

SUPPORTING INFORMATION

Theoretical tuning the singlet-triplet energy gap to achieve efficient long-wavelength TADF emitters: the Impact of Substituents

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Contents

Table S1 Computed dihedral angles (θ_1 , θ_2 , and θ_3) and bond lengths (l_1 , l_2 , and l_3) of molecule 1 based on the optimized S_0 geometries using different functionals and 6-31G* basis set (the unit of dihedral angles is degree, and bond lengths is angstroms)

Table S2 Computed transition energies (E_{VA} and E_{VE}), oscillator strengths (f_{VA} and f_{VE}) and configuration interaction (CI) description of S_1 and T_1 transitions using TD-B3LYP and TD-BMK, and 6-31G* basis set in toluene based on the optimized S_0 and S_1 geometries (HOMO is abbreviated as "H", and LUMO as "L").

Table S3 The excitation and emission energies and absorption and emission wavelengths of molecule 1 using BMK functional in toluene and gas phase.

Table S4 The excitation and emission energies and absorption and emission wavelengths, as well as the singlet-triplet energy gap (ΔE_{ST}) of molecule 1 obtained using PBE0/6-311G(d), M06-2X/6-311G(d) and CAM-B3LYP/6-311G(d) methods in toluene.

Figure S1 The HOMO, LUMO distributions of the designed molecules at the lowest singlet state (S_1).

Figure S2 The electron-hole (e-h) distribution and the overlap of e-h for S_1 of molecules 2 to 8.

Figure S3-S12 Natural transition orbitals of the S_1 , S_2 , T_1 , T_2 and T_3 states for molecules 2-11.

Figure S13 The energy landscape of vertical excitation for molecules 2 to 8 based on the S_0 geometry in toluene using BMK functional.

The Cartesian coordinates of the investigated molecules for S_0 and S_1 geometry optimization.

Table S1 Computed dihedral angles (θ_1 , θ_2 , and θ_3) and bond lengths (l_1 , l_2 , and l_3) of molecule 1 based on the optimized S_0 geometries using different functionals and 6-31G* basis set (the unit of dihedral angles is degree, and bond lengths is angstroms)

Compd 1	$\theta_1/\theta_2/\theta_3(\text{deg})$	$l_1/l_2/l_3(\text{\AA})$
B3LYP	-19.2/51.8/48.1	1.482/1.417/1.427
MPW1B95	-21.0/49.5/44.3	1.473/1.405/1.414
BMK	-19.3/51.2/48.5	1.482/1.416/1.426
M062X	-24.7/49.6/47.0	1.482/1.412/1.421
PBE0	-21.2/50.8/47.9	1.477/1.409/1.418
CAM-B3LYP	-22.8/52.8/50.6	1.482/1.414/1.423

Table S2 Computed transition energies (E_{VA} and E_{VE}), oscillator strengths (f_{VA} and f_{VE}) and configuration interaction (CI) description of S_1 and T_1 transitions using TD-B3LYP and TD-BMK, and 6-31G* basis set in toluene based on the optimized S_0 and S_1 geometries (HOMO is abbreviated as “H”, and LUMO as “L”)

	Functional		S_0 geometry in toluene				S_1 geometry in toluene			
			E_{VA} (eV)	CI	cj %	f_{VA}	E_{VE} (eV)	CI	cj %	f_{VE}
1	BMK	S_1	3.1650	H→L	90.4	0.3483	2.5469	H→L	95.0	0.1740
		S_2	3.6011	H-1→L	96.3	0.0128	3.1469	H-1→L	97.4	0.0083
		S_3	3.6261	H→L+2	91.4	0.0367	3.4406	H→L+2	93.1	0.0355
		T_1	2.7527	H-4→L	34.9	0.0000	2.3207	H→L	42.7	0.0000
		T_2	3.1129	H→L+2	75.0	0.0000	2.6411	H→L	48.5	0.0000
		T_3	3.1197	H-12→L	61.1	0.0000	2.8421	H→L+2	84.3	0.0000
		T_4	3.1495	H→L	36.3	0.0000				
		T_5	3.2406	H-3→L	32.7	0.0000				
	B3LYP	S_1	2.2709	H→L	99.2	0.1325	1.7223	H→L	99.3	0.1045
		S_2	2.5505	H-1→L	99.6	0.0046	2.1742	H-1→L	99.5	0.0050
		S_3	3.1585	H→L+2	59.6	0.1348	2.8095	H→L+1	97.8	0.0586
		T_1	2.1920	H→L	89.9	0.0000	1.6626	H→L	96.0	0.0000
		T_2	2.5393	H-1→L	98.1	0.0000	2.1648	H-1→L	99.0	0.0000
		T_3	2.6282	H-4→L	46.0	0.0000	2.2622	H-4→L	59.9	0.0000
2	BMK	S_1	3.1282	H→L	92.3	0.1757	2.4831	H→L	95.3	0.1527
		S_2	3.5274	H-1→L	97.5	0.0046	3.0737	H-1→L	97.5	0.0061
		S_3	3.6688	H→L+2	91.4	0.0417	3.4565	H→L+2	92.3	0.0338
		T_1	2.7711	H-4→L	25.9	0.0000	2.2657	H→L	43.6	0.0000
		T_2	3.1115	H-13→L	42.7	0.0000	2.5885	H→L	48.9	0.0000
		T_3	3.1312	H-13→L	37.8	0.0000	2.8564	H→L+2	83.6	0.0000
		T_4	3.1467	H→L+2	79.5	0.0000				
		T_5	3.2684	H-3→L+2	35.1	0.0000				
	B3LYP	S_1	2.2000	H→L	99.2	0.0653	1.6663	H→L	99.4	0.0925
		S_2	2.4717	H-1→L	99.6	0.0021	2.1155	H-1→L	99.5	0.0042
		S_3	3.0959	H→L+1	96.5	0.0958	2.7403	H→L+1	97.9	0.0512
		T_1	2.1569	H→L	93.8	0.0000	1.6100	H→L	96.1	0.0000
		T_2	2.4662	H-1→L	98.8	0.0000	2.1070	H-1→L	98.6	0.0000
		T_3	2.5898	H-4→L	28.9	0.0000	2.2055	H-4→L	37.7	0.0000
3	BMK	S_1	3.2043	H→L	93.2	0.0944	2.5511	H→L	95.5	0.0462
		S_2	3.5897	H-1→L	97.5	0.0023	3.1435	H-1→L	97.6	0.0019
		S_3	3.6382	H→L+2	92.0	0.0417	3.4314	H→L+2	93.3	0.0409
		T_1	2.8388	H-4→L	54.7	0.0000	2.3931	H-4→L	44.0	0.0000
		T_2	3.1180	H→L+2	80.4	0.0000	2.5811	H→L	71.1	0.0000
		T_3	3.1198	H-13→L	43.7	0.0000	2.8282	H→L+2	84.7	0.0000
		T_4	3.1861	H→L	74.3	0.0000				
		T_5	3.2640	H-3→L+2	37.0	0.0000				
	B3LYP	S_1	2.2465	H→L	99.2	0.0341	1.6939	H→L	99.2	0.0274
		S_2	2.5177	H-1→L	99.6	0.0011	2.1588	H-1→L	99.5	0.0012

