000
C	-6.840599000	0.051628000	-5.885006000
H	-6.126761000	-0.090180000	-6.708155000
C	9.809771000	0.253981000	-0.039511000
H	9.231993000	1.186181000	-0.023419000
C	11.187120000	0.310153000	-0.049177000
H	11.753202000	-0.631406000	-0.065338000
C	1.023570000	2.941190000	0.025244000
H	2.040067000	3.353897000	0.019999000
C	-0.060212000	3.793617000	0.039970000

H	-1.070273000	3.362685000	0.044893000
C	11.995574000	1.598294000	-0.039149000
H	12.661448000	1.643406000	0.844227000
H	12.647332000	1.666046000	-0.931566000
H	11.339120000	2.483609000	-0.022677000
C	0.041194000	5.310382000	0.049804000
H	-0.455018000	5.734178000	0.944096000
H	1.091673000	5.644583000	0.043900000
H	-0.468900000	5.746541000	-0.830629000
C	-8.246784000	0.303024000	6.304986000
H	-8.885359000	0.436074000	5.416258000
H	-8.678732000	-0.507022000	6.924022000
H	-8.299466000	1.228192000	6.911034000
C	-8.277408000	0.371829000	-6.268471000
H	-8.332715000	1.303098000	-6.864864000
H	-8.712016000	-0.431908000	-6.893840000
H	-8.912146000	0.495819000	-5.375696000

Species 9a, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	0.753065000	0.000063000	-0.000087000
C	1.457024000	-0.873333000	-0.873698000
C	1.457009000	0.873491000	0.873501000
N	2.876792000	0.887475000	0.887441000
N	2.876810000	-0.887298000	-0.887624000
B	3.781068000	-0.000423000	0.000431000
C	0.986588000	1.851778000	1.851895000
C	2.141721000	2.423925000	2.423918000
C	3.307155000	1.819844000	1.819853000
C	0.986628000	-1.851478000	-1.852255000
C	2.141777000	-2.423405000	-2.424463000
C	3.307195000	-1.819485000	-1.820205000
C	-0.753065000	0.000039000	-0.000059000
C	-1.456975000	-0.873645000	0.873299000
N	-2.876760000	-0.887652000	0.887266000
B	-3.781069000	-0.000184000	-0.000143000
N	-2.876842000	0.887674000	-0.887246000
C	-1.457057000	0.873724000	-0.873355000
C	-3.307089000	-1.820228000	1.819486000
C	-2.141633000	-2.424364000	2.423455000
C	-0.986518000	-1.852116000	1.851498000
C	-3.307262000	1.820297000	-1.819377000
C	-2.141866000	2.424535000	-2.423356000
C	-0.986698000	1.852293000	-1.851498000
F	-4.646029000	0.823789000	0.824245000
F	-4.645365000	-0.824545000	-0.824845000
F	4.646692000	0.823479000	-0.823331000
F	4.644702000	-0.825365000	0.825249000
C	-0.444094000	-2.219901000	-2.220953000
H	-0.437096000	-2.998432000	-3.000183000
H	-1.006906000	-2.607546000	-1.356223000
H	-1.006973000	-1.354853000	-2.607782000
C	-0.444149000	2.220285000	2.220455000
H	-1.007099000	1.355274000	2.607263000
H	-0.437181000	2.998843000	2.999658000
H	-1.006867000	2.607927000	1.355659000
C	0.444015000	2.220937000	-2.220017000
H	0.436994000	2.999669000	-2.999047000
H	1.006730000	2.608419000	-1.355146000
H	1.006995000	1.356039000	-2.607026000
C	0.444229000	-2.220643000	2.219997000
H	1.007168000	-1.355687000	2.606939000
H	0.437283000	-2.999329000	2.999072000
H	1.006951000	-2.608134000	1.355137000
C	4.719500000	-2.079156000	-2.079944000
H	5.444574000	-1.502878000	-1.503750000
C	5.172593000	-3.004379000	-3.005180000

H	4.456683000	-3.591885000	-3.592614000
C	4.719454000	2.079572000	2.079567000
H	5.444542000	1.503512000	1.503173000
C	5.172528000	3.004646000	3.004962000
H	4.456607000	3.591954000	3.592579000
C	6.595530000	-3.255988000	-3.256862000
H	7.315835000	-2.670995000	-2.671906000
C	7.056115000	-4.174656000	-4.175547000
H	6.323991000	-4.753993000	-4.754844000
C	6.595461000	3.256320000	3.256604000
H	7.315775000	2.671497000	2.671490000
C	7.056032000	4.174848000	4.175436000
H	6.323899000	4.754016000	4.754891000
C	-4.719577000	2.080088000	-2.078941000
H	-5.444629000	1.503756000	-1.502772000
C	-5.172710000	3.005525000	-3.003943000
H	-4.456826000	3.593105000	-3.591334000
C	-4.719377000	-2.080064000	2.079147000
H	-5.444488000	-1.503689000	1.503096000
C	-5.172411000	-3.005578000	3.004121000
H	-4.456464000	-3.593195000	3.591397000
C	-6.595659000	3.257251000	-3.255442000
H	-7.315935000	2.672165000	-2.670544000
C	-7.056290000	4.176133000	-4.173889000
H	-6.324195000	4.755562000	-4.753131000
C	-6.595332000	-3.257353000	3.255729000
H	-7.315674000	-2.672242000	2.670937000
C	-7.055856000	-4.176311000	4.174154000
H	-6.323693000	-4.755763000	4.753287000
C	-8.525523000	-4.453299000	4.450953000
H	-9.177379000	-3.824562000	3.822572000
H	-8.774402000	-5.514381000	4.255938000
H	-8.774424000	-4.258910000	5.512144000
C	-8.525989000	4.453068000	-4.450567000
H	-9.177770000	3.824315000	-3.822124000
H	-8.774891000	5.514143000	-4.255540000
H	-8.774975000	4.258660000	-5.511735000
C	8.525713000	4.451725000	4.452269000
H	8.774680000	4.256879000	5.513360000
H	9.177535000	3.823264000	3.823576000
H	8.774575000	5.512892000	4.257696000
C	8.525800000	-4.451472000	-4.452421000
H	8.774692000	-4.256779000	-5.513559000
H	9.177614000	-3.822864000	-3.823868000
H	8.774748000	-5.512590000	-4.257693000
H	-2.152546000	-3.191749000	3.190608000
H	-2.152855000	3.192009000	-3.190419000
H	2.152662000	3.191234000	3.191146000
H	2.152739000	-3.190445000	-3.191959000

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	x(Å)	y(Å)	z(Å)
C	5.008001000	-3.733605000	-0.305197000
N	5.464748000	-2.396598000	-0.249205000
B	4.539952000	-1.155939000	-0.095754000
N	3.061187000	-1.641165000	-0.111478000
C	2.665806000	-2.990642000	-0.169552000
C	3.630971000	-4.027856000	-0.260751000
C	1.921266000	-0.849658000	-0.021937000
C	0.760971000	-1.719182000	-0.034814000
C	1.220678000	-3.057148000	-0.127580000
C	6.162941000	-4.620120000	-0.413065000
C	7.296301000	-3.786665000	-0.419811000
C	6.848550000	-2.409322000	-0.316000000
C	6.117323000	-6.136118000	-0.502206000
C	7.639539000	-1.186798000	-0.277652000
C	0.371522000	-4.315150000	-0.198896000

C	2.023848000	0.602526000	0.061315000
F	4.769681000	-0.221757000	-1.175794000
F	4.828163000	-0.469597000	1.141095000
C	-0.683407000	-1.325541000	-0.037127000
C	-1.385152000	-1.141091000	1.188902000
N	-2.764620000	-0.822538000	1.189089000
B	-3.670910000	-0.870854000	-0.067696000
N	-2.752268000	-0.904711000	-1.316580000
C	-1.365154000	-1.176667000	-1.284452000
C	-3.156828000	-0.804610000	-2.639319000
C	-2.002845000	-1.001015000	-3.484987000
C	-0.880419000	-1.234110000	-2.665676000
C	-0.924564000	-1.173040000	2.580535000
C	-2.046311000	-0.860881000	3.371005000
C	-3.178679000	-0.644866000	2.498389000
C	0.534124000	-1.461469000	-3.179178000
C	-4.539611000	-0.549075000	-3.019891000
C	0.470958000	-1.456892000	3.115532000
C	-4.549156000	-0.296495000	2.847052000
F	-4.493974000	-2.061810000	-0.031464000
F	-4.555820000	0.265958000	-0.118082000
C	-4.974105000	-0.500981000	-4.338133000
C	-4.996316000	-0.176241000	4.155783000
C	9.026359000	-1.171197000	-0.339863000
C	0.975473000	1.468411000	0.343432000
H	3.302225000	-5.066039000	-0.301446000
H	8.329221000	-4.111282000	-0.490068000
H	7.135594000	-6.550044000	-0.552563000
H	5.615332000	-6.577340000	0.376792000
H	5.571283000	-6.471039000	-1.401910000
H	7.094817000	-0.244281000	-0.196611000
H	-0.013371000	-4.481154000	-1.221747000
H	0.944584000	-5.209351000	0.092352000
H	-0.504604000	-4.238687000	0.464911000
H	3.020446000	1.020355000	-0.095143000
H	-1.997575000	-0.963395000	-4.569355000
H	-2.055727000	-0.778453000	4.452760000
H	0.538838000	-1.416531000	-4.279081000
H	1.235618000	-0.697041000	-2.807000000
H	0.932862000	-2.443996000	-2.877062000
H	-5.254729000	-0.385485000	-2.212084000
H	0.453953000	-1.447263000	4.216104000
H	0.847171000	-2.439468000	2.786805000
H	1.202389000	-0.701177000	2.784159000
H	-5.238880000	-0.111841000	2.022015000
H	-4.276839000	-0.661432000	-5.164557000
H	-4.321983000	-0.353180000	4.997641000
H	9.592634000	-2.102509000	-0.422864000
H	-0.030668000	1.094654000	0.534009000
C	-6.371366000	0.187102000	4.450492000
H	-7.045527000	0.372711000	3.609910000
C	-6.894032000	0.316346000	5.739976000
C	-6.365413000	-0.241854000	-4.663496000
H	-7.064941000	-0.079804000	-3.838818000
C	-6.874910000	-0.186602000	-5.963916000
C	9.771799000	0.075642000	-0.297538000
H	9.210194000	1.009964000	-0.213584000
C	11.164756000	0.160301000	-0.357087000
C	1.188393000	2.904228000	0.427758000
H	2.179307000	3.298054000	0.185239000
C	0.202454000	3.816221000	0.811998000
C	-1.128672000	3.370904000	1.203975000
N	-2.196094000	2.957631000	1.537297000
C	11.839642000	1.447493000	-0.309281000
N	12.386874000	2.506799000	-0.269873000
C	12.000635000	-1.028123000	-0.469640000
N	12.665462000	-2.014371000	-0.562039000

C	-6.077189000	0.088421000	6.924847000
N	-5.391445000	-0.104653000	7.881998000
C	-8.285166000	0.683103000	5.951259000
N	-9.427892000	0.982984000	6.118131000
C	-8.284334000	0.075814000	-6.206153000
N	-9.442172000	0.290629000	-6.398416000
C	-6.023978000	-0.390649000	-7.128879000
N	-5.308728000	-0.561977000	-8.068500000
C	0.479281000	5.242407000	0.867458000
N	0.714223000	6.411281000	0.908383000