		S ₃	3.1583	H→L+1	91.9	0.0630	2.8027	H→L+1	97.9	0.0154
		T ₁	2.2255	H→L	96.5	0.0000	1.6768	H→L	98.2	0.0000
		T ₂	2.5139	H-1→L	99.1	0.0000	2.1546	H-1→L	99.2	0.0000
		T ₃	2.6156	H-4→L	61.5	0.0000	2.2274	H-4→L	73.3	0.0000
4	BMK	S ₁	2.9517	H→L	92.1	0.0007	2.2684	H→L	94.3	0.0003
		S ₂	3.3147	H-1→L	96.8	0.0036	2.8539	H-1→L	96.7	0.0019
		S ₃	3.6580	H-14→L	87.1	0.0033	3.4706	H→L+3	92.9	0.0410
		T ₁	2.8505	H-4→L	72.8	0.0000	2.2639	H→L	94.0	0.0000
		T ₂	2.9467	H→L	90.9	0.0000	2.4600	H-4→L	85.8	0.0000
		T ₃	3.1086	H-13→L	79.5	0.0000	2.8478	H-1→L	95.8	0.0000
		T ₄	3.1580	H→L+2	79.7	0.0000				
		T ₅	3.2738	H-2→L+2	38.4	0.0000				
	B3LYP	S ₁	2.0186	H→L	98.7	0.0003	1.4523	H→L	98.8	0.0002
		S ₂	2.2756	H→L	99.4	0.0019	1.9119	H-1→L	99.3	0.0013
		S ₃	2.9184	H→L+1	96.1	0.0003	2.5742	H→L+1	97.7	0.0001
		T ₁	2.0167	H→L	98.6	0.0000	1.4496	H→L	98.7	0.0000
		T ₂	2.2730	H-1→L	99.3	0.0000	1.9075	H-1→L	99.2	0.0000
		T ₃	2.5989	H-6→L	78.6	0.0000	2.2427	H-4→L	88.5	0.0000
5	BMK	S ₁	3.1655	H→L	95.3	0.0100	2.4891	H→L	97.3	0.0066
		S ₂	3.5583	H-1→L	97.9	0.0025	3.1013	H-1→L	98.1	0.0068
		S ₃	3.6300	H→L+2	92.4	0.0436	3.4206	H→L+2	93.5	0.0355
		T ₁	2.8587	H-4→L	59.7	0.0000	2.3811	H→L	47.4	0.0000
		T ₂	3.1012	H-12→L	36.8	0.0000	2.5190	H→L	47.2	0.0000
		T ₃	3.1134	H→L+2	67.4	0.0000	2.8141	H→L+2	84.9	0.0000
		T ₄	3.1412	H→L	45.1	0.0000				
		T ₅	3.2605	H-3→L+2	36.7	0.0000				
	B3LYP	S ₁	2.2149	H→L	99.2	0.0047	1.6347	H→L	99.5	0.0046
		S ₂	2.4979	H-1→L	99.5	0.0007	2.1250	H-1→L	99.6	0.0033
		S ₃	3.1541	H→L+1	97.3	0.0024	2.7612	H→L+1	98.7	0.0024
		T ₁	2.1927	H→L	97.4	0.0000	1.6105	H→L	98.5	0.0000
		T ₂	2.4952	H-1→L	98.7	0.0000	2.1184	H-1→L	96.2	0.0000
		T ₃	2.6252	H-4→L	66.5	0.0000	2.2428	H-4→L	75.7	0.0000
6	BMK	S ₁	3.2550	H→L	96.5	0.0042	2.5928	H→L	97.9	0.0042
		S ₂	3.6116	H-1→L	98.4	0.0021	3.1802	H-1→L	98.5	0.0020
		S ₃	3.6739	H→L+2	87.4	0.0448	3.4445	H→L+2	89.6	0.0371
		T ₁	2.8008	H-4→L	42.6	0.0000	2.3924	H-2→L	47.9	0.0000
		T ₂	3.1360	H-12→L	79.0	0.0000	2.5952	H→L	82.8	0.0000
		T ₃	3.1472	H→L+2	72.8	0.0000	2.8387	H→L+2	82.3	0.0000
		T ₄	3.2370	H→L	77.1	0.0000				
		T ₅	3.2842	H-3→L+2	35.8	0.0000				
	B3LYP	S ₁	2.2862	H→L	99.4	0.0020	1.7152	H→L	99.6	0.0029
		S ₂	2.5527	H→L	99.7	0.0005	2.1932	H-1→L	99.7	0.0008
		S ₃	3.1983	H→L+2	77.0	0.0196	2.8852	H→L+1	97.2	0.0023
		T ₁	2.2742	H→L	97.5	0.0000	1.6984	H→L	98.6	0.0000

		T ₂	2.5439	H-1→L	55.8	0.0000	2.1855	H-1→L	70.4	0.0000
		T ₃	2.5619	H-4→L	28.3	0.0000	2.2083	H-1→L	29.2	0.0000
7	BMK	S ₁	3.2241	H→L	96.3	0.0075	2.5646	H→L	97.6	0.0078
		S ₂	3.5842	H-1→L	98.2	0.0017	3.1562	H-1→L	98.3	0.0052
		S ₃	3.6395	H→L+2	87.7	0.0423	3.4187	H→L+2	90.3	0.0375
		T ₁	2.8523	H-4→L	64.5	0.0000	2.4330	H-4→L	62.7	0.0000
		T ₂	3.1131	H→L+2	21.2	0.0000	2.5529	H→L	89.1	0.0000
		T ₃	3.1213	H-12→L	59.0	0.0000	2.8143	H→L+2	83.2	0.0000
		T ₄	3.2175	H→L	80.9	0.0000				
		T ₅	3.2728	H-3→L+2	32.8	0.0000				
	B3LYP	S ₁	2.2507	H→L	99.4	0.0034	1.6911	H→L	99.5	0.0053
		S ₂	2.5196	H-1→L	99.7	0.0008	2.1702	H-1→L	99.6	0.0024
		S ₃	3.1616	H→L+2	65.7	0.0229	2.8276	H→L+1	98.3	0.0037
		T ₁	2.2446	H→L	99.0	0.0000	1.6791	H→L	99.2	0.0000
		T ₂	2.5175	H-1→L	98.3	0.0000	2.1636	H-1→L	92.7	0.0000
		T ₃	2.6028	H-4→L	67.9	0.0000	2.2335	H-4→L	73.5	0.0000
8	BMK	S ₁	2.9086	H→L	95.1	0.0016	2.1746	H→L	96.5	0.0014
		S ₂	3.2506	H-1→L	97.8	0.0081	2.7432	H-1→L	97.7	0.0157
		S ₃	3.6469	H-13→L	86.4	0.0028	3.4293	H→L+1	94.5	0.0029
		T ₁	2.8459	H-4→L	49.7	0.0000	2.1675	H→L	96.3	0.0000
		T ₂	2.9010	H→L	92.5	0.0000	2.4455	H-4→L	83.8	0.0000
		T ₃	3.1002	H-13→L	78.4	0.0000	2.7438	H-1→L	95.3	0.0000
		T ₄	3.1600	H→L+2	80.0	0.0000				
		T ₅	3.2474	H-1→L	96.1	0.0000				
	B3LYP	S ₁	1.9775	H→L	99.2	0.0010	1.3617	H→L	99.2	0.0010
		S ₂	2.2300	H-1→L	99.6	0.0041	1.8214	H-1→L	99.5	0.0107
		S ₃	2.8727	H→L+1	98.0	0.0016	2.4819	H→L+1	98.7	0.0014
		T ₁	1.9744	H→L	99.0	0.0000	1.3566	H→L	99.2	0.0000
		T ₂	2.2278	H-1→L	99.4	0.0000	1.8147	H-1→L	99.1	0.0000
		T ₃	2.5961	H-6→L	78.8	0.0000	2.4769	H→L+1	98.3	0.0000
9	BMK	S ₁	3.0194	H→L	91.9	0.3096	2.3753	H→L	95.9	0.0851
		S ₂	3.4394	H-1→L	97.3	0.0097	2.9594	H-1→L	97.8	0.0037
		S ₃	3.6219	H→L+2	91.8	0.0444	3.4379	H→L+2	92.5	0.0331
		T ₁	2.7188	H→L	38.6	0.0000	2.2837	H→L	71.6	0.0000
		T ₂	3.1115	H→L+2	70.2	0.0000	2.5540	H-4→L	52.0	0.0000
		T ₃	3.1184	H→L	35.0	0.0000	2.8346	H→L+2	84.5	0.0000
		T ₄	3.1885	H-13→L	78.4	0.0000				
		T ₅	3.2251	H-3→L+2	29.3	0.0000				
	B3LYP	S ₁	2.1327	H→L	99.3	0.1268	1.5375	H→L	99.4	0.0559
		S ₂	2.4068	H-1→L	99.6	0.0045	1.9935	H-1→L	99.6	0.0029
		S ₃	3.0591	H→L+1	96.6	0.1836	2.6611	H→L+1	98.0	0.0343
		T ₁	2.0652	H→L	93.6	0.0000	1.5060	H→L	98.3	0.0000
		T ₂	2.3980	H-1→L	98.8	0.0000	1.9879	H-1→L	99.4	0.0000
		T ₃	2.6424	H-2→L	28.8	0.0000	2.2750	H-4→L	69.0	0.0000

10	BMK	S ₁	2.8182	H→L	93.5	0.2838	2.1536	H→L	96.7	0.0401
		S ₂	3.2246	H-1→L	97.8	0.0086	2.7265	H-1→L	98.2	0.0019
		S ₃	3.6179	H→L+2	89.7	0.0771	3.3402	H→L+1	91.3	0.0295
		T ₁	2.5607	H→L	45.6	0.0000	2.1161	H→L	87.9	0.0000
		T ₂	2.9149	H→L	37.1	0.0000	2.3722	H-4→L	75.8	0.0000
		T ₃	3.1135	H→L+2	82.1	0.0000	2.7194	H-1→L	97.2	0.0000
		T ₄	3.1515	H-1→L	58.1	0.0000				
		T ₅	3.2221	H-14→L	84.2	0.0000				
	B3LYP	S ₁	1.9559	H→L	99.5	0.1318	1.3229	H→L	99.4	0.0300
		S ₂	2.2222	H-1→L	99.6	0.0053	1.7793	H-1→L	99.6	0.0019
		S ₃	2.8550	H→L+1	98.2	0.1384	2.4571	H→L+1	98.3	0.0155
		T ₁	1.8867	H→L	94.8	0.0000	1.3043	H→L	99.0	0.0000
		T ₂	2.2140	H-1→L	99.1	0.0000	1.7753	H-1→L	99.5	0.0000
		T ₃	2.4845	H-4→L	40.2	0.0000	2.1290	H-4→L	85.4	0.0000
11	BMK	S ₁	2.7317	H→L	94.3	0.3165	2.1002	H→L	97.0	0.0851
		S ₂	3.1337	H-1→L	98.2	0.0077	2.6651	H-1→L	98.3	0.0031
		S ₃	3.5974	H-13→L	73.9	0.0027	3.4226	H→L+1	74.4	0.0418
		T ₁	2.5176	H→L	55.6	0.0000	2.0470	H→L	88.2	0.0000
		T ₂	2.9044	H→L	32.5	0.0000	2.4013	H-4→L	67.9	0.0000
		T ₃	3.0708	H-13→L	64.1	0.0000	2.6560	H-1→L	97.2	0.0000
		T ₄	3.0899	H-1→L	75.2	0.0000				
		T ₅	3.1121	H→L+2	81.7	0.0000				
	B3LYP	S ₁	1.8485	H→L	99.5	0.1561	1.2619	H→L	99.5	0.0661
		S ₂	2.1116	H-1→L	99.7	0.0055	1.7041	H-1→L	99.6	0.0035
		S ₃	2.8353	H→L+1	98.2	0.0944	2.4884	H→L+1	98.1	0.0224
		T ₁	1.7843	H→L	96.2	0.0000	1.2294	H→L	98.9	0.0000
		T ₂	2.1037	H-1→L	99.3	0.0000	1.6986	H-1→L	99.5	0.0000
		T ₃	2.4876	H-2→L	32.5	0.0000	2.1611	H-4→L	71.8	0.0000

Table S3 The excitation and emission energies and absorption and emission wavelengths of molecule 1 using BMK functional in toluene and gas phase.

Methods	BMK(Toluene)	BMK(Gas)
$E_{VA}S_1$ (eV)	3.17	3.13
λ_{ab} (nm)	392	396
$E_{VE}S_1$ (eV)	2.55	2.43
λ_{em} (nm)	487	511
$\lambda_{em,expt}$ (nm)	526 nm in doped film, 544 nm in toluene	

Table S4 The excitation and emission energies and absorption and emission wavelengths, as well as the singlet-triplet energy gap (ΔE_{ST}) of molecule 1 obtained using PBE0/6-311G(d), M06-2X/6-311G(d) and CAM-B3LYP/6-311G(d) methods in toluene.

Methods	PBE0/6-311G(d)	M06-2X/6-311G(d)	CAM-B3LYP/6-311G(d)
$E_{VA}S_1$ (eV)	2.49	3.54	3.71
$E_{VA}T_1$ (eV)	2.34	3.05	2.60
$\Delta E_{ST, \text{Vertical}}$ (eV)	0.15	0.49	1.11
λ_{ab} (nm)	498	350	334
$E_{VE}S_1$ (eV)	1.85	2.93	3.05
$E_{VE}T_1$ (eV)	1.76	2.13	1.52
$\Delta E_{ST, \text{Adiabatic}}$ (eV)	0.09	0.80	1.53
λ_{em} (nm)	670	423	407

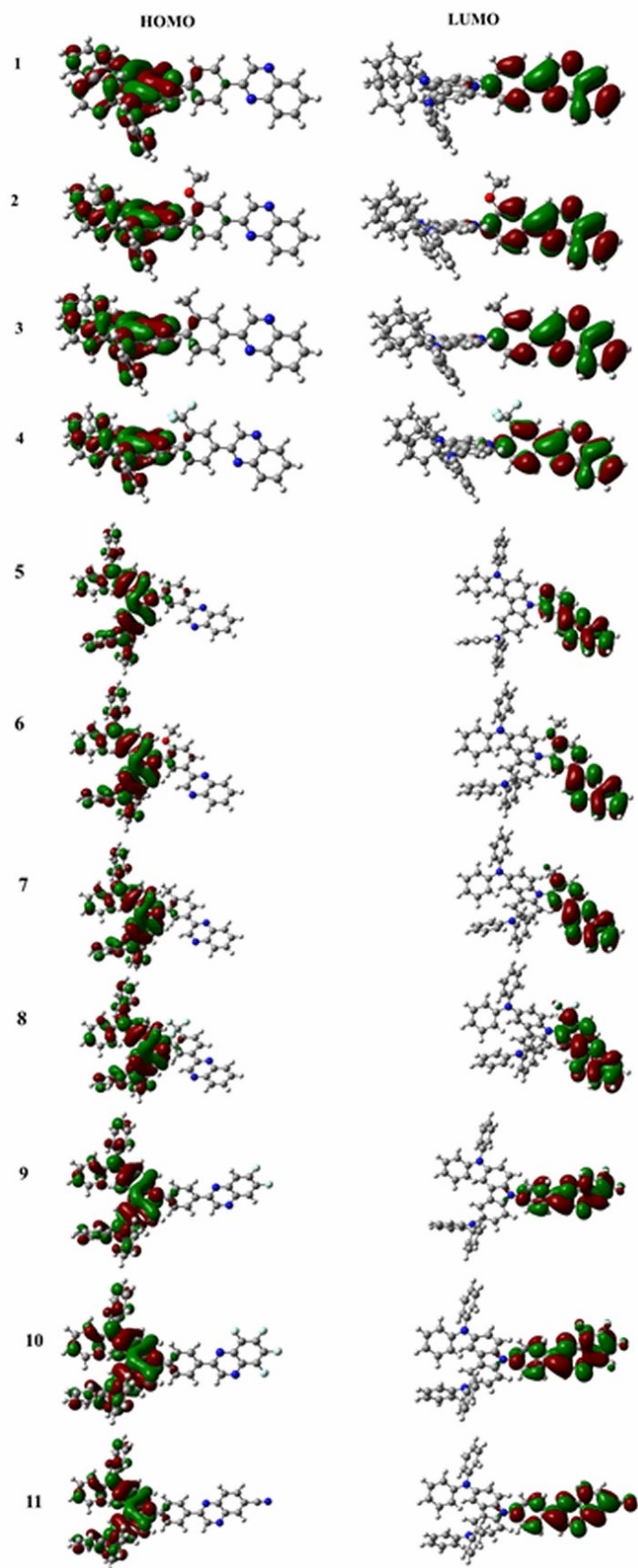


Figure S1 The HOMO, LUMO distributions of the designed molecules at the lowest singlet state (S_1) based on BMK/6-31G(d) level.