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	x(Å)	y(Å)	z(Å)
C	-0.752830000	-0.000030000	-0.000030000
C	-1.456268000	0.874749000	0.874950000
C	-1.456309000	-0.874793000	-0.874997000
N	-2.870822000	-0.886529000	-0.886681000
N	-2.870780000	0.886517000	0.886674000
B	-3.779110000	-0.000048000	0.000061000
C	-0.982983000	-1.855649000	-1.855984000
C	-2.138330000	-2.426019000	-2.426470000
C	-3.300221000	-1.818941000	-1.819269000
C	-0.982888000	1.855619000	1.855895000
C	-2.138204000	2.425994000	2.426438000
C	-3.300128000	1.818975000	1.819240000
C	0.752830000	-0.000038000	-0.000042000
C	1.456288000	-0.875043000	0.874699000
N	2.870801000	-0.886742000	0.886456000
B	3.779110000	0.000072000	0.000070000
N	2.870801000	0.886696000	-0.886507000
C	1.456289000	0.874979000	-0.874769000
C	3.300173000	-1.819365000	1.818845000
C	2.138265000	-2.426590000	2.425867000
C	0.982934000	-1.856069000	1.855500000
C	3.300176000	1.819270000	-1.818944000
C	2.138269000	2.426520000	-2.425943000
C	0.982937000	1.856001000	-1.855576000
F	4.636655000	-0.823243000	-0.823469000
F	4.636289000	0.823578000	0.823801000
F	-4.636573000	0.823506000	-0.823325000
F	-4.636371000	-0.823687000	0.823573000
C	0.446432000	2.225657000	2.225814000
H	0.437428000	3.003565000	3.004109000
H	1.008952000	1.362051000	2.616314000
H	1.008658000	2.616733000	1.362267000
C	0.446315000	-2.225703000	-2.225974000
H	1.008587000	-2.616758000	-1.362448000
H	0.437263000	-3.003632000	-3.004247000
H	1.008816000	-1.362110000	-2.616531000
C	-0.446371000	2.225983000	-2.225597000
H	-0.437342000	3.004293000	-3.003490000
H	-1.008636000	1.362467000	-2.616685000
H	-1.008867000	2.616491000	-1.361979000
C	-0.446376000	-2.226058000	2.225508000
H	-1.008860000	-2.616580000	1.361888000
H	-0.437349000	-3.004359000	3.003410000
H	-1.008651000	-1.362542000	2.616580000
C	-4.711781000	2.073445000	2.073600000
H	-5.434802000	1.495605000	1.495397000
C	-5.167324000	3.000671000	3.001016000
H	-4.464446000	3.592538000	3.593175000
C	-4.711887000	-2.073355000	-2.073609000
H	-5.434877000	-1.495463000	-1.495420000
C	-5.167480000	-3.000592000	-3.000990000
H	-4.464634000	-3.592514000	-3.593131000
C	-6.587994000	3.216703000	3.216791000
H	-7.294359000	2.626707000	2.626487000

C	-7.115024000	4.131435000	4.131647000
C	-6.588162000	-3.216570000	-3.216744000
H	-7.294496000	-2.626524000	-2.626452000
C	-7.115240000	-4.131308000	-4.131565000
C	4.711835000	2.073595000	-2.073410000
H	5.434841000	1.495361000	-1.495580000
C	5.167405000	3.001024000	-3.000610000
H	4.464543000	3.593217000	-3.592462000
C	4.711832000	-2.073715000	2.073289000
H	5.434839000	-1.495539000	1.495404000
C	5.167399000	-3.001101000	3.000533000
H	4.464536000	-3.593234000	3.592445000
C	6.588081000	3.216773000	-3.216629000
H	7.294430000	2.626438000	-2.626645000
C	7.115136000	4.131641000	-4.131334000
C	6.588075000	-3.216875000	3.216530000
H	7.294425000	-2.626592000	2.626496000
C	7.115128000	-4.131705000	4.131275000
C	-8.551991000	4.289126000	4.289092000
N	-9.732053000	4.413128000	4.412890000
C	-6.256306000	4.963714000	4.964330000
N	-5.534120000	5.635025000	5.635975000
C	-8.552215000	-4.288943000	-4.288990000
N	-9.732284000	-4.412898000	-4.412773000
C	-6.256567000	-4.963650000	-4.964230000
N	-5.534415000	-5.635011000	-5.635863000
C	6.256432000	-4.964360000	4.963604000
N	5.534263000	-5.635985000	5.634954000
C	8.552099000	-4.289148000	4.288931000
N	9.732165000	-4.412945000	4.412903000
C	8.552107000	4.289058000	-4.289015000
N	9.732173000	4.412831000	-4.413009000
C	6.256441000	4.964366000	-4.963595000
N	5.534272000	5.636044000	-5.634892000
H	2.151120000	3.193733000	-3.193050000
H	2.151114000	-3.193822000	3.192955000
H	-2.151033000	3.193122000	3.193630000
H	-2.151201000	-3.193140000	-3.193668000

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	x(Å)	y(Å)	z(Å)
C	5.059093000	-3.671359000	-0.076721000
N	5.504687000	-2.326763000	-0.051147000
B	4.563019000	-1.091078000	-0.003632000
N	3.090464000	-1.587621000	-0.026196000
C	2.708260000	-2.946332000	-0.049861000
C	3.683309000	-3.975469000	-0.074312000
C	1.941673000	-0.803796000	-0.009545000
C	0.792254000	-1.684319000	-0.022517000
C	1.265256000	-3.020984000	-0.047241000
C	6.223162000	-4.545947000	-0.104642000
C	7.350552000	-3.702025000	-0.095027000
C	6.889384000	-2.326639000	-0.061131000
C	6.194989000	-6.065415000	-0.138386000
C	7.669018000	-1.092522000	-0.038070000
C	0.421344000	-4.284598000	-0.067753000
C	2.029330000	0.654127000	0.014458000
F	4.819868000	-0.222502000	-1.134004000
F	4.814072000	-0.319007000	1.195717000
C	-0.656516000	-1.311196000	-0.015018000
C	-1.350517000	-1.179342000	1.223473000
N	-2.744207000	-0.914746000	1.247457000
B	-3.651006000	-0.842293000	-0.004533000
N	-2.748970000	-0.887582000	-1.261175000
C	-1.354996000	-1.151044000	-1.247873000
C	-3.168365000	-0.766269000	-2.576050000
C	-2.023585000	-0.946436000	-3.436769000

C	-0.889747000	-1.186783000	-2.633091000
C	-0.880601000	-1.247165000	2.605935000
C	-2.011301000	-1.023001000	3.418668000
C	-3.158799000	-0.822007000	2.566151000
C	0.521156000	-1.406967000	-3.159636000
C	-4.560203000	-0.503126000	-2.933935000
C	0.531671000	-1.481799000	3.122363000
C	-4.549019000	-0.564785000	2.934390000
F	-4.581718000	-1.954988000	-0.014773000
F	-4.442893000	0.370919000	0.009955000
C	-5.009247000	-0.415657000	-4.238537000
C	-4.993599000	-0.503893000	4.242015000
C	9.051560000	-1.062316000	-0.044617000
C	0.959941000	1.532474000	0.040750000
H	3.364845000	-5.017554000	-0.092983000
H	8.388078000	-4.019630000	-0.110410000
H	7.218730000	-6.470090000	-0.150990000
H	5.677964000	-6.479997000	0.745268000
H	5.671851000	-6.440215000	-1.036150000
H	7.110685000	-0.155391000	-0.014817000
H	-0.244661000	-4.304321000	-0.948070000
H	1.045790000	-5.191038000	-0.092982000
H	-0.228738000	-4.343273000	0.822763000
H	3.039586000	1.066448000	0.009198000
H	-2.031170000	-0.895778000	-4.520697000
H	-2.015125000	-0.996418000	4.503470000
H	0.515917000	-1.368806000	-4.260366000
H	1.220113000	-0.635581000	-2.796594000
H	0.930564000	-2.383502000	-2.852365000
H	-5.264950000	-0.366785000	-2.112608000
H	0.529486000	-1.473553000	4.223723000
H	0.940131000	-2.449651000	2.787607000
H	1.230006000	-0.701018000	2.778740000
H	-5.256324000	-0.410291000	2.118498000
H	-4.322548000	-0.547545000	-5.079003000
H	-4.304404000	-0.654032000	5.077362000
H	9.632453000	-1.988268000	-0.068379000
H	-0.071920000	1.179718000	0.047096000
C	-6.397450000	-0.239698000	4.568963000
H	-7.120120000	-0.083002000	3.765840000
C	-6.867463000	-0.175897000	5.846331000
C	-6.414470000	-0.146730000	-4.555537000
H	-7.134765000	-0.007233000	-3.747126000
C	-6.888677000	-0.057891000	-5.829850000
C	9.797737000	0.198035000	-0.019988000
H	9.259078000	1.147176000	0.004659000
C	11.159357000	0.257770000	-0.025896000
C	1.176533000	2.981719000	0.062167000
H	2.194352000	3.376813000	0.056919000
C	0.160352000	3.889793000	0.088857000
F	11.897447000	1.423279000	-0.002954000
F	12.005850000	-0.837716000	-0.055621000
F	0.335540000	5.259176000	0.109537000
F	-1.186702000	3.583944000	0.099427000
F	-8.181566000	0.070083000	6.193189000
F	-6.102355000	-0.347842000	6.988863000
F	-8.204175000	0.193369000	-6.167609000
F	-6.127006000	-0.205859000	-6.978068000

Species 9c, 8,8‘ Dimer , Electronic state S_0

	x(Å)	**y(Å)**	**z(Å)**
C	0.752944000	-0.000929000	0.000712000
C	1.456739000	-0.871694000	0.877544000
C	1.455205000	0.870801000	-0.876319000
N	2.873759000	0.884436000	-0.889765000
N	2.875308000	-0.884090000	0.889715000
B	3.779707000	-0.002695000	-0.003651000

C	0.984006000	1.847120000	-1.857824000
C	2.139639000	2.417493000	-2.430971000
C	3.302389000	1.814002000	-1.824122000
C	0.987348000	-1.847056000	1.860779000
C	2.144005000	-2.415545000	2.433799000
C	3.305657000	-1.812022000	1.824860000
C	-0.752974000	-0.001473000	0.001327000
C	-1.455978000	0.875831000	0.872243000
N	-2.874531000	0.888599000	0.885353000
B	-3.779709000	0.004597000	-0.004659000
N	-2.874605000	-0.892797000	-0.881255000
C	-1.456023000	-0.879521000	-0.868756000
C	-3.303983000	1.823289000	1.814215000
C	-2.141758000	2.430773000	2.418052000
C	-0.985639000	1.857838000	1.848391000
C	-3.304130000	-1.829513000	-1.807958000
C	-2.141947000	-2.438365000	-2.410584000
C	-0.985772000	-1.863651000	-1.842882000
F	-4.630025000	0.831445000	-0.838451000
F	-4.655590000	-0.809034000	0.815809000
F	4.636662000	-0.831860000	-0.828366000
F	4.649053000	0.820720000	0.813942000
C	-0.442054000	-2.215982000	2.232954000
H	-0.432912000	-2.989063000	3.016909000
H	-1.006078000	-1.349786000	2.615436000
H	-1.003977000	-2.611651000	1.371243000
C	-0.446039000	2.215582000	-2.227876000
H	-1.007286000	2.609995000	-1.365171000
H	-0.438302000	2.989446000	-3.011071000
H	-1.009993000	1.349454000	-2.610599000
C	0.443933000	-2.235351000	-2.211070000
H	0.435446000	-3.017283000	-2.986199000
H	1.006852000	-1.372930000	-2.603612000
H	1.006655000	-2.620490000	-1.345158000
C	0.444108000	2.228523000	2.217426000
H	1.007228000	2.614288000	1.352051000
H	0.435709000	3.009697000	2.993326000
H	1.006504000	1.365434000	2.609287000
C	4.721131000	-2.066122000	2.080407000
H	5.441527000	-1.488923000	1.499290000
C	5.175585000	-2.986204000	3.006969000
H	4.473928000	-3.576906000	3.602031000
C	4.717380000	2.069583000	-2.080829000
H	5.438769000	1.493512000	-1.499810000
C	5.170031000	2.989950000	-3.007999000
H	4.467121000	3.579522000	-3.602697000
C	6.604942000	-3.212972000	3.235198000
H	7.342302000	-2.645934000	2.663851000
C	7.081135000	-4.112583000	4.141420000
C	6.598892000	3.218412000	-3.237585000
H	7.337527000	2.652392000	-2.666882000
C	7.073041000	4.118437000	-4.144486000
C	-4.719376000	-2.086375000	-2.061999000
H	-5.440285000	-1.506543000	-1.484149000
C	-5.172980000	-3.012882000	-2.982558000
H	-4.470775000	-3.606681000	-3.573879000
C	-4.719202000	2.079873000	2.068719000
H	-5.440090000	1.496799000	1.494094000
C	-5.172652000	3.009154000	2.986556000
H	-4.470257000	3.605953000	3.574617000
C	-6.602120000	-3.242578000	-3.209206000
H	-7.340032000	-2.672377000	-2.641735000
C	-7.077424000	-4.148811000	-4.109280000
C	-6.601721000	3.238432000	3.214064000
H	-7.339843000	2.665812000	2.649311000
C	-7.076688000	4.147362000	4.111603000
H	2.150785000	3.182901000	-3.200050000

H	2.156629000	-3.179375000	3.204410000
H	-2.153564000	3.199904000	3.183398000
H	-2.153920000	-3.210169000	-3.173216000
F	-8.414066000	-4.393730000	-4.351210000
F	-6.294870000	-4.958952000	-4.915214000
F	-6.293763000	4.960781000	4.913901000
F	-8.413204000	4.392221000	4.354197000
F	6.289390000	4.922599000	-4.955347000
F	8.418021000	-4.354551000	4.384995000
F	6.299379000	-4.917957000	4.952899000
F	8.409336000	4.362040000	-4.389534000

Species 9d, 8,2' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	5.827460000	8.434066000	0.929671000
N	5.376061000	9.432538000	1.821888000
B	3.883754000	9.691617000	2.178612000
N	3.010819000	8.652129000	1.412451000
C	3.518098000	7.681190000	0.532956000
C	4.913740000	7.571135000	0.293501000
C	1.626223000	8.533628000	1.449960000
C	1.237060000	7.447635000	0.568565000
C	2.415706000	6.910731000	-0.005925000
C	7.284587000	8.506569000	0.838617000
C	7.675679000	9.559422000	1.685056000
C	6.481679000	10.124094000	2.288695000
C	8.170343000	7.608136000	-0.007157000
C	6.366068000	11.226373000	3.234039000
C	2.528779000	5.762597000	-0.995106000
C	0.823781000	9.420974000	2.280174000
F	3.506370000	11.031018000	1.801432000
F	3.678550000	9.559701000	3.600787000
C	-0.141574000	6.922031000	0.313545000
C	-0.632015000	5.829579000	1.094533000
N	-1.885493000	5.247615000	0.803543000
B	-2.747749000	5.599109000	-0.437946000
N	-2.210299000	6.930133000	-1.026205000
C	-0.940691000	7.475347000	-0.728460000
C	-2.785810000	7.677871000	-2.039449000
C	-1.868993000	8.732823000	-2.411238000
C	-0.715611000	8.623676000	-1.614189000
C	-0.065247000	5.139038000	2.257598000
C	-1.005398000	4.156745000	2.624241000
C	-2.124141000	4.228152000	1.712796000
C	0.484551000	9.555415000	-1.681389000
C	-4.099393000	7.376951000	-2.591510000
C	1.246392000	5.397898000	2.984114000
C	-3.325028000	3.405467000	1.675509000
F	-2.628881000	4.548526000	-1.424701000
F	-4.135989000	5.713450000	-0.079786000
C	-4.661286000	8.098184000	-3.638877000
C	-3.547921000	2.351342000	2.554899000
C	7.460708000	11.946426000	3.695998000
C	-0.565629000	9.457338000	2.311901000
H	5.281697000	6.808527000	-0.392735000
H	8.691845000	9.894350000	1.864801000
H	9.224978000	7.905926000	0.089274000
H	8.087356000	6.552108000	0.305213000
H	7.898884000	7.663319000	-1.075955000
H	5.363571000	11.480040000	3.584496000
H	2.865520000	6.118686000	-1.985200000
H	3.253144000	5.003925000	-0.652252000
H	1.557915000	5.264783000	-1.133310000
H	1.379922000	10.117894000	2.910679000
H	-2.047259000	9.487504000	-3.169774000
H	-0.909254000	3.467111000	3.456179000
H	0.344037000	10.281271000	-2.496557000

H	0.617004000	10.124142000	-0.746043000
H	1.422862000	9.007931000	-1.867751000
H	-4.651638000	6.548363000	-2.144560000
H	1.339524000	4.705091000	3.834144000
H	2.118787000	5.249413000	2.326597000
H	1.304603000	6.425437000	3.378907000
H	-4.071268000	3.644813000	0.915796000
H	-4.131863000	8.922271000	-4.113699000
H	-2.817815000	2.077010000	3.314180000
H	8.474768000	11.709068000	3.378557000
H	-1.175518000	8.813914000	1.684513000
C	-4.770241000	1.577584000	2.450230000
C	-5.166667000	0.514618000	3.245752000
C	-5.977601000	7.737589000	-4.131554000
H	-6.490411000	6.899362000	-3.650926000
C	-6.694586000	8.348853000	-5.146847000
C	7.260626000	13.035790000	4.636313000
H	6.238864000	13.249195000	4.963413000
C	8.225506000	13.873682000	5.165849000
C	-1.231125000	10.410857000	3.181665000
H	-0.609455000	11.046307000	3.819254000
C	-2.594095000	10.605743000	3.318956000
N	7.836270000	14.907565000	6.151759000
O	8.712166000	15.280053000	7.017058000
O	6.611956000	15.326878000	6.106811000
N	9.655017000	13.835774000	4.810899000
O	10.290940000	14.950158000	4.736500000
O	10.171980000	12.675277000	4.543463000
N	-3.095015000	11.653533000	4.235652000
O	-4.229498000	12.200003000	3.972680000
O	-2.320384000	11.987399000	5.218762000
N	-3.624088000	9.833082000	2.603279000
O	-4.713908000	9.553313000	3.222749000
O	-3.341558000	9.440967000	1.397388000
N	-6.435412000	-0.184559000	2.947961000
O	-6.536812000	-1.426506000	3.270790000
O	-7.345794000	0.493442000	2.323407000
N	-4.415540000	0.011149000	4.405917000
O	-5.076970000	-0.421210000	5.420513000
N	-6.250098000	9.540843000	-5.886148000
O	-4.973383000	9.678621000	-6.083292000
O	-7.136055000	10.398899000	-6.249781000
N	-8.011134000	7.801595000	-5.540885000
O	-8.662351000	7.135892000	-4.640465000
O	-8.400261000	7.967470000	-6.756565000
O	-3.119171000	0.082698000	4.354486000
H	-5.485706000	1.855315000	1.670723000

Species 9d, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-0.752656000	-0.006072000	-0.006126000
C	-1.449965000	0.861577000	0.881575000
C	-1.461275000	-0.869149000	-0.889267000
N	-2.874336000	-0.875075000	-0.896367000
N	-2.862866000	0.876765000	0.897940000
B	-3.778956000	0.003450000	0.004026000
C	-0.993123000	-1.840753000	-1.884329000
C	-2.152189000	-2.399335000	-2.457756000
C	-3.309253000	-1.794019000	-1.839093000
C	-0.968831000	1.830172000	1.873436000
C	-2.120418000	2.396391000	2.454381000
C	-3.285488000	1.798636000	1.843408000
C	0.753016000	-0.010673000	-0.010867000
C	1.456020000	-0.897263000	0.853275000
N	2.869015000	-0.912213000	0.860494000
B	3.779284000	-0.009706000	-0.010067000
N	2.868912000	0.877832000	-0.895769000

C	1.455925000	0.870720000	-0.880413000
C	3.297795000	-1.857719000	1.779476000
C	2.136723000	-2.470583000	2.383046000
C	0.981388000	-1.890293000	1.823846000
C	3.297600000	1.815934000	-1.822360000
C	2.136472000	2.431803000	-2.422738000
C	0.981192000	1.860955000	-1.853777000
F	4.617290000	0.813293000	0.828690000
F	4.646113000	-0.818362000	-0.834286000
F	-4.632011000	0.839385000	-0.806784000
F	-4.630921000	-0.827640000	0.820929000
C	0.462627000	2.191441000	2.242944000
H	0.458324000	2.958528000	3.031567000
H	1.024219000	1.321527000	2.620478000
H	1.022566000	2.593698000	1.383002000
C	0.433386000	-2.211558000	-2.263455000
H	0.996003000	-2.618786000	-1.407569000
H	0.418490000	-2.977835000	-3.052748000
H	0.998515000	-1.345236000	-2.643992000
C	-0.447832000	2.236367000	-2.218608000
H	-0.438276000	3.025419000	-2.985212000
H	-1.009731000	1.378902000	-2.623477000
H	-1.010546000	2.615234000	-1.350002000
C	-0.447596000	-2.261773000	2.192829000
H	-1.014439000	-2.636893000	1.325284000
H	-0.437997000	-3.052748000	2.957448000
H	-1.005386000	-1.403424000	2.601493000
C	-4.695089000	2.052545000	2.109041000
H	-5.424086000	1.477988000	1.534551000
C	-5.135253000	2.976149000	3.049223000
H	-4.437640000	3.554303000	3.652816000
C	-4.722229000	-2.038531000	-2.095485000
H	-5.443622000	-1.458755000	-1.516657000
C	-5.174758000	-2.959533000	-3.032335000
H	-4.485012000	-3.542756000	-3.640083000
C	-6.560456000	3.169991000	3.250655000
H	-7.247954000	2.567561000	2.649787000
C	-7.175495000	4.059914000	4.113626000
C	-6.602556000	-3.143556000	-3.224441000
H	-7.281971000	-2.535991000	-2.619564000
C	-7.229344000	-4.029646000	-4.082875000
C	4.708852000	2.068332000	-2.080605000
H	5.434116000	1.477055000	-1.518487000
C	5.155008000	3.010548000	-2.999249000
H	4.461131000	3.605864000	-3.590337000
C	4.709061000	-2.121613000	2.025897000
H	5.434312000	-1.546765000	1.446972000
C	5.155228000	-3.061343000	2.947074000
H	4.461347000	-3.665488000	3.529134000
C	6.581452000	3.201273000	-3.194761000
H	7.265092000	2.582053000	-2.606700000
C	7.202189000	4.106881000	-4.037088000
C	6.581663000	-3.261971000	3.132513000
H	7.265336000	-2.660206000	2.526635000
C	7.202311000	-4.125502000	4.017979000
H	-2.172438000	-3.154476000	-3.236517000
H	-2.130549000	3.151778000	3.233098000
H	2.151909000	-3.250176000	3.137445000
H	2.151582000	3.202142000	-3.186586000
N	-6.532508000	-5.007089000	-4.935713000
O	-5.369550000	-4.667274000	-5.403086000
O	-7.085971000	-6.151581000	-5.125730000
N	-8.707407000	-4.039047000	-4.169204000
O	-9.248193000	-4.394177000	-5.281017000
O	-9.356569000	-3.630946000	-3.125464000
N	-6.466456000	5.031917000	4.962591000
O	-5.302571000	4.684049000	5.421696000

O	-7.011095000	6.179823000	5.157476000
N	-8.652895000	4.079703000	4.209286000
O	-9.311497000	3.677837000	3.169051000
O	-9.184118000	4.437016000	5.324998000
N	8.679742000	4.120487000	-4.131363000
O	9.213847000	4.501786000	-5.237742000
O	9.335266000	3.689412000	-3.100922000
N	6.499082000	5.101259000	-4.864857000
O	5.334419000	4.769246000	-5.333641000
O	7.049239000	6.250785000	-5.032686000
N	6.499223000	-4.975680000	4.993292000
O	7.050017000	-5.170488000	6.138241000
O	5.334068000	-5.435917000	4.651204000
N	8.679782000	-4.221176000	4.028528000
O	9.335887000	-3.181314000	3.621663000
O	9.213222000	-5.336702000	4.383200000