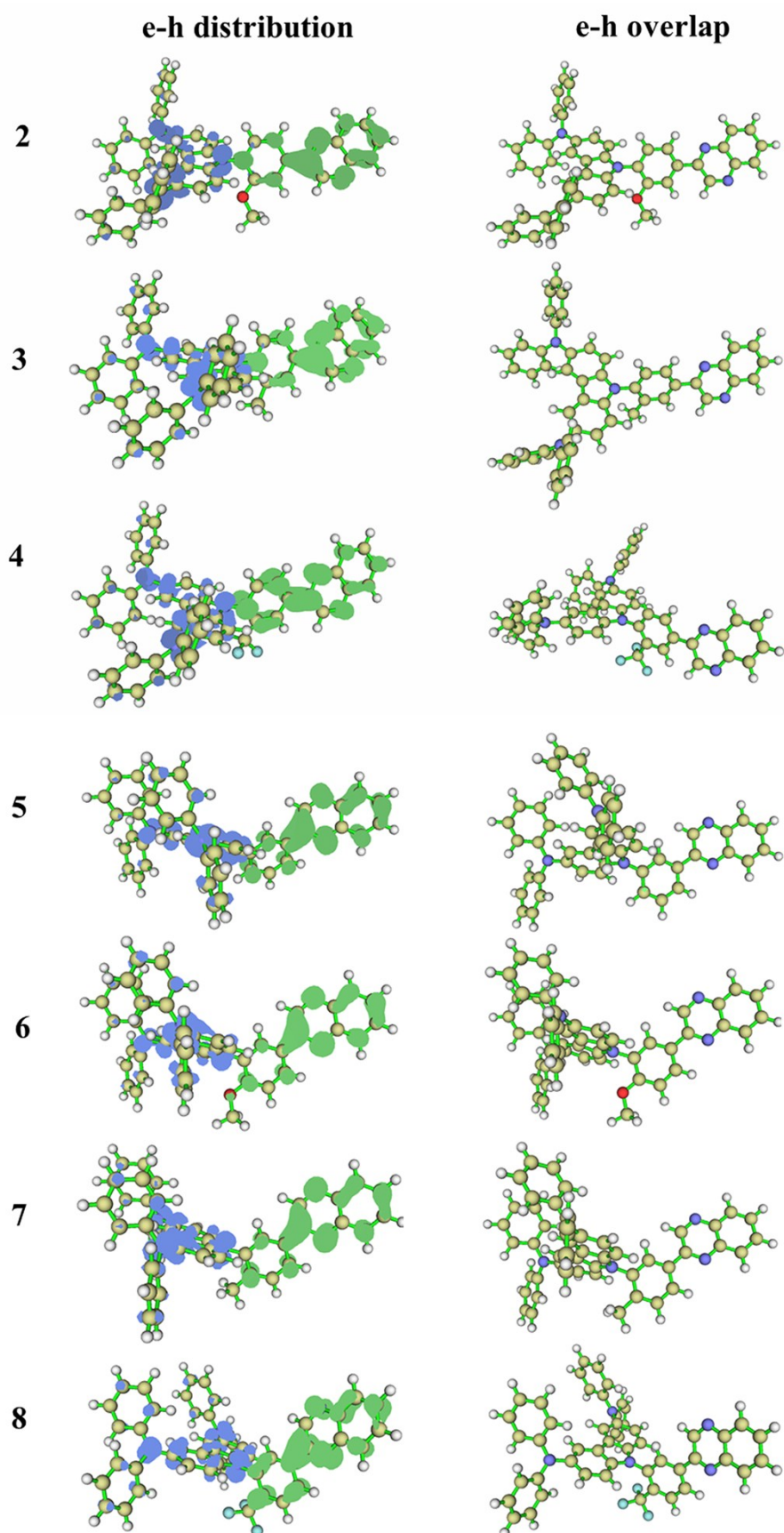


Figure S2 The electron-hole (e-h) distribution and the overlap of e-h for S_1 of molecules 2 to 8.

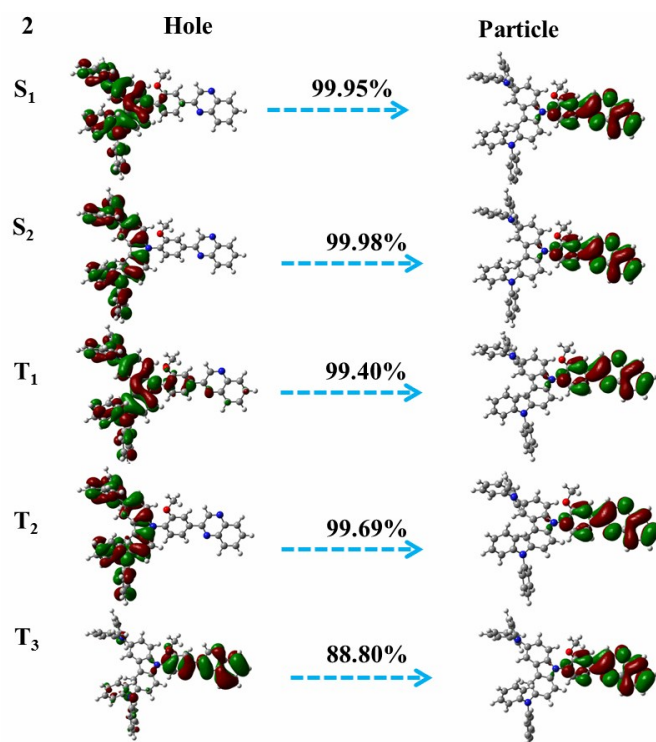


Figure S3 Natural transition orbitals of the S₁, S₂, T₁, T₂ and T₃ states for molecule 2.

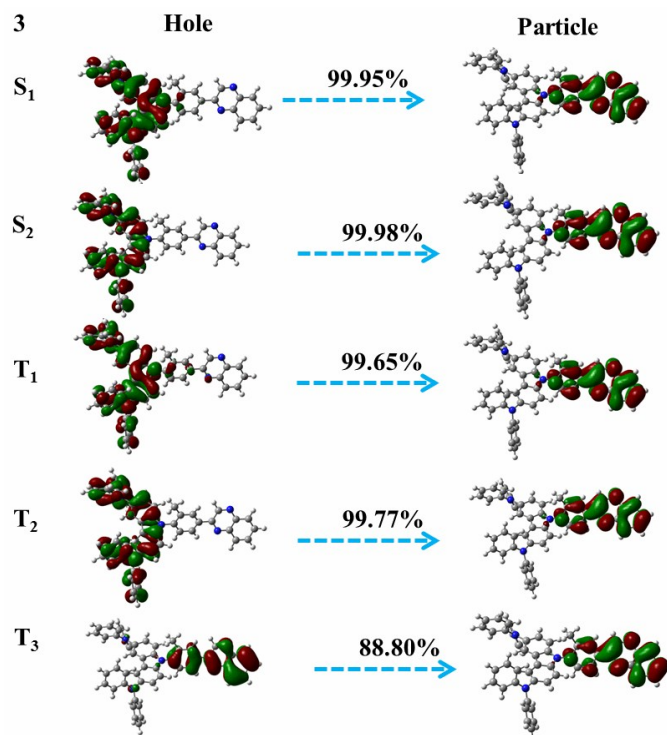


Figure S4 Natural transition orbitals of the S₁, S₂, T₁, T₂ and T₃ states for molecule 3.

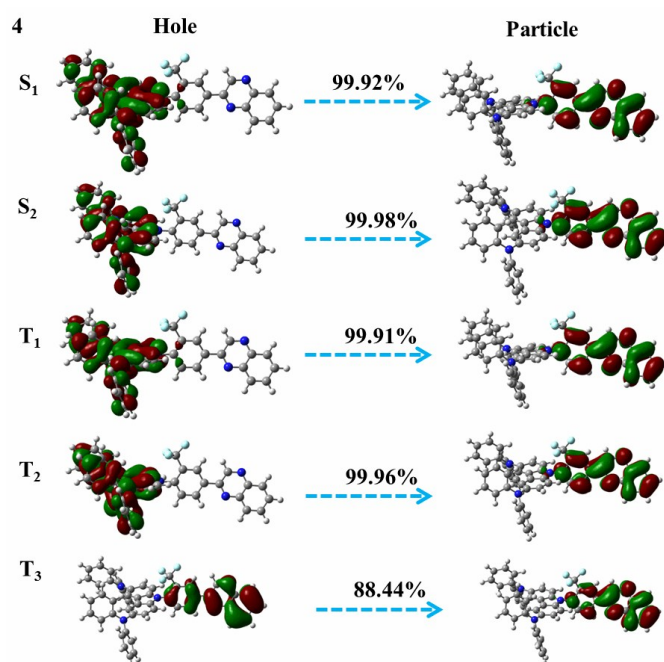


Figure S5 Natural transition orbitals of the S₁, S₂, T₁, T₂ and T₃ states for molecule 4.