Species 9I, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
6	0.752968000	0.000331000	0.000262000
6	1.455739000	0.962150000	-0.779212000
6	1.456663000	-0.960830000	0.779749000
7	2.870598000	-0.978354000	0.794545000
7	2.869676000	0.981063000	-0.794008000
5	3.772680000	0.001570000	0.000063000
6	0.971488000	-2.030334000	1.646274000
6	2.133458000	-2.662205000	2.158527000
6	3.318629000	-2.003597000	1.625153000
6	0.969542000	2.031173000	-1.645805000
6	2.130886000	2.663957000	-2.158282000
6	3.316725000	2.006471000	-1.624927000
6	-0.752967000	-0.000379000	0.000246000
6	-1.455823000	-0.780147000	-0.961291000
7	-2.869742000	-0.795459000	-0.979644000
5	-3.772676000	-0.001231000	-0.000291000
7	-2.870528000	0.792923000	0.979914000
6	-1.456576000	0.778753000	0.961738000
6	-3.316868000	-1.626421000	-2.004995000
6	-2.131110000	-2.159468000	-2.662823000
6	-0.969701000	-1.646594000	-2.030433000
6	-3.318483000	1.623602000	2.005128000
6	-2.133227000	2.157352000	2.663331000
6	-0.971324000	1.645441000	2.031111000
9	-4.630061000	-0.908553000	0.734814000
9	-4.629383000	0.906138000	-0.735973000
9	4.629760000	0.737333000	0.907112000
9	4.629691000	-0.733597000	-0.907462000
6	-0.473871000	2.402332000	-1.947574000
1	-0.509167000	3.255482000	-2.638870000
1	-1.020773000	1.566636000	-2.412177000
1	-1.021822000	2.683140000	-1.034220000
6	-0.471553000	-2.402854000	1.948121000
1	-1.019091000	-2.684830000	1.034870000
1	-0.505987000	-3.255619000	2.639937000
1	-1.019420000	-1.567470000	2.412142000
6	0.471755000	1.947638000	2.403223000
1	0.506276000	2.639365000	3.256056000
1	1.019617000	1.034497000	2.684942000
1	1.019241000	2.411880000	1.567723000
6	0.473673000	-1.947876000	-2.402112000
1	1.020920000	-2.412662000	-1.566744000
1	0.508880000	-2.638842000	-3.255534000
1	1.021335000	-1.034287000	-2.682738000
53	-2.061434000	3.495746000	4.314679000
53	2.057635000	4.314407000	-3.497706000
53	2.061835000	-4.312651000	3.497969000
53	-2.058003000	-3.498725000	-4.313353000

6	4.751110000	2.222750000	-1.799987000
1	5.386916000	1.533116000	-1.244488000
6	5.387111000	3.180833000	-2.572168000
1	4.828179000	3.910567000	-3.159490000
6	4.753226000	-2.218556000	1.799981000
1	5.388345000	-1.527301000	1.245695000
6	5.390319000	-3.177235000	2.570503000
1	4.832270000	-3.908786000	3.156433000
6	6.853232000	3.262434000	-2.638501000
1	7.419537000	2.531169000	-2.049920000
6	7.519011000	4.200346000	-3.393962000
1	6.977775000	4.942130000	-3.991030000
6	6.856545000	-3.257159000	2.636713000
1	7.421935000	-2.524126000	2.049458000
6	7.523487000	-4.195654000	3.390427000
1	6.983174000	-4.939211000	3.986126000
1	8.611599000	4.239103000	-3.425595000
1	8.616121000	-4.233135000	3.421955000
6	-4.753059000	1.797952000	2.220714000
1	-5.388256000	1.240384000	1.532189000
6	-5.389921000	2.571856000	3.176834000
1	-4.831648000	3.161563000	3.905148000
6	-4.751276000	-1.801666000	-2.220863000
1	-5.386988000	-1.246401000	-1.530941000
6	-5.387563000	-2.573693000	-3.178868000
1	-4.828907000	-3.160824000	-3.908992000
6	-6.856117000	2.637134000	3.257939000
1	-7.421738000	2.046208000	2.528037000
6	-7.522779000	3.394389000	4.193774000
1	-6.982253000	3.993810000	4.934176000
6	-6.853720000	-2.640110000	-3.259860000
1	-7.419734000	-2.051700000	-2.528235000
6	-7.519861000	-3.395395000	-4.197661000
1	-6.978910000	-3.992264000	-4.939814000
1	-8.615404000	3.425161000	4.232185000
1	-8.612462000	-3.427055000	-4.235972000

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	x(Å)	y(Å)	z(Å)
C	-0.753014000	-0.001608000	-0.001542000
C	-1.456400000	0.895289000	-0.854345000
C	-1.457576000	-0.899406000	0.849367000
N	-2.871970000	-0.918295000	0.863137000
N	-2.870744000	0.912871000	-0.871501000
B	-3.773259000	-0.002565000	-0.004721000
C	-0.972565000	-1.896800000	1.797545000
C	-2.134460000	-2.488146000	2.355719000
C	-3.321176000	-1.876294000	1.771192000
C	-0.970016000	1.892819000	-1.801701000
C	-2.131136000	2.483165000	-2.362561000
C	-3.318672000	1.870741000	-1.780378000
C	0.752982000	-0.000676000	0.000750000
C	1.455030000	0.853048000	0.897844000
N	2.869383000	0.870469000	0.917259000
B	3.773239000	0.001118000	0.005467000
N	2.873274000	-0.869351000	-0.908946000
C	1.458880000	-0.853584000	-0.894066000
C	3.315886000	1.780105000	1.875039000
C	2.127433000	2.362778000	2.485253000
C	0.967190000	1.801315000	1.893804000
C	3.323928000	-1.777642000	-1.866077000
C	2.138165000	-2.361146000	-2.480635000
C	0.975354000	-1.801728000	-1.892234000
F	4.631304000	-0.844272000	0.812344000
F	4.632787000	0.847410000	-0.798537000
F	-4.631361000	-0.805801000	-0.853621000
F	-4.632773000	0.800254000	0.842640000

C	0.473648000	2.239298000	-2.130744000
H	0.509451000	3.037094000	-2.885347000
H	1.021715000	2.588367000	-1.241398000
H	1.020255000	1.370034000	-2.529528000
C	0.470678000	-2.243408000	2.128353000
H	1.018966000	-1.372689000	2.521318000
H	0.505491000	-3.036617000	2.887821000
H	1.017692000	-2.599091000	1.240851000
C	-0.467311000	-2.133196000	-2.240574000
H	-0.500771000	-2.887767000	-3.038493000
H	-1.014563000	-2.532832000	-1.372161000
H	-1.016265000	-1.244657000	-2.590470000
C	-0.476997000	2.131169000	2.237382000
H	-1.027806000	1.241092000	2.580064000
H	-0.513965000	2.881722000	3.038938000
H	-1.020081000	2.535596000	1.368463000
I	2.066669000	-3.831661000	-4.017312000
I	-2.055084000	4.026755000	-3.825575000
I	-2.060450000	-4.037418000	3.812842000
I	2.049047000	3.832535000	4.022325000
C	-4.751433000	2.074414000	-1.970248000
H	-5.388093000	1.437333000	-1.356348000
C	-5.385451000	2.965652000	-2.822128000
H	-4.818932000	3.636993000	-3.469643000
C	-4.754181000	-2.081885000	1.957148000
H	-5.389981000	-1.458065000	1.328937000
C	-5.389243000	-2.959430000	2.822350000
H	-4.823563000	-3.614875000	3.486660000
C	-6.847868000	3.052909000	-2.897900000
H	-7.424933000	2.381124000	-2.250703000
C	-7.509846000	3.928208000	-3.732797000
H	-6.917145000	4.594288000	-4.374472000
C	-6.851698000	-3.051160000	2.892067000
H	-7.427893000	-2.395351000	2.227926000
C	-7.514700000	-3.911650000	3.741410000
H	-6.922853000	-4.561642000	4.400142000
C	4.757249000	-1.967872000	-2.065426000
H	5.392125000	-1.371610000	-1.410071000
C	5.393688000	-2.799269000	-2.974106000
H	4.828973000	-3.425547000	-3.666788000
C	4.748327000	1.971463000	2.079555000
H	5.386095000	1.369283000	1.432491000
C	5.380749000	2.810966000	2.983591000
H	4.813028000	3.444450000	3.667186000
C	6.856337000	-2.878431000	-3.054193000
H	7.431527000	-2.252027000	-2.361412000
C	7.520752000	-3.691691000	-3.947831000
H	6.929918000	-4.312219000	-4.635252000
C	6.843036000	2.890215000	3.070127000
H	7.421321000	2.256905000	2.386258000
C	7.503430000	3.711839000	3.959078000
H	6.909516000	4.339541000	4.637269000
C	9.015818000	3.815741000	4.073558000
H	9.520397000	3.150917000	3.353749000
H	9.357562000	4.852352000	3.888223000
H	9.356084000	3.547380000	5.092332000
C	9.033655000	-3.795742000	-4.055361000
H	9.534996000	-3.136799000	-3.327916000
H	9.373578000	-4.834002000	-3.875499000
H	9.379541000	-3.520541000	-5.070314000
C	-9.027310000	-4.030862000	3.836261000
H	-9.379576000	-3.807233000	4.861713000
H	-9.529808000	-3.340740000	3.139187000
H	-9.359382000	-5.061415000	3.605016000
C	-9.022400000	4.043134000	-3.833586000
H	-9.367973000	3.840465000	-4.865661000
H	-9.525811000	3.335843000	-3.154619000

H	-9.360192000	5.067002000	-3.581847000

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	x(Å)	y(Å)	z(Å)
C	5.136559000	-3.763374000	-0.113260000
N	5.563806000	-2.412250000	-0.102566000
B	4.603042000	-1.191005000	-0.066342000
N	3.137899000	-1.708009000	-0.068067000
C	2.776169000	-3.074099000	-0.077984000
C	3.764799000	-4.088101000	-0.099941000
C	1.977347000	-0.940115000	-0.050137000
C	0.841315000	-1.842585000	-0.048155000
C	1.334400000	-3.169793000	-0.065022000
C	6.311374000	-4.620506000	-0.139667000
C	7.427623000	-3.761623000	-0.144188000
C	6.949842000	-2.391129000	-0.120523000
C	6.304223000	-6.140891000	-0.159077000
C	7.711220000	-1.146329000	-0.113867000
C	0.509684000	-4.446379000	-0.069449000
C	2.036786000	0.518651000	-0.039075000
F	4.838171000	-0.334475000	-1.212921000
F	4.854647000	-0.392392000	1.117685000
C	-0.607250000	-1.472373000	-0.033631000
C	-1.289619000	-1.316734000	1.207623000
N	-2.670897000	-0.989421000	1.240847000
B	-3.543989000	-0.717197000	-0.005137000
N	-2.691464000	-0.974183000	-1.268469000
C	-1.309721000	-1.301094000	-1.261693000
C	-3.119937000	-0.862446000	-2.582867000
C	-1.993099000	-1.120900000	-3.447826000
C	-0.862322000	-1.390107000	-2.648895000
C	-0.819753000	-1.422819000	2.586102000
C	-1.937106000	-1.162393000	3.406609000
C	-3.077767000	-0.893105000	2.563316000
C	0.531507000	-1.684352000	-3.184594000
C	-4.498538000	-0.528630000	-2.930405000
C	0.582485000	-1.724626000	3.095006000
C	-4.450432000	-0.563046000	2.937033000
F	-4.724733000	-1.561519000	-0.000636000
F	-4.016895000	0.659359000	0.007180000
C	-4.937282000	-0.393341000	-4.232272000
C	-4.867258000	-0.438660000	4.247144000
C	9.091652000	-1.105456000	-0.130384000
C	-6.312973000	-0.054544000	-4.662087000
C	-6.235844000	-0.104367000	4.702508000
C	-7.389421000	0.175180000	-3.738667000
C	-8.684240000	0.498123000	-4.212754000
C	-8.938154000	0.599930000	-5.612926000
C	-7.881393000	0.374710000	-6.538720000
C	-6.582771000	0.050663000	-6.066974000
C	-6.481768000	-0.008335000	6.112418000
C	-7.772542000	0.311092000	6.608244000
C	-8.845240000	0.540659000	5.702056000
C	-8.615149000	0.447869000	4.297150000
C	-7.328203000	0.129648000	3.799047000
C	0.938917000	1.358439000	-0.016935000
C	0.977411000	2.837519000	-0.007239000
C	9.932077000	0.112520000	-0.124548000
C	11.358054000	-0.042253000	-0.144344000
C	12.214466000	1.089135000	-0.139717000
C	11.660203000	2.399482000	-0.115146000
C	10.243682000	2.568150000	-0.095315000
C	9.386134000	1.441354000	-0.099911000
C	2.197271000	3.596142000	-0.019847000
C	2.159481000	5.011637000	-0.009812000
C	0.910291000	5.700829000	0.012855000
C	-0.305141000	4.960801000	0.025436000
C	-0.272164000	3.542358000	0.015467000

H	3.461867000	-5.135000000	-0.107732000
H	8.468960000	-4.066036000	-0.162261000
H	7.333809000	-6.531366000	-0.173694000
H	5.797826000	-6.555056000	0.731138000
H	5.781334000	-6.532101000	-1.050192000
H	7.129716000	-0.225632000	-0.094921000
H	-0.162039000	-4.483903000	-0.945103000
H	1.148158000	-5.343370000	-0.091588000
H	-0.133856000	-4.508053000	0.825883000
H	3.040143000	0.941625000	-0.051232000
H	-2.010345000	-1.104957000	-4.532602000
H	-1.936765000	-1.159695000	4.491633000
H	0.514598000	-1.672364000	-4.286137000
H	1.265559000	-0.934236000	-2.847352000
H	0.905118000	-2.668791000	-2.857820000
H	-5.184863000	-0.387134000	-2.097116000
H	0.583091000	-1.730206000	4.196728000
H	0.951382000	-2.703396000	2.746636000
H	1.310882000	-0.968736000	2.758321000
H	-5.150830000	-0.414933000	2.116694000
H	-4.221572000	-0.541812000	-5.048541000
H	-4.137766000	-0.592720000	5.050070000
H	9.646901000	-2.049896000	-0.149789000
H	-7.214085000	0.102385000	-2.663977000
H	-9.493143000	0.670515000	-3.498366000
H	-8.067041000	0.450750000	-7.612900000
H	-5.771335000	-0.121439000	-6.779920000
H	-5.658079000	-0.183782000	6.810335000
H	-7.939923000	0.380233000	7.685888000
H	-9.436346000	0.623522000	3.597740000
H	-7.171241000	0.063638000	2.721076000
H	-0.064395000	0.930346000	-0.004857000
H	11.785031000	-1.049029000	-0.163214000
H	13.298353000	0.951827000	-0.154944000
H	9.814875000	3.573076000	-0.076395000
H	8.305057000	1.589602000	-0.084605000
H	3.161714000	3.085356000	-0.037372000
H	3.094363000	5.577572000	-0.019610000
H	-1.265687000	5.480914000	0.042733000
H	-1.206904000	2.974885000	0.024957000
H	12.316167000	3.273643000	-0.111430000
H	0.888099000	6.793645000	0.020429000
H	-9.840931000	0.787026000	6.079514000
H	-9.939806000	0.849920000	-5.971772000

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	x(Å)	y(Å)	z(Å)
C	0.753032000	0.000931000	0.000955000
C	1.456120000	-0.875806000	-0.869685000
C	1.457275000	0.877275000	0.871096000
N	2.876848000	0.892066000	0.883268000
N	2.875705000	-0.891548000	-0.882759000
B	3.779793000	0.000089000	-0.000170000
C	0.987482000	1.859241000	1.845880000
C	2.142839000	2.434493000	2.414217000
C	3.307459000	1.828682000	1.811350000
C	0.984979000	-1.857622000	-1.844111000
C	2.139597000	-2.433670000	-2.413067000
C	3.305033000	-1.828533000	-1.811040000
C	-0.753009000	0.001202000	0.001368000
C	-1.456703000	-0.874473000	0.872647000
N	-2.876289000	-0.888758000	0.886165000
B	-3.779633000	-0.010710000	-0.010716000
N	-2.876233000	0.891763000	-0.882943000
C	-1.456659000	0.877956000	-0.868806000
C	-3.306342000	-1.821330000	1.818554000
C	-2.141374000	-2.424542000	2.423370000

C	-0.986331000	-1.852159000	1.851538000
C	-3.306169000	1.829119000	-1.810587000
C	-2.141111000	2.436510000	-2.411057000
C	-0.986148000	1.860990000	-1.842223000
F	-4.670351000	0.797776000	0.802843000
F	-4.623261000	-0.843718000	-0.849042000
F	4.646862000	0.819449000	-0.828110000
F	4.647459000	-0.819509000	0.826919000
C	-0.445805000	-2.225884000	-2.212217000
H	-0.439316000	-2.997187000	-2.998451000
H	-1.004990000	-2.623040000	-1.349365000
H	-1.011756000	-1.358718000	-2.589434000
C	-0.442846000	2.228374000	2.214888000
H	-1.009463000	1.361135000	2.590967000
H	-0.435400000	2.998540000	3.002239000
H	-1.001746000	2.627355000	1.352650000
C	0.444446000	2.232058000	-2.208227000
H	0.437633000	3.002878000	-2.994941000
H	1.001161000	2.631060000	-1.344588000
H	1.012951000	1.365867000	-2.583802000
C	0.444173000	-2.220078000	2.221060000
H	1.010111000	-1.352462000	2.597273000
H	0.437113000	-2.990290000	3.008368000
H	1.003607000	-2.618629000	1.359003000
C	4.719503000	-2.087035000	-2.063579000
H	5.429014000	-1.503904000	-1.478844000
C	5.165004000	-3.013304000	-2.985478000
H	4.426842000	-3.584716000	-3.559251000
C	4.722290000	2.086265000	2.062892000
H	5.430988000	1.502567000	1.477739000
C	5.169111000	3.012233000	2.984442000
H	4.431781000	3.584230000	3.558707000
C	-4.720808000	2.084543000	-2.065357000
H	-5.429953000	1.500798000	-1.480788000
C	-5.166922000	3.008709000	-2.989062000
H	-4.429154000	3.581166000	-3.562303000
C	-4.721012000	-2.077286000	2.072587000
H	-5.430068000	-1.490484000	1.490979000
C	-5.167260000	-3.004485000	2.993186000
H	-4.429572000	-3.579848000	3.563610000
C	6.582092000	3.327792000	3.292860000
C	6.857859000	4.324204000	4.287234000
C	7.689072000	2.682867000	2.642451000
C	8.192647000	4.668478000	4.624391000
C	9.019784000	3.028813000	2.981340000
C	9.279487000	4.021727000	3.972349000
H	6.023355000	4.822125000	4.789160000
H	7.509413000	1.921203000	1.881842000
H	8.383168000	5.430010000	5.384467000
H	9.852096000	2.530141000	2.478534000
H	10.309052000	4.283844000	4.228871000
C	6.577518000	-3.329926000	-3.294899000
C	6.851799000	-4.326684000	-4.289339000
C	7.685455000	-2.685734000	-2.645394000
C	8.186078000	-4.672012000	-4.627424000
C	9.015656000	-3.032723000	-2.985218000
C	9.273879000	-4.025982000	-3.976271000
H	6.016553000	-4.824050000	-4.790578000
H	7.506919000	-1.923822000	-1.884767000
H	8.375469000	-5.433796000	-5.387529000
H	9.848714000	-2.534600000	-2.483105000
H	10.303057000	-4.288910000	-4.233513000
C	-6.580050000	-3.317743000	3.304800000
C	-7.687452000	-2.668027000	2.659895000
C	-6.855179000	-4.316464000	4.297033000
C	-9.017952000	-3.011698000	3.001912000
C	-8.189757000	-4.658394000	4.637389000

C	-9.277018000	-4.006929000	3.990762000
H	-7.508271000	-1.904404000	1.901139000
H	-6.020350000	-4.818015000	4.794785000
H	-9.850595000	-2.509437000	2.503243000
H	-8.379796000	-5.421733000	5.395770000
H	-10.306424000	-4.267176000	4.249814000
C	-6.579667000	3.321434000	-3.301405000
C	-7.687149000	2.674829000	-2.653519000
C	-6.854659000	4.316461000	-4.297378000
C	-9.017602000	3.017917000	-2.996296000
C	-8.189193000	4.657826000	-4.638476000
C	-9.276536000	4.009470000	-3.988872000
H	-7.508057000	1.913983000	-1.891957000
H	-6.019761000	4.815569000	-4.797466000
H	-9.850314000	2.518001000	-2.495391000
H	-8.379135000	5.418291000	-5.399764000
H	-10.305908000	4.269242000	-4.248534000
H	2.153335000	3.205162000	3.177910000
H	2.149077000	-3.204428000	-3.176679000
H	-2.151076000	3.208319000	-3.173603000
H	-2.151439000	-3.190641000	3.191651000

Species 10a, 8,2' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	-3.722057000	5.247738000	0.000000000
N	-2.359309000	5.636652000	0.000000000
B	-1.166067000	4.641647000	0.000000000
N	-1.724021000	3.192314000	0.000000000
C	-3.100280000	2.868827000	0.000000000
C	-4.086066000	3.885058000	0.000000000
C	-0.988017000	2.010482000	0.000000000
C	-1.923865000	0.899581000	0.000000000
C	-3.235647000	1.429790000	0.000000000
C	-4.545128000	6.446078000	0.000000000
C	-3.655302000	7.538210000	0.000000000
C	-2.298328000	7.022601000	0.000000000
C	-6.065457000	6.482078000	0.000000000
C	-1.033778000	7.748398000	0.000000000
C	-4.535307000	0.641811000	0.000000000
C	0.470339000	2.025004000	0.000000000
F	-0.329840000	4.861633000	1.165561000
F	-0.329840000	4.861633000	-1.165561000
C	-1.582897000	-0.556151000	0.000000000
C	-1.421754000	-1.249375000	-1.234609000
N	-1.085729000	-2.629392000	-1.254741000
B	-0.763787000	-3.471364000	0.000000000
N	-1.085729000	-2.629392000	1.254741000
C	-1.421754000	-1.249375000	1.234609000
C	-0.985378000	-3.048436000	2.574076000
C	-1.264719000	-1.917364000	3.427292000
C	-1.530783000	-0.793724000	2.617176000
C	-1.530783000	-0.793724000	-2.617176000
C	-1.264719000	-1.917364000	-3.427292000
C	-0.985378000	-3.048436000	-2.574076000
C	-1.842629000	0.601223000	3.139946000
C	-0.639741000	-4.419203000	2.936420000
C	-1.842630000	0.601223000	-3.139947000
C	-0.639741000	-4.419203000	-2.936420000
F	-1.519358000	-4.710704000	0.000000000
F	0.646501000	-3.842996000	0.000000000
C	-0.496776000	-4.842947000	4.243780000
C	-0.496776000	-4.842947000	-4.243780000
C	-0.954734000	9.128627000	0.000000000
C	-0.146069000	-6.207450000	4.687913000
C	-0.146069000	-6.207450000	-4.687913000
C	0.084379000	-7.300090000	3.777863000
C	0.419660000	-8.582270000	4.256036000