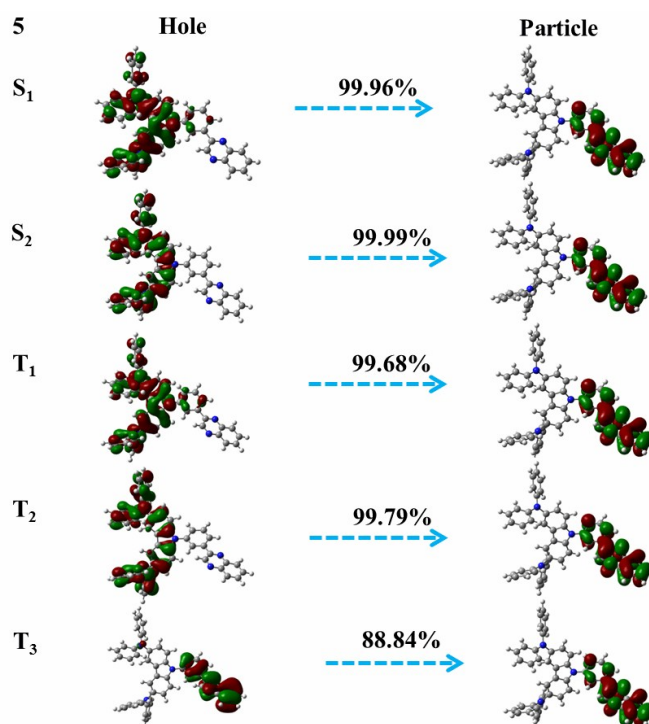


Figure S6 Natural transition orbitals of the S₁, S₂, T₁, T₂ and T₃ states for molecule 5.

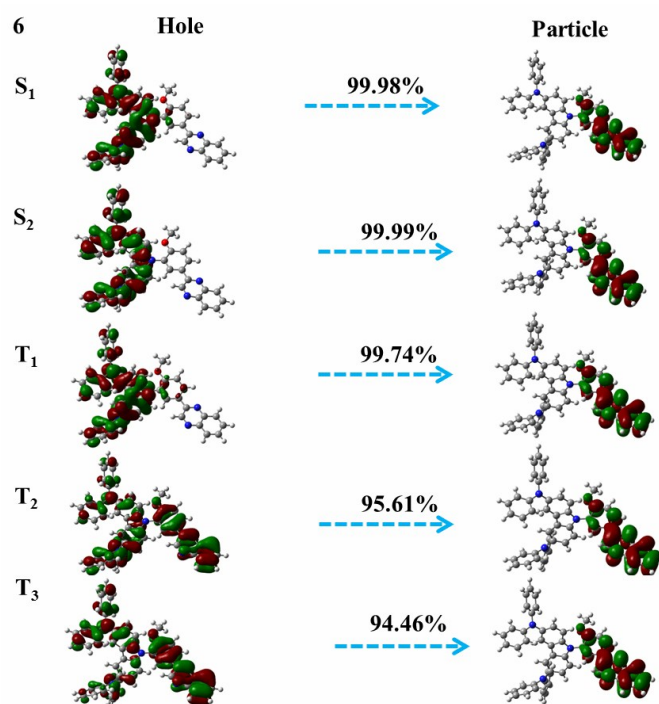


Figure S7 Natural transition orbitals of the S_1 , S_2 , T_1 , T_2 and T_3 states for molecule 6.

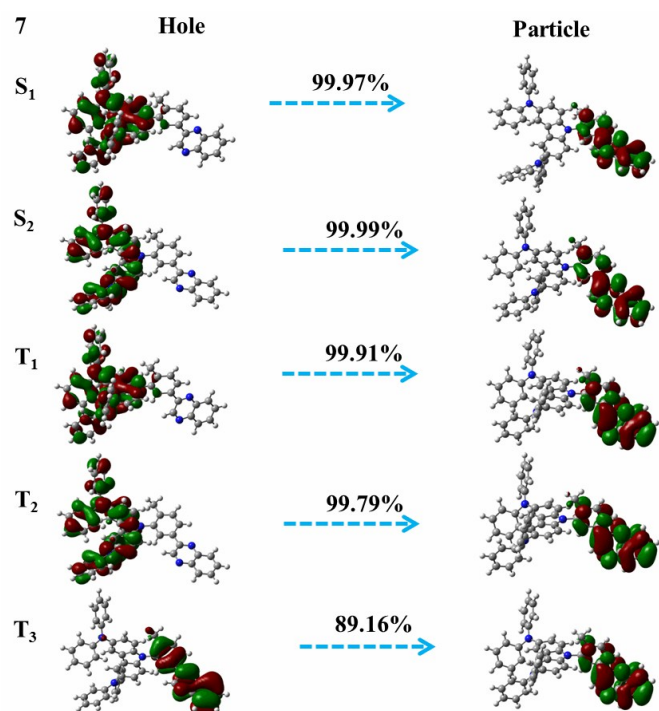


Figure S8 Natural transition orbitals of the S_1 , S_2 , T_1 , T_2 and T_3 states for molecule 7.

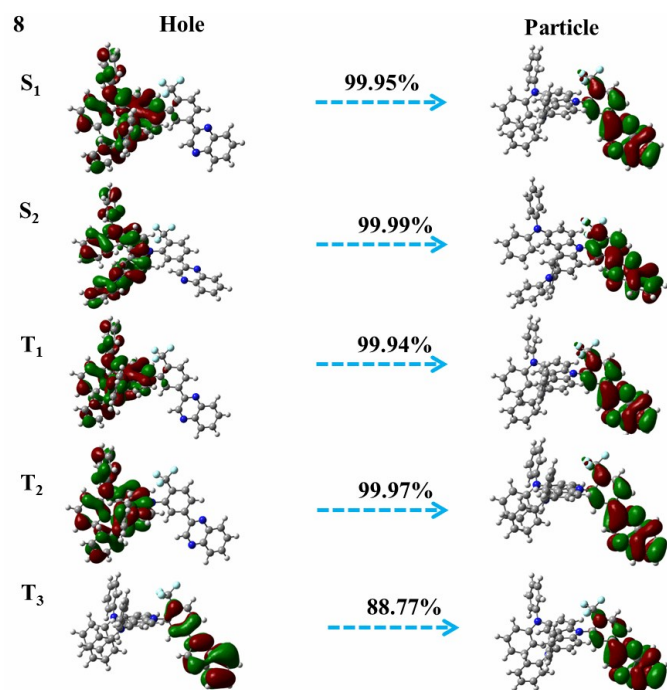


Figure S9 Natural transition orbitals of the S₁, S₂, T₁, T₂ and T₃ states for molecule 8.

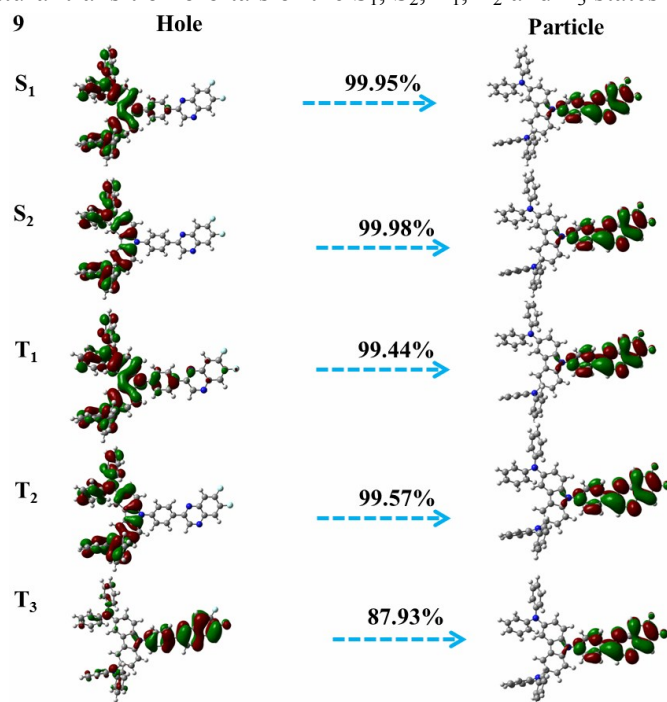


Figure S10 Natural transition orbitals of the S₁, S₂, T₁, T₂ and T₃ states for molecule 9.