C	0.536266000	-8.814623000	5.661976000
C	0.313343000	-7.753882000	6.587134000
C	-0.024635000	-6.467126000	6.090280000
C	-0.024635000	-6.467126000	-6.090280000
C	0.313342000	-7.753882000	-6.587133000
C	0.536266000	-8.814623000	-5.661976000
C	0.419659000	-8.582271000	-4.256036000
C	0.084379000	-7.300090000	-3.777863000
O	0.875620000	-10.128412000	6.025047000
O	0.875620000	-10.128412000	-6.025046000
C	1.272920000	0.897011000	0.000000000
C	2.747180000	0.873910000	0.000000000
C	0.280911000	9.936049000	0.000000000
C	0.171679000	11.363393000	0.000000000
C	1.317490000	12.201650000	0.000000000
C	2.611045000	11.603012000	0.000001000
C	2.747684000	10.179479000	0.000000000
C	1.601649000	9.360430000	0.000000000
C	3.564429000	2.059771000	0.000000000
C	4.970124000	1.967268000	0.000000000
C	5.601841000	0.683941000	0.000000000
C	4.817763000	-0.506737000	0.000000000
C	3.402970000	-0.399734000	0.000000000
O	7.005392000	0.709350000	0.000000000
O	3.817994000	12.319334000	0.000001000
H	-5.141233000	3.612252000	0.000000000
H	-3.930778000	8.587805000	0.000000000
H	-6.426809000	7.522515000	0.000000000
H	-6.482938000	5.978984000	-0.890688000
H	-6.482938000	5.978984000	0.890687000
H	-0.129250000	7.141658000	0.000000000
H	-4.603945000	-0.014331000	0.885699000
H	-5.413768000	1.306071000	0.000000000
H	-4.603945000	-0.014331000	-0.885699000
H	0.926081000	3.014129000	0.000000000
H	-1.265507000	-1.927457000	4.512350000
H	-1.265507000	-1.927457000	-4.512350000
H	-1.847559000	0.590826000	4.241773000
H	-1.092368000	1.338214000	2.809594000
H	-2.824084000	0.966847000	2.795809000
H	-0.495305000	-5.113774000	2.110555000
H	-1.847559000	0.590826000	-4.241773000
H	-2.824084000	0.966847000	-2.795810000
H	-1.092369000	1.338213000	-2.809595000
H	-0.495305000	-5.113774000	-2.110555000
H	-0.647405000	-4.117982000	5.051586000
H	-0.647406000	-4.117982000	-5.051586000
H	-1.885012000	9.707890000	0.000000000
H	0.000638000	-7.142704000	2.701390000
H	0.595651000	-9.414749000	3.573726000
H	0.397057000	-7.910737000	7.662489000
H	-0.195028000	-5.652478000	6.799710000
H	-0.195029000	-5.652478000	-6.799710000
H	0.397056000	-7.910737000	-7.662489000
H	0.595651000	-9.414749000	-3.573725000
H	0.000638000	-7.142704000	-2.701390000
H	0.807061000	-0.088778000	0.000000000
H	-0.821171000	11.821864000	0.000000000
H	1.192230000	13.284372000	0.000001000
H	3.751135000	9.752315000	0.000000000
H	1.726669000	8.276493000	0.000000000
H	3.098807000	3.046839000	0.000000000
H	5.599229000	2.858166000	0.000000000
H	5.279943000	-1.493552000	0.000000000
H	2.800743000	-1.312373000	0.000000000
C	1.017074000	-10.444203000	-7.448365000
H	0.067283000	-10.275911000	-7.987454000

H	1.821731000	-9.842955000	-7.908850000
H	1.281137000	-11.508539000	-7.481964000
C	1.017074000	-10.444202000	7.448366000
H	0.067284000	-10.275910000	7.987454000
H	1.281137000	-11.508538000	7.481964000
H	1.821731000	-9.842955000	7.908850000
C	7.726203000	-0.566637000	0.000000000
H	7.487871000	-1.155022000	0.904112000
H	7.487871000	-1.155022000	-0.904113000
H	8.789417000	-0.295860000	0.000000000
C	3.761907000	13.783465000	0.000001000
H	3.250694000	14.159348000	-0.904530000
H	3.250694000	14.159347000	0.904532000
H	4.808903000	14.110953000	0.000001000

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	x(Å)	y(Å)	z(Å)
C	0.753173000	-0.001727000	-0.003137000
C	1.457699000	0.884014000	-0.863608000
C	1.457300000	-0.888484000	0.856625000
N	2.877249000	-0.902889000	0.870554000
N	2.877631000	0.898839000	-0.876334000
B	3.780043000	0.012427000	0.012097000
C	0.987173000	-1.883984000	1.817092000
C	2.141925000	-2.466980000	2.378693000
C	3.307885000	-1.852401000	1.786380000
C	0.988191000	1.873776000	-1.830211000
C	2.143245000	2.453436000	-2.394654000
C	3.308862000	1.843416000	-1.797003000
C	-0.752866000	-0.001168000	-0.002735000
C	-1.458096000	-0.863201000	-0.886431000
N	-2.878021000	-0.876978000	-0.899201000
B	-3.779974000	-0.004486000	0.003437000
N	-2.876223000	0.876792000	0.895858000
C	-1.456295000	0.861893000	0.881331000
C	-3.309930000	-1.797471000	-1.843639000
C	-2.144790000	-2.392834000	-2.456747000
C	-0.989318000	-1.828074000	-1.878181000
C	-3.306180000	1.799418000	1.839006000
C	-2.139754000	2.395195000	2.449422000
C	-0.985420000	1.828722000	1.870398000
F	-4.639643000	-0.842196000	0.822696000
F	-4.658236000	0.824024000	-0.804728000
F	4.620468000	0.837600000	0.863298000
F	4.677083000	-0.783362000	-0.808428000
C	-0.442331000	2.245401000	-2.196425000
H	-0.434958000	3.032588000	-2.966961000
H	-1.004304000	1.384338000	-2.593317000
H	-1.006269000	2.622964000	-1.327981000
C	-0.443513000	-2.259607000	2.178558000
H	-1.003224000	-2.639643000	1.308393000
H	-0.436514000	-3.046198000	2.949696000
H	-1.009603000	-1.400051000	2.572621000
C	0.445538000	2.192386000	2.242834000
H	0.439089000	2.956651000	3.036105000
H	1.010598000	1.321352000	2.612416000
H	1.006022000	2.596516000	1.384126000
C	0.440962000	-2.191265000	-2.253713000
H	1.003368000	-2.595022000	-1.396076000
H	0.433105000	-2.955624000	-3.046899000
H	1.004704000	-1.319878000	-2.624652000
C	4.722217000	2.103699000	-2.047023000
H	5.431947000	1.508894000	-1.474395000
C	5.167750000	3.045854000	-2.954675000
H	4.427335000	3.627815000	-3.515023000
C	4.721067000	-2.112258000	2.037890000
H	5.431318000	-1.521458000	1.461806000

C	5.165769000	-3.050984000	2.949504000
H	4.424815000	-3.629304000	3.512902000
C	-4.719212000	2.052706000	2.097879000
H	-5.429669000	1.476540000	1.507363000
C	-5.163529000	2.967258000	3.033929000
H	-4.422346000	3.531184000	3.611421000
C	-4.723517000	-2.049773000	-2.100463000
H	-5.432673000	-1.472211000	-1.509751000
C	-5.169928000	-2.964590000	-3.035226000
H	-4.430051000	-3.529913000	-3.613051000
C	6.573168000	-3.372188000	3.259862000
C	6.851035000	-4.379444000	4.238243000
C	7.690894000	-2.721049000	2.625685000
C	8.179978000	-4.738894000	4.585733000
C	9.014870000	-3.067151000	2.960244000
C	9.265299000	-4.077073000	3.941196000
H	6.017796000	-4.886778000	4.732450000
H	7.519862000	-1.947994000	1.874925000
H	8.349952000	-5.511036000	5.335821000
H	9.866864000	-2.579361000	2.485265000
C	6.575471000	3.367012000	-3.263653000
C	6.854360000	4.378728000	-4.237138000
C	7.692547000	2.711497000	-2.632855000
C	8.183662000	4.738349000	-4.583076000
C	9.016868000	3.057664000	-2.965969000
C	9.268324000	4.072096000	-3.941987000
H	6.021626000	4.889542000	-4.728608000
H	7.520760000	1.935098000	-1.885729000
H	8.354425000	5.514033000	-5.329325000
H	9.868366000	2.566639000	-2.493439000
C	-6.577962000	-3.276067000	-3.352622000
C	-7.694407000	-2.639083000	-2.702030000
C	-6.857826000	-4.258592000	-4.355283000
C	-9.019063000	-2.974978000	-3.044210000
C	-8.187480000	-4.607498000	-4.710731000
C	-9.271498000	-3.960145000	-4.049515000
H	-7.521866000	-1.885041000	-1.932517000
H	-6.025585000	-4.754965000	-4.862144000
H	-9.870091000	-2.497849000	-2.556832000
H	-8.358988000	-5.360815000	-5.479389000
C	-6.570795000	3.279951000	3.353421000
C	-7.688794000	2.644979000	2.703532000
C	-6.848243000	4.261681000	4.357539000
C	-9.012623000	2.982036000	3.047763000
C	-8.177029000	4.611726000	4.715064000
C	-9.262633000	3.966371000	4.054494000
H	-7.518086000	1.891563000	1.932995000
H	-6.014787000	4.756474000	4.863946000
H	-9.864822000	2.506405000	2.560968000
H	-8.346672000	5.364341000	5.484811000
H	2.151169000	-3.248706000	3.131166000
H	2.152969000	3.228956000	-3.153520000
H	-2.148459000	3.153670000	3.225326000
H	-2.155084000	-3.149326000	-3.234579000
O	10.623931000	4.335371000	-4.195274000
C	10.963167000	5.362613000	-5.183373000
H	10.571984000	5.095437000	-6.181607000
H	10.571553000	6.349616000	-4.877879000
H	12.059699000	5.387492000	-5.206951000
O	10.620641000	-4.340726000	4.195530000
C	10.958817000	-5.362895000	5.189236000
H	10.567743000	-5.089965000	6.185949000
H	10.566363000	-6.351199000	4.889047000
H	12.055324000	-5.388640000	5.213093000
O	-10.627363000	-4.215532000	-4.309439000
C	-10.967574000	-5.213024000	-5.327230000
H	-10.576986000	-4.916568000	-6.317397000

H	-10.576049000	-6.208739000	-5.051314000
H	-12.064130000	-5.236895000	-5.350778000
O	-10.617864000	4.223027000	4.316430000
C	-10.955676000	5.219641000	5.335890000
H	-10.564197000	4.921512000	6.325202000
H	-10.563384000	6.215265000	5.060737000
H	-12.052173000	5.244714000	5.360838000

Species 10I, 8,8' Dimer , Electronic state S_0

	x(Å)	y(Å)	z(Å)
C	0.752450000	-0.007384000	-0.007355000
C	1.443443000	0.869779000	0.875425000
C	1.468524000	-0.874608000	-0.879675000
N	2.883059000	-0.888173000	-0.879276000
N	2.857556000	0.902976000	0.895974000
B	3.771371000	0.013460000	0.015095000
C	0.997324000	-1.842082000	-1.864679000
C	2.167102000	-2.410691000	-2.430791000
C	3.344593000	-1.813393000	-1.814403000
C	0.944069000	1.831743000	1.852157000
C	2.097358000	2.417063000	2.434775000
C	3.292112000	1.835146000	1.837114000
C	-0.753445000	-0.017664000	-0.018218000
C	-1.456955000	0.869770000	-0.880408000
N	-2.871299000	0.882335000	-0.902001000
B	-3.772265000	-0.021706000	-0.022405000
N	-2.871271000	-0.936808000	0.845416000
C	-1.456909000	-0.912316000	0.836585000
C	-3.319015000	1.835419000	-1.816097000
C	-2.132198000	2.446793000	-2.400280000
C	-0.971020000	1.861615000	-1.833571000
C	-3.319096000	-1.884710000	1.764578000
C	-2.132657000	-2.488246000	2.357370000
C	-0.971273000	-1.898330000	1.795946000
F	-4.642772000	-0.827611000	-0.860928000
F	-4.626542000	0.788771000	0.821278000
F	4.632971000	-0.801230000	0.850752000
F	4.634107000	0.839900000	-0.807569000
C	-0.503819000	2.157049000	2.183983000
H	-0.549743000	2.902807000	2.989433000
H	-1.039214000	2.566456000	1.312465000
H	-1.056428000	1.264325000	2.516080000
C	-0.440980000	-2.185843000	-2.218798000
H	-0.998235000	-1.300659000	-2.563456000
H	-0.464756000	-2.935190000	-3.021891000
H	-0.985873000	-2.598015000	-1.354527000
C	0.472001000	-2.240147000	2.131221000
H	0.507203000	-3.003355000	2.920716000
H	1.011023000	-2.634133000	1.254840000
H	1.027849000	-1.358348000	2.486397000
C	0.472436000	2.206187000	-2.165250000
H	1.028915000	1.326929000	-2.525940000
H	0.508207000	2.974816000	-2.949435000
H	1.010475000	2.594258000	-1.285737000
I	-2.055414000	-4.045043000	3.806125000
I	1.999751000	3.942061000	3.915739000
I	2.112696000	-3.934612000	-3.915044000
I	-2.053487000	3.963824000	-3.890593000
C	4.723760000	2.052235000	2.027691000
H	5.352166000	1.516011000	1.320258000
C	5.332591000	2.836440000	2.988907000
H	4.726368000	3.366531000	3.723861000
C	4.781942000	-2.010978000	-1.982831000
H	5.391948000	-1.468116000	-1.264488000
C	5.416474000	-2.784933000	-2.935666000
H	4.829352000	-3.321642000	-3.681243000
C	-4.753626000	-2.090550000	1.945626000

H	-5.374084000	-1.526311000	1.253214000
C	-5.374178000	-2.895109000	2.882226000
H	-4.776107000	-3.457031000	3.599967000
C	-4.753700000	2.027807000	-2.009914000
H	-5.374638000	1.342971000	-1.437269000
C	-5.375214000	2.964227000	-2.814029000
H	-4.777855000	3.672120000	-3.388859000
C	6.883008000	-2.952231000	-3.057333000
C	7.382235000	-3.769304000	-4.126062000
C	7.826358000	-2.343106000	-2.161151000
C	8.775663000	-3.971717000	-4.299896000
C	9.216503000	-2.547970000	-2.337004000
C	9.698818000	-3.361127000	-3.405362000
H	6.672954000	-4.238799000	-4.813401000
H	7.478054000	-1.719747000	-1.336054000
H	9.137021000	-4.596375000	-5.120240000
H	9.922816000	-2.079448000	-1.647251000
H	10.773140000	-3.514639000	-3.534980000
C	6.794501000	3.024059000	3.133856000
C	7.265118000	3.848086000	4.210200000
C	7.760337000	2.427948000	2.252994000
C	8.652650000	4.069769000	4.406251000
C	9.144514000	2.652049000	2.451032000
C	9.598308000	3.471892000	3.526766000
H	6.538434000	4.307689000	4.885940000
H	7.433744000	1.799899000	1.422603000
H	8.992219000	4.699428000	5.232063000
H	9.868258000	2.193388000	1.772833000
H	10.668185000	3.640297000	3.673550000
C	-6.840267000	3.112628000	-2.971670000
C	-7.797722000	2.271664000	-2.308232000
C	-7.323271000	4.151590000	-3.835611000
C	-9.185505000	2.471392000	-2.506993000
C	-8.714340000	4.349505000	-4.031788000
C	-9.651496000	3.509384000	-3.367626000
H	-7.461973000	1.471451000	-1.646765000
H	-6.603192000	4.797040000	-4.346328000
H	-9.902793000	1.824328000	-1.996158000
H	-9.063168000	5.146505000	-4.692723000
H	-10.724124000	3.657715000	-3.515935000
C	-6.838686000	-3.065822000	3.021642000
C	-7.796151000	-2.420673000	2.166583000
C	-7.320990000	-3.923682000	4.065902000
C	-9.183408000	-2.630877000	2.358038000
C	-8.711570000	-4.131530000	4.255352000
C	-9.648782000	-3.485257000	3.401458000
H	-7.460766000	-1.764247000	1.362063000
H	-6.600846000	-4.420490000	4.722031000
H	-9.900760000	-2.133873000	1.700366000
H	-9.059966000	-4.787599000	5.056558000
H	-10.720998000	-3.642464000	3.543483000

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	x(Å)	y(Å)	z(Å)
C	5.143458000	0.066601000	-3.844209000
N	5.599808000	0.041617000	-2.504656000
B	4.667159000	-0.021386000	-1.257918000
N	3.186476000	0.021317000	-1.744603000
C	2.798367000	0.038345000	-3.099051000
C	3.765181000	0.061228000	-4.135708000
C	2.043719000	0.001816000	-0.955300000
C	0.887481000	0.009735000	-1.832938000
C	1.354556000	0.032225000	-3.170876000
C	6.299525000	0.098477000	-4.730733000
C	7.433106000	0.091363000	-3.896669000
C	6.983528000	0.054854000	-2.516523000
C	6.257908000	0.134440000	-6.249503000

C	7.773972000	0.031164000	-1.285131000
C	0.523275000	0.052412000	-4.443413000
C	2.147514000	-0.011717000	0.505377000
F	4.909332000	-1.239678000	-0.524066000
F	4.935154000	1.094366000	-0.383525000
C	-0.558509000	0.019001000	-1.447478000
C	-1.268006000	-1.210565000	-1.321382000
N	-2.657441000	-1.218829000	-1.043521000
B	-3.550095000	0.047870000	-0.973612000
N	-2.623816000	1.292244000	-0.984610000
C	-1.234957000	1.261136000	-1.263060000
C	-3.021507000	2.610640000	-0.841131000
C	-1.864682000	3.456409000	-1.021469000
C	-0.746920000	2.639798000	-1.286623000
C	-0.813821000	-2.598870000	-1.401008000
C	-1.951140000	-3.397683000	-1.168631000
C	-3.087038000	-2.531396000	-0.952671000
C	0.667169000	3.150887000	-1.520642000
C	-4.408730000	2.984701000	-0.558909000
C	0.588451000	-3.132448000	-1.655080000
C	-4.482809000	-2.882597000	-0.684001000
F	-4.359341000	0.032069000	0.219104000
F	-4.438663000	0.086239000	-2.114879000
C	-4.788076000	4.309421000	-0.459831000
C	-4.891850000	-4.201042000	-0.630264000
C	9.155155000	0.034205000	-1.320771000
C	-6.137896000	4.832662000	-0.179276000
C	-6.252840000	-4.704077000	-0.367544000
C	-7.321125000	4.052463000	0.034649000
C	-8.581791000	4.635608000	0.298493000
C	-8.715236000	6.045452000	0.360336000
C	-7.573587000	6.858702000	0.154809000
C	-6.326131000	6.251953000	-0.107032000
C	-6.470698000	-6.120689000	-0.339441000
C	-7.730806000	-6.709110000	-0.097161000
C	-8.855574000	-5.878959000	0.132374000
C	-8.692802000	-4.470981000	0.113716000
C	-7.419906000	-3.906396000	-0.131127000
C	1.064538000	-0.156092000	1.351950000
C	1.100948000	-0.181923000	2.827769000
C	10.080124000	0.011035000	-0.172835000
C	11.491129000	0.017813000	-0.425745000
C	12.463916000	-0.002972000	0.596965000
C	12.050274000	-0.032232000	1.951753000
C	10.665258000	-0.040159000	2.254431000
C	9.710960000	-0.018983000	1.211495000
C	2.249877000	0.044546000	3.653721000
C	2.194500000	0.004273000	5.065803000
C	0.968270000	-0.269306000	5.721767000
C	-0.195981000	-0.498509000	4.947707000
C	-0.114664000	-0.451232000	3.538716000
H	3.435498000	0.076372000	-5.174718000
H	8.466591000	0.110633000	-4.226191000
H	7.277908000	0.142424000	-6.663098000
H	5.732767000	-0.745936000	-6.660510000
H	5.736264000	1.035529000	-6.618163000
H	7.228034000	0.011745000	-0.344920000
H	-0.551341000	0.070485000	-4.209893000
H	0.750119000	0.940614000	-5.059314000
H	0.717933000	-0.839335000	-5.065592000
H	3.152284000	0.093552000	0.907440000
H	-1.851860000	4.539376000	-0.957636000
H	-1.964787000	-4.482273000	-1.147243000
H	0.673178000	4.251517000	-1.486165000
H	1.369829000	2.784824000	-0.754027000
H	1.063640000	2.836168000	-2.499920000
H	-5.123051000	2.176348000	-0.424902000

H	0.571746000	-4.233493000	-1.649626000
H	0.987065000	-2.800573000	-2.627877000
H	1.302933000	-2.801427000	-0.883508000
H	-5.178424000	-2.063047000	-0.522263000
H	-4.036259000	5.087654000	-0.598233000
H	-4.157118000	-4.990673000	-0.793617000
H	9.658924000	0.055105000	-2.288216000
H	0.066796000	-0.284848000	0.936754000
F	10.253510000	-0.069013000	3.578438000
F	8.368287000	-0.028340000	1.575288000
F	12.988831000	-0.052839000	2.969828000
F	13.816101000	0.005105000	0.285568000
F	11.942041000	0.046542000	-1.748146000
F	-1.283398000	-0.686682000	2.814478000
F	-1.402113000	-0.769424000	5.577037000
F	3.483374000	0.329605000	3.075233000
F	3.337990000	0.234597000	5.817007000
F	0.909576000	-0.311904000	7.104911000
F	-7.259682000	2.663421000	-0.013806000
F	-9.695634000	3.832795000	0.497892000
F	-9.948838000	6.621371000	0.618700000
F	-7.688541000	8.241030000	0.212233000
F	-5.226221000	7.092273000	-0.303530000
F	-5.388389000	-6.977357000	-0.561136000
F	-7.874506000	-8.089852000	-0.082556000
F	-9.790105000	-3.651602000	0.336177000
F	-7.329728000	-2.518203000	-0.137847000
F	-10.101220000	-6.436764000	0.371914000

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	x(Å)	y(Å)	z(Å)
C	0.752885000	-0.000659000	-0.000932000
C	1.454213000	0.872012000	0.876235000
C	1.454924000	-0.872920000	-0.877962000
N	2.871529000	-0.886330000	-0.891089000
N	2.870835000	0.886029000	0.889877000
B	3.779621000	0.000944000	-0.001341000
C	0.982207000	-1.849376000	-1.860133000
C	2.137729000	-2.418856000	-2.432476000
C	3.300701000	-1.814895000	-1.824526000
C	0.980666000	1.847951000	1.858621000
C	2.135747000	2.417666000	2.431574000
C	3.299220000	1.814407000	1.823846000
C	-0.752978000	-0.000891000	-0.001139000
C	-1.454710000	0.878940000	-0.870851000
N	-2.871330000	0.892914000	-0.883868000
B	-3.779658000	0.006286000	0.006287000
N	-2.871239000	-0.895556000	0.880935000
C	-1.454628000	-0.881480000	0.867848000
C	-3.300179000	1.828644000	-1.810273000
C	-2.137025000	2.436757000	-2.413713000
C	-0.981674000	1.862549000	-1.845798000
C	-3.299964000	-1.834276000	1.804379000
C	-2.136719000	-2.444645000	2.405366000
C	-0.981458000	-1.868389000	1.839342000
F	-4.643983000	-0.806520000	-0.817403000
F	-4.614392000	0.834329000	0.845500000
F	4.631004000	-0.826032000	0.821866000
F	4.627438000	0.830082000	-0.826095000
C	-0.449129000	2.215609000	2.229845000
H	-0.440901000	2.987045000	3.015088000
H	-1.010443000	2.613368000	1.368757000
H	-1.013365000	1.348980000	2.610897000
C	-0.447311000	-2.217798000	-2.231678000
H	-1.011557000	-1.351546000	-2.613638000
H	-0.438492000	-2.989809000	-3.016355000
H	-1.008843000	-2.615090000	-1.370502000