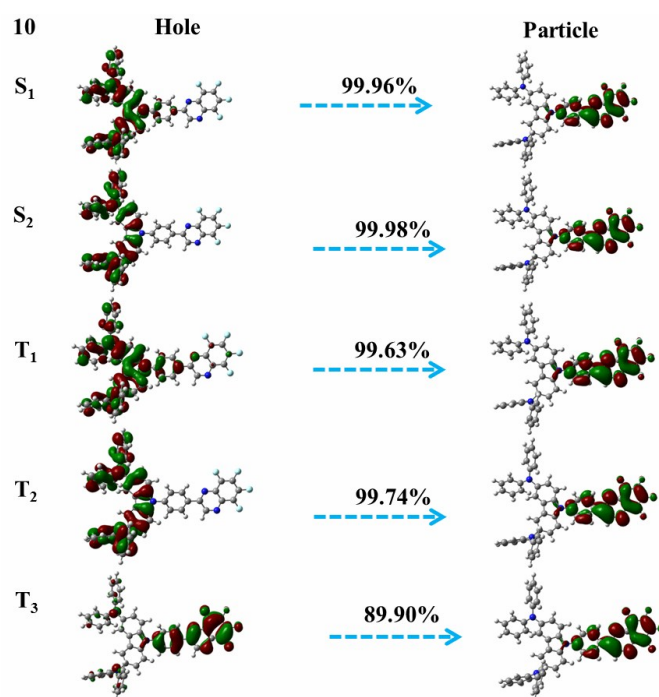


Figure S11 Natural transition orbitals of the S_1 , S_2 , T_1 , T_2 and T_3 states for molecule 10.

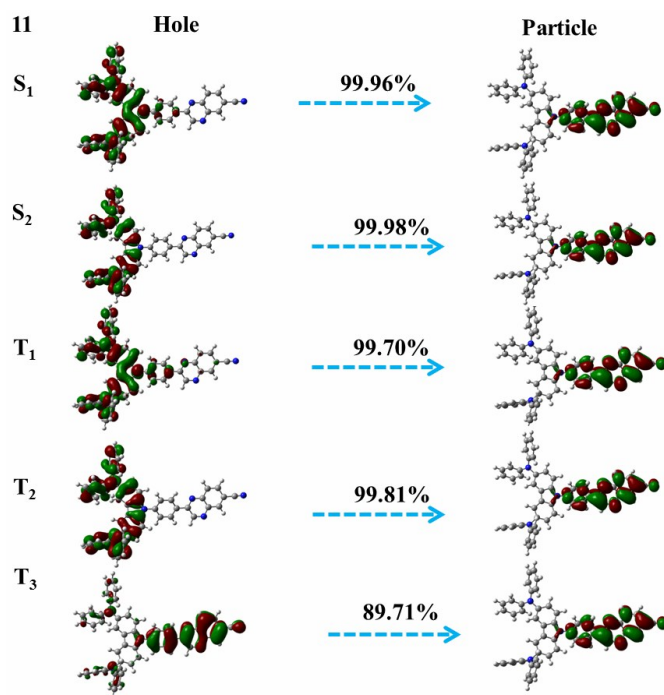


Figure S12 Natural transition orbitals of the S_1 , S_2 , T_1 , T_2 and T_3 states for molecule 11.

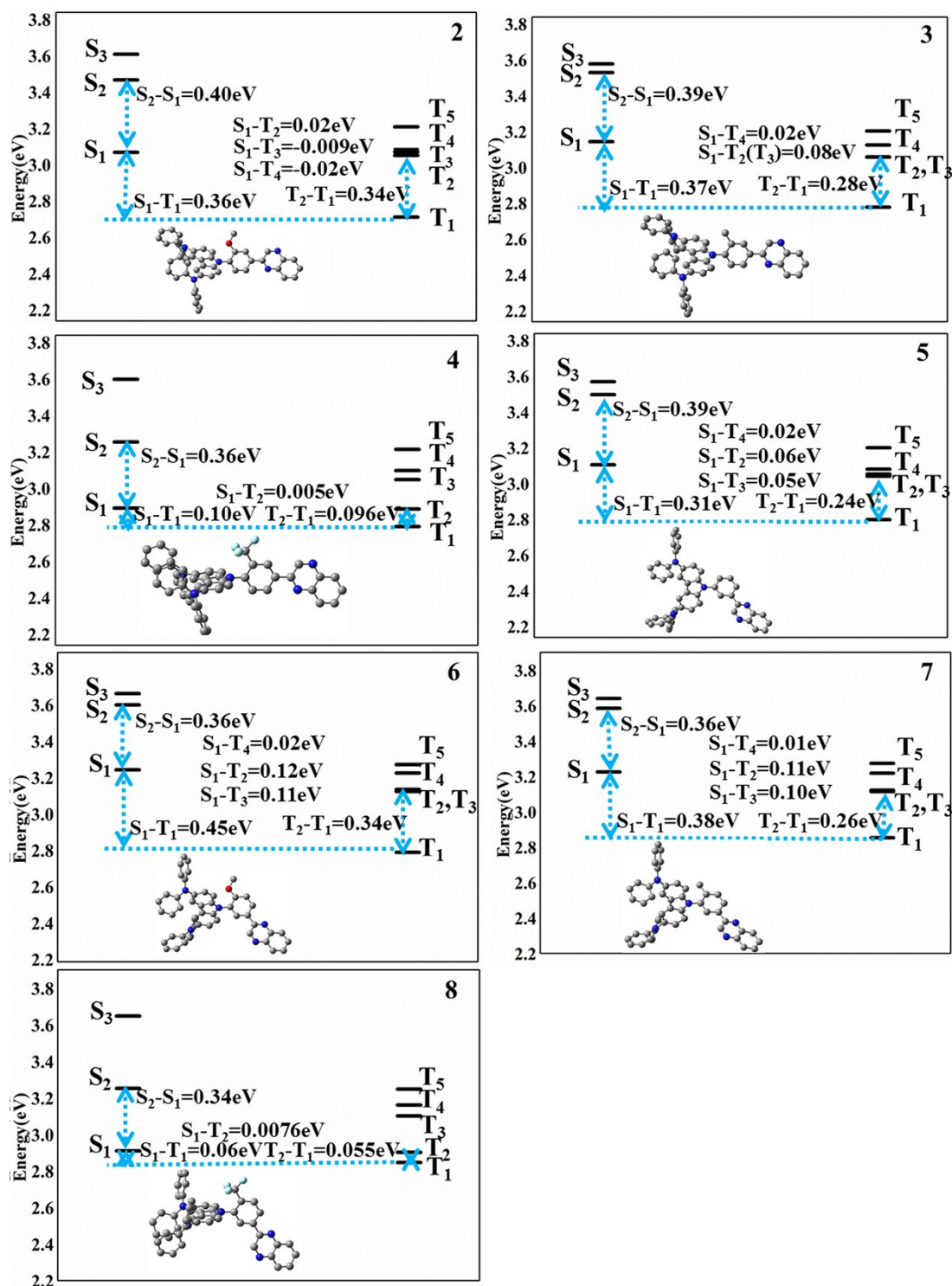


Figure S13 The energy landscape of vertical excitation for molecules 2 to 8 based on the S_0 geometry in toluene using BMK functional.

The Cartesian coordinates of the investigated molecules for S_0 and S_1 geometry optimization:

Cartesian coordinates of molecule 1 for S_0 and S_1 geometry optimization

S_0	B3LYP/6-31G(d)			S_1	BMK/6-31G(d)		
C	9.30033300	-0.91079300	-0.71977400	C	9.29714200	-0.92175200	-0.71765000
C	8.67951100	0.16626400	-0.01476500	C	8.67953800	0.16552900	-0.02531400
C	9.49365700	1.14692500	0.60931400	C	9.49649800	1.15330600	0.58379100
C	10.86526300	1.05475200	0.52689000	C	10.86812000	1.05822100	0.49975100
C	11.47932400	-0.01309900	-0.17666300	C	11.47902400	-0.01986200	-0.19100700
C	10.71337300	-0.98067800	-0.78941200	C	10.71007700	-0.99449000	-0.78939000
N	8.54301800	-1.87811200	-1.31575300	N	8.53584400	-1.89534000	-1.29967700
C	7.24030200	-1.75178600	-1.21941300	C	7.23295700	-1.76622900	-1.20202900
C	6.60073100	-0.66331500	-0.53888300	C	6.59746600	-0.66832600	-0.53301800
N	7.32557000	0.26962400	0.06045500	N	7.32527100	0.27172500	0.05174800
C	5.12489000	-0.55281100	-0.45875100	C	5.12172900	-0.55753900	-0.45010300
C	4.54200200	0.26920700	0.52153000	C	4.53928700	0.25328400	0.53978600
C	3.16276200	0.38747100	0.63283600	C	3.15976100	0.37206700	0.65114600
C	2.32005500	-0.30028300	-0.25364200	C	2.31861500	-0.30436100	-0.24508800
C	2.88850100	-1.10880400	-1.24645000	C	2.88601100	-1.10273200	-1.24647300
C	4.27120400	-1.23769500	-1.33948700	C	4.26885800	-1.23251900	-1.33957700
C	-2.19638700	-2.95482300	0.11193500	C	-2.20207700	-2.95269000	0.11439800
C	-0.88059900	-3.45973100	0.01494500	C	-0.88677000	-3.45935500	0.01813400
C	0.22188800	-2.61657000	-0.06955800	C	0.21709800	-2.61762500	-0.06462700
C	-0.00250700	-1.23715200	-0.08817300	C	-0.00615000	-1.23769000	-0.08149200
C	-1.31433400	-0.71074100	0.01108900	C	-1.31789600	-0.70965400	0.01631100
C	-2.40843900	-1.57318800	0.12147600	C	-2.41348600	-1.57109000	0.12473400
N	0.91358600	-0.17762200	-0.14777900	N	0.91093100	-0.17987000	-0.13984700
C	0.19453300	1.02427500	-0.08552300	C	0.19415500	1.02266100	-0.07855200
C	-1.18866200	0.73257600	0.00987600	C	-1.19011000	0.73344700	0.01499400
C	0.64855300	2.34467000	-0.14979900	C	0.65140300	2.34235600	-0.14081700
C	-0.29449500	3.36525900	-0.10071100	C	-0.29001900	3.36470300	-0.09321000
C	-1.67527100	3.09589100	0.02674200	C	-1.67168500	3.09756900	0.03097000
C	-2.12013900	1.77211400	0.08345000	C	-2.11995100	1.77502900	0.08715500
N	-2.60454500	4.17671600	0.08289600	N	-2.59978600	4.18060900	0.08446900
N	-3.29733800	-3.85716600	0.19963200	N	-3.30453600	-3.85470800	0.20034000
C	-3.76337000	4.15030700	-0.73749200	C	-3.74675200	4.16331900	-0.75243100
C	-5.00539700	4.58030400	-0.24067400	C	-4.99503300	4.59406400	-0.27126700
C	-6.13671900	4.55326300	-1.05384500	C	-6.11496200	4.57452800	-1.10086200
C	-6.05983700	4.08152200	-2.36589200	C	-6.02050200	4.10964200	-2.41466600
C	-4.82921900	3.64291100	-2.85923900	C	-4.78366200	3.67033000	-2.89274800
C	-3.68843100	3.68274400	-2.06030300	C	-3.65424700	3.70267200	-2.07688900
C	-2.37157100	5.25339100	0.97733900	C	-2.37537500	5.24860700	0.99118400
C	-2.66228500	6.57588700	0.60000200	C	-2.66104700	6.57533100	0.62375800
C	-2.42824600	7.62777800	1.48291300	C	-2.43429100	7.61889600	1.51888000

C	-1.88456700	7.38978100	2.74734200	C	-1.90293300	7.36828000	2.78657800
C	-1.58489800	6.07849800	3.12168000	C	-1.60810800	6.05277700	3.15130800
C	-1.83167100	5.01710800	2.25291900	C	-1.84763300	4.99978000	2.26981000
C	-4.43807700	-3.65559400	-0.62182600	C	-4.43517700	-3.66321000	-0.63693300
C	-3.25206300	-4.92957300	1.12829100	C	-3.26669400	-4.91721700	1.14053100
C	-5.73337900	-3.84708700	-0.11208400	C	-5.73671700	-3.85796100	-0.14356000
C	-6.84693900	-3.64947400	-0.92623400	C	-6.84060000	-3.66954700	-0.97346300
C	-6.69593300	-3.24019300	-2.25271900	C	-6.67394300	-3.26619300	-2.30034600
C	-5.41033900	-3.03832600	-2.75938200	C	-5.38224600	-3.06082500	-2.79091000
C	-4.28981600	-3.25065900	-1.95902100	C	-4.27127300	-3.26393500	-1.97436800
C	-3.76621200	-6.19327200	0.79010400	C	-3.77588200	-6.18571400	0.81167500
C	-3.71612700	-7.24198400	1.70584400	C	-3.73145900	-7.22497200	1.73893000
C	-3.13865400	-7.06192200	2.96484100	C	-3.16464400	-7.03050700	3.00109500
C	-2.61758000	-5.81079800	3.30036000	C	-2.64840100	-5.77455400	3.32762600
C	-2.67881300	-4.75009600	2.39846700	C	-2.70402500	-4.72344000	2.41366400
H	2.72825400	0.99755600	1.41825500	H	2.72592700	0.97382300	1.44325700
H	9.00170500	1.95624200	1.14000300	H	9.00847200	1.97088700	1.10541500
H	11.48839300	1.80637200	1.00366700	H	11.49324100	1.81502900	0.96514900
H	12.56326700	-0.06410300	-0.22874300	H	12.56259100	-0.07324400	-0.24486900
H	11.15713500	-1.81003300	-1.33153900	H	11.15404400	-1.83051300	-1.32114800
H	6.64470800	-2.54200000	-1.67103400	H	6.63382300	-2.55986400	-1.64218200
H	5.19411800	0.80155300	1.20503600	H	5.18908900	0.77640400	1.23251500
H	2.24454900	-1.61529400	-1.95801400	H	2.24313200	-1.60118000	-1.96457200
H	4.67960000	-1.85040100	-2.13683200	H	4.67713000	-1.83691600	-2.14308700
H	-0.73291500	-4.53483700	0.01355000	H	-0.73976800	-4.53458400	0.01469100
H	1.22385200	-3.02819200	-0.12650900	H	1.21831400	-3.03067200	-0.12314600
H	-3.41723500	-1.18256400	0.21249900	H	-3.42175500	-1.17890400	0.21519200
H	1.70250500	2.57688700	-0.25821500	H	1.70609800	2.57281400	-0.24512200
H	0.03173800	4.39849500	-0.16187800	H	0.03909500	4.39711500	-0.15362000
H	-3.18168900	1.56226900	0.17086200	H	-3.18195500	1.56689300	0.17350600
H	-5.07702100	4.93386900	0.78286700	H	-5.08165700	4.94179400	0.75312800
H	-7.08839400	4.88977000	-0.65042200	H	-7.07135300	4.91133500	-0.70910900
H	-6.94575700	4.05464500	-2.99386700	H	-6.89735200	4.08862100	-3.05543000
H	-4.75004000	3.27767600	-3.88000600	H	-4.69054800	3.31039800	-3.91418100
H	-2.73308300	3.35163200	-2.45463200	H	-2.69457900	3.37091400	-2.46005100
H	-3.07041600	6.77135100	-0.38639600	H	-3.05896200	6.78174700	-0.36459300
H	-2.65961600	8.64328000	1.17155700	H	-2.66147500	8.63747500	1.21472100
H	-1.69700000	8.21379300	3.42981300	H	-1.72097900	8.18557400	3.47854300
H	-1.16771500	5.87400000	4.10447500	H	-1.20034100	5.83830800	4.13587600
H	-1.60975100	3.99921800	2.55691300	H	-1.62916200	3.97913200	2.56702400
H	-5.86007400	-4.15005000	0.92228900	H	-5.87694400	-4.15572800	0.89057500
H	-7.84054400	-3.80227600	-0.51264100	H	-7.83876400	-3.82480800	-0.57204000
H	-7.56688100	-3.07950100	-2.88164400	H	-7.53717400	-3.11276300	-2.94156800

H	-5.27414600	-2.72501100	-3.79133100	H	-5.23351100	-2.75196700	-3.82243100
H	-3.29348300	-3.10348600	-2.36332200	H	-3.27076400	-3.11392900	-2.36715700
H	-4.20269000	-6.34581900	-0.19173900	H	-4.20367400	-6.35068500	-0.17198600
H	-4.11908400	-8.21168200	1.42473500	H	-4.13030200	-8.19825100	1.46457200
H	-3.09501100	-7.88442500	3.67302900	H	-3.12537500	-7.84538500	3.71825900
H	-2.17044300	-5.65087700	4.27820400	H	-2.20944100	-5.60331300	4.30720700
H	-2.28431200	-3.77682400	2.67205100	H	-2.31310400	-3.74694500	2.68091000