C	0.448225000	-2.241156000	2.205873000
H	0.439788000	-3.016354000	2.987400000
H	1.006681000	-2.636258000	1.341633000
H	1.015349000	-1.377715000	2.589752000
C	0.447931000	2.233409000	-2.214566000
H	1.013140000	1.369317000	-2.599848000
H	0.439305000	3.008986000	-2.995715000
H	1.008442000	2.627253000	-1.351120000
C	4.718447000	2.068026000	2.078115000
H	5.437825000	1.495414000	1.498265000
C	5.124410000	2.996704000	3.016703000
H	4.368570000	3.548929000	3.577057000
C	4.720141000	-2.067917000	-2.078213000
H	5.439029000	-1.495042000	-1.498015000
C	5.126920000	-2.996580000	-3.016459000
H	4.371571000	-3.549261000	-3.577029000
C	-4.719263000	-2.090167000	2.055937000
H	-5.438487000	-1.512375000	1.481050000
C	-5.125455000	-3.028204000	2.985056000
H	-4.369747000	-3.586104000	3.539951000
C	-4.719521000	2.084346000	-2.061775000
H	-5.438635000	1.502353000	-1.491003000
C	-5.125903000	3.026430000	-2.986715000
H	-4.370314000	3.588464000	-3.537579000
C	6.511669000	-3.354352000	-3.376064000
C	6.726477000	-4.349301000	-4.385431000
C	7.704187000	-2.798260000	-2.808026000
C	8.008202000	-4.766451000	-4.805230000
C	8.998941000	-3.198625000	-3.210753000
C	9.158174000	-4.187397000	-4.214080000
C	6.508837000	3.354990000	3.377028000
C	6.722731000	4.349896000	4.386631000
C	7.701860000	2.799448000	2.809513000
C	8.004078000	4.767525000	4.807110000
C	8.996249000	3.200299000	3.212926000
C	9.154577000	4.189020000	4.216447000
C	-6.510496000	3.388569000	-3.342514000
C	-7.703256000	2.820496000	-2.786987000
C	-6.724860000	4.400947000	-4.334495000
C	-8.997836000	3.225919000	-3.185188000
C	-8.006403000	4.823459000	-4.749458000
C	-9.156632000	4.232148000	-4.171080000
C	-6.509969000	-3.390220000	3.341284000
C	-7.702854000	-2.827485000	2.780616000
C	-6.724110000	-4.396742000	4.339252000
C	-8.997344000	-3.232367000	3.179663000
C	-8.005559000	-4.818575000	4.755199000
C	-9.155919000	-4.232624000	4.171648000
H	2.146385000	-3.183880000	-3.201671000
H	2.143789000	3.182247000	3.201213000
H	-2.145038000	-3.218458000	3.165725000
H	-2.145460000	3.206864000	-3.177823000
F	5.619497000	-4.946320000	-4.994785000
F	8.148333000	-5.735497000	-5.788649000
F	10.424642000	-4.582636000	-4.611784000
F	10.120379000	-2.627478000	-2.627480000
F	7.617615000	-1.823728000	-1.818663000
F	7.616172000	1.824968000	1.820024000
F	10.118214000	2.629679000	2.630148000
F	10.420684000	4.584730000	4.614821000
F	8.143329000	5.736501000	5.790719000
F	5.615207000	4.946349000	4.995537000
F	-5.617612000	5.010536000	-4.930769000
F	-8.146105000	5.809682000	-5.715710000
F	-10.422926000	4.632505000	-4.564184000
F	-10.119532000	2.642528000	-2.614667000
F	-7.617103000	1.828460000	-1.815139000

F	-7.616925000	-1.841599000	1.802512000
F	-10.119167000	-2.654392000	2.603904000
F	-10.422123000	-4.632419000	4.565615000
F	-8.145040000	-5.798988000	5.727378000
F	-5.616729000	-5.000988000	4.940696000

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	x(Å)	y(Å)	z(Å)
N	-3.290720000	-1.806137000	0.007312000
C	-2.224033000	-2.132100000	-0.789391000
C	-3.109544000	-0.724851000	0.792442000
C	-0.949260000	-1.392529000	-0.829602000
C	-1.878533000	0.091336000	0.840436000
C	-0.766246000	-0.258081000	-0.001528000
C	-4.080453000	-0.154030000	1.739468000
C	-3.453740000	0.965953000	2.338718000
C	-2.108117000	1.140422000	1.808378000
C	-2.148764000	-3.231466000	-1.720882000
C	-0.840713000	-3.177089000	-2.335455000
C	-0.094935000	-2.077879000	-1.817259000
C	0.508314000	0.541941000	0.001801000
C	0.690748000	1.677823000	-0.842370000
C	1.607062000	0.212911000	0.850734000
C	1.960641000	2.424900000	-0.794227000
C	2.830329000	1.034526000	0.810410000
N	3.012866000	2.117917000	0.009831000
C	1.838591000	-0.836048000	1.840440000
C	3.162460000	-0.645830000	2.375036000
C	3.787712000	0.487163000	1.763384000
C	-0.149122000	2.341582000	-1.836145000
C	0.598087000	3.453385000	-2.365364000
C	1.886990000	3.525546000	-1.746920000
H	-3.901003000	1.612575000	3.091333000
H	-0.473552000	-3.873186000	-3.087355000
H	3.612108000	-1.279609000	3.137110000
H	0.225370000	4.134401000	-3.128185000
C	-3.250520000	-4.236314000	-1.984858000
H	-3.553539000	-4.225131000	-3.048884000
H	-2.913052000	-5.265821000	-1.760314000
H	-4.129995000	-4.010092000	-1.364801000
C	-5.472377000	-0.695110000	1.989641000
H	-6.079588000	-0.657838000	1.066866000
H	-5.432647000	-1.756808000	2.291691000
H	-5.988790000	-0.119892000	2.775064000
C	-1.162440000	2.249114000	2.237418000
H	-1.610291000	2.847859000	3.046491000
H	-0.197693000	1.846214000	2.591120000
H	-0.924676000	2.925405000	1.396721000
C	1.319767000	-1.708816000	-2.228919000
H	2.017803000	-1.763107000	-1.374611000
H	1.681914000	-2.389009000	-3.016544000
H	1.375329000	-0.673220000	-2.607814000
C	-1.556093000	1.965000000	-2.266726000
H	-1.919043000	2.653134000	-3.046829000
H	-1.596365000	0.935005000	-2.662711000
H	-2.261642000	1.996830000	-1.417649000
C	0.890423000	-1.945267000	2.262307000
H	0.665962000	-2.626992000	1.422418000
H	1.329443000	-2.537851000	3.080822000
H	-0.080142000	-1.543185000	2.601242000
C	5.171365000	1.046752000	2.024043000
H	5.286562000	1.351458000	3.081229000
H	5.953121000	0.290782000	1.821753000
H	5.354004000	1.922204000	1.384049000
C	2.991814000	4.530507000	-2.001618000
H	3.861215000	4.309413000	-1.365512000
H	3.313438000	4.511092000	-3.059832000

H	2.651138000	5.561338000	-1.789393000

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	x(Å)	y(Å)	z(Å)
N	-3.569647000	-2.212360000	-0.071503000
C	-2.522160000	-2.525244000	-0.876324000
C	-3.385293000	-1.150434000	0.753994000
C	-1.234601000	-1.800429000	-0.906412000
C	-2.151435000	-0.340093000	0.824346000
C	-1.086000000	-0.699991000	-0.031834000
C	-4.340725000	-0.608694000	1.709197000
C	-3.701931000	0.509454000	2.348573000
C	-2.377579000	0.696413000	1.834579000
C	-2.458060000	-3.607327000	-1.847926000
C	-1.157311000	-3.543569000	-2.457081000
C	-0.394812000	-2.461624000	-1.908064000
N	0.179676000	0.075221000	-0.015828000
C	0.332807000	1.155140000	-0.856987000
C	1.197512000	-0.287186000	0.837976000
C	1.581061000	1.930950000	-0.853654000
C	2.456221000	0.471214000	0.861792000
C	2.648742000	1.586727000	0.010555000
C	1.289636000	-1.383157000	1.823755000
C	2.579185000	-1.267990000	2.412721000
C	3.312484000	-0.154364000	1.851767000
C	-0.585171000	1.744662000	-1.852149000
C	0.113896000	2.845807000	-2.420303000
C	1.429880000	2.986651000	-1.837536000
H	-4.153703000	1.132358000	3.117371000
H	-0.793959000	-4.219260000	-3.228145000
H	3.578814000	2.156299000	0.020602000
H	2.958203000	-1.933870000	3.184345000
H	-0.294717000	3.492936000	-3.192845000
C	4.714081000	0.267241000	2.231837000
H	4.783242000	0.461766000	3.317492000
H	5.436879000	-0.540316000	2.012005000
H	5.038264000	1.172168000	1.697324000
C	2.449832000	4.044705000	-2.193618000
H	3.393832000	3.917975000	-1.643628000
H	2.673218000	4.023846000	-3.275739000
H	2.056333000	5.054682000	-1.974692000
C	-1.988752000	1.324234000	-2.245276000
H	-2.380473000	2.010097000	-3.010664000
H	-2.009144000	0.299905000	-2.654268000
H	-2.676504000	1.334475000	-1.383350000
C	0.268496000	-2.444031000	2.188400000
H	-0.018010000	-3.054294000	1.315582000
H	0.684555000	-3.111404000	2.957320000
H	-0.660880000	-1.998178000	2.581255000
C	-1.416174000	1.783782000	2.286007000
H	-1.881794000	2.409906000	3.061576000
H	-0.486701000	1.358891000	2.706657000
H	-1.121706000	2.443416000	1.449611000
C	1.024201000	-2.102649000	-2.317984000
H	1.724628000	-2.168235000	-1.465584000
H	1.382278000	-2.786731000	-3.101700000
H	1.088608000	-1.072245000	-2.712102000
C	-3.570050000	-4.590833000	-2.133172000
H	-3.868960000	-4.552373000	-3.196932000
H	-3.241147000	-5.627708000	-1.934639000
H	-4.448506000	-4.373381000	-1.510050000
C	-5.731673000	-1.147995000	1.953457000
H	-5.934722000	-2.005936000	1.297766000
H	-5.852414000	-1.467898000	3.005047000
H	-6.495560000	-0.370019000	1.770236000

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	x(Å)	y(Å)	z(Å)
C	-3.153749000	-2.009572000	-0.059210000
C	-3.046276000	-0.884278000	-0.914290000
C	-2.074337000	-2.270474000	0.821642000
C	-1.856189000	-0.019370000	-0.887671000
C	-0.886069000	-1.403006000	0.847178000
N	-0.836817000	-0.321814000	-0.008463000
C	-1.850679000	-3.309971000	1.809163000
C	-0.550234000	-3.060982000	2.410179000
C	0.066090000	-1.911417000	1.852624000
C	-3.938802000	-0.331458000	-1.916212000
C	-3.286426000	0.842065000	-2.474373000
C	-2.019704000	1.063796000	-1.875509000
N	0.340570000	0.533274000	0.015309000
C	1.395430000	0.229383000	-0.820588000
C	0.355870000	1.613982000	0.872623000
C	2.587214000	1.092170000	-0.796502000
C	1.545787000	2.479122000	0.898167000
C	2.660917000	2.216520000	0.063374000
C	-0.637465000	2.124139000	1.836650000
C	-0.042842000	3.271660000	2.421209000
C	1.282654000	3.518221000	1.876268000
C	1.598328000	-0.853176000	-1.801661000
C	2.889411000	-0.633029000	-2.346768000
C	3.520097000	0.538557000	-1.760543000
C	2.198989000	4.650751000	2.266546000
C	4.891785000	1.064369000	-2.102290000
C	-5.294238000	-0.859431000	-2.314758000
C	-2.779772000	-4.445472000	2.158609000
H	-4.035159000	-2.651115000	-0.078152000
H	-0.104204000	-3.675170000	3.188968000
H	-3.711988000	1.471061000	-3.252756000
H	3.543545000	2.856354000	0.082192000
H	-0.520368000	3.886573000	3.180499000
H	3.345797000	-1.262236000	-3.107347000
H	2.411732000	4.622085000	3.351403000
H	3.154858000	4.629102000	1.724664000
H	1.712854000	5.625904000	2.076543000
H	4.968717000	1.274787000	-3.185029000
H	5.144698000	1.981019000	-1.551206000
H	5.664091000	0.303083000	-1.883672000
H	-5.560932000	-1.785599000	-1.786572000
H	-6.078344000	-0.105782000	-2.111517000
H	-5.331892000	-1.053276000	-3.402507000
H	-3.717946000	-4.417574000	1.586877000
H	-2.288414000	-5.419095000	1.973473000
H	-3.026463000	-4.428252000	3.236357000
C	1.426233000	-1.368833000	2.255399000
H	1.864417000	-2.012021000	3.031057000
H	2.129923000	-1.342031000	1.405809000
H	1.358124000	-0.347176000	2.667703000
C	-1.074292000	2.199473000	-2.226373000
H	-0.861888000	2.845515000	-1.357191000
H	-0.109265000	1.828547000	-2.612850000
H	-1.526107000	2.827934000	-3.006260000
C	0.667248000	-1.987184000	-2.193928000
H	1.147284000	-2.608934000	-2.962250000
H	0.426005000	-2.640449000	-1.337649000
H	-0.284424000	-1.615050000	-2.611034000
C	-2.015912000	1.585579000	2.178137000
H	-2.684440000	1.572586000	1.300138000
H	-1.971339000	0.559069000	2.581325000
H	-2.481682000	2.223360000	2.942108000