Cartesian coordinates of molecule 2 for S_0 and S_1 geometry optimization

S_0	B3LYP/6-31G(d)			S_1	BMK/6-31G(d)		
C	9.30033300	-0.91079300	-0.71977400	C	9.19993100	-0.68661200	-0.51382000
C	8.67951100	0.16626400	-0.01476500	C	8.55707300	0.29914100	0.29772500
C	9.49365700	1.14692500	0.60931400	C	9.35110500	1.20617900	1.04684700
C	10.86526300	1.05475200	0.52689000	C	10.72494400	1.13196600	0.98221900
C	11.47932400	-0.01309900	-0.17666300	C	11.36096500	0.15549000	0.17288000
C	10.71337300	-0.98067800	-0.78941200	C	10.61486700	-0.73976200	-0.56243800
N	8.54301800	-1.87811200	-1.31575300	N	8.46096600	-1.58375500	-1.23110200
C	7.24030200	-1.75178600	-1.21941300	C	7.15494900	-1.47589800	-1.14761400
C	6.60073100	-0.66331500	-0.53888300	C	6.49525100	-0.47518100	-0.36099000
N	7.32557000	0.26962400	0.06045500	N	7.20053300	0.38627300	0.35650100
C	5.12489000	-0.55281100	-0.45875100	C	5.01539300	-0.38503100	-0.29919100
C	4.54200200	0.26920700	0.52153000	C	4.40414400	0.23800600	0.79734200
C	3.16276200	0.38747100	0.63283600	C	3.01683300	0.30981500	0.87327200
C	2.32005500	-0.30028300	-0.25364200	C	2.20982100	-0.21151400	-0.14029200
C	2.88850100	-1.10880400	-1.24645000	C	2.81739300	-0.81801900	-1.26382000
C	4.27120400	-1.23769500	-1.33948700	C	4.21079100	-0.90939700	-1.32609500
C	-2.19638700	-2.95482300	0.11193500	C	-2.27102500	-2.91292000	0.26445700
C	-0.88059900	-3.45973100	0.01494500	C	-0.94921700	-3.40354100	0.17099400
C	0.22188800	-2.61657000	-0.06955800	C	0.14133700	-2.54751700	0.06804200
C	-0.00250700	-1.23715200	-0.08817300	C	-0.10443200	-1.17297500	0.03179000
C	-1.31433400	-0.71074100	0.01108900	C	-1.42257800	-0.65940000	0.11994300
C	-2.40843900	-1.57318800	0.12147600	C	-2.50503200	-1.53546100	0.24844200
N	0.91358600	-0.17762200	-0.14777900	N	0.79721600	-0.10940500	-0.05581200
C	0.19453300	1.02427500	-0.08552300	C	0.07073000	1.08491600	-0.02051100
C	-1.18866200	0.73257600	0.00987600	C	-1.31118000	0.78497100	0.08360900
C	0.64855300	2.34467000	-0.14979900	C	0.52230300	2.40519200	-0.09366000
C	-0.29449500	3.36525900	-0.10071100	C	-0.42555200	3.42243200	-0.05969800
C	-1.67527100	3.09589100	0.02674200	C	-1.80535000	3.14643700	0.06485300
C	-2.12013900	1.77211400	0.08345000	C	-2.24661900	1.82254300	0.14153700
N	-2.60454500	4.17671600	0.08289600	N	-2.74227700	4.22470600	0.10183000
N	-3.29733800	-3.85716600	0.19963200	N	-3.36067900	-3.83121300	0.37235100
C	-3.76337000	4.15030700	-0.73749200	C	-3.86801400	4.20232100	-0.76214000
C	-5.00539700	4.58030400	-0.24067400	C	-5.12849300	4.63560900	-0.31540900
C	-6.13671900	4.55326300	-1.05384500	C	-6.22778100	4.60840200	-1.17186500

C	-6.05983700	4.08152200	-2.36589200	C	-6.10133300	4.13338600	-2.47936500
C	-4.82921900	3.64291100	-2.85923900	C	-4.85282300	3.69118400	-2.92316800
C	-3.68843100	3.68274400	-2.06030300	C	-3.74365400	3.73072000	-2.08034900
C	-2.37157100	5.25339100	0.97733900	C	-2.54319000	5.28918800	1.01748400
C	-2.66228500	6.57588700	0.60000200	C	-2.83767300	6.61564900	0.65507200
C	-2.42824600	7.62777800	1.48291300	C	-2.63379800	7.65567400	1.55970400
C	-1.88456700	7.38978100	2.74734200	C	-2.11675700	7.40278100	2.83286900
C	-1.58489800	6.07849800	3.12168000	C	-1.81266400	6.08804600	3.19271100
C	-1.83167100	5.01710800	2.25291900	C	-2.02902000	5.03831700	2.30144800
C	-4.43807700	-3.65559400	-0.62182600	C	-4.47723800	-3.69692200	-0.49298000
C	-3.25206300	-4.92957300	1.12829100	C	-3.31639500	-4.85102500	1.35718500
C	-5.73337900	-3.84708700	-0.11208400	C	-5.78422800	-3.91190300	-0.02190800
C	-6.84693900	-3.64947400	-0.92623400	C	-6.87433500	-3.77746500	-0.87992100
C	-6.69593300	-3.24019300	-2.25271900	C	-6.69004900	-3.40863400	-2.21451700
C	-5.41033900	-3.03832600	-2.75938200	C	-5.39373800	-3.18244000	-2.68321000
C	-4.28981600	-3.25065900	-1.95902100	C	-4.29569900	-3.33140000	-1.83805900
C	-3.76621200	-6.19327200	0.79010400	C	-3.80633100	-6.14012400	1.08204300
C	-3.71612700	-7.24198400	1.70584400	C	-3.75261200	-7.13730800	2.05385500
C	-3.13865400	-7.06192200	2.96484100	C	-3.19543500	-6.88072600	3.30920900
C	-2.61758000	-5.81079800	3.30036000	C	-2.69783300	-5.60471800	3.58263700
C	-2.67881300	-4.75009600	2.39846700	C	-2.76242800	-4.59530600	2.62348000
H	2.72825400	0.99755600	1.41825500	H	2.53735500	0.76707900	1.73342400
H	9.00170500	1.95624200	1.14000300	H	8.84405600	1.94668000	1.65774400
H	11.48839300	1.80637200	1.00366700	H	11.33269300	1.82695300	1.55468600
H	12.56326700	-0.06410300	-0.22874300	H	12.44590700	0.11696300	0.13720200
H	11.15713500	-1.81003300	-1.33153900	H	11.07836600	-1.49782900	-1.18633600
H	6.64470800	-2.54200000	-1.67103400	H	6.57199600	-2.21362800	-1.69423900
H	5.19411800	0.80155300	1.20503600	H	5.02327700	0.64492400	1.58800600
H	4.67960000	-1.85040100	-2.13683200	H	4.67275300	-1.35053200	-2.19997200
H	-0.73291500	-4.53483700	0.01355000	H	-0.78909000	-4.47699700	0.18447500
H	1.22385200	-3.02819200	-0.12650900	H	1.14992100	-2.94183900	0.00508900
H	-3.41723500	-1.18256400	0.21249900	H	-3.51983500	-1.15853100	0.33198600
H	1.70250500	2.57688700	-0.25821500	H	1.57801200	2.63616400	-0.19134900
H	0.03173800	4.39849500	-0.16187800	H	-0.10425100	4.45684400	-0.12941800
H	-3.18168900	1.56226900	0.17086200	H	-3.30758300	1.61125100	0.23432200
H	-5.07702100	4.93386900	0.78286700	H	-5.24101700	4.99082800	0.70385800
H	-7.08839400	4.88977000	-0.65042200	H	-7.19368900	4.94714800	-0.80586200
H	-6.94575700	4.05464500	-2.99386700	H	-6.96234400	4.10637700	-3.14106700
H	-4.75004000	3.27767600	-3.88000600	H	-4.73446900	3.32255700	-3.93891000
H	-2.73308300	3.35163200	-2.45463200	H	-2.77513200	3.39551500	-2.43714700
H	-3.07041600	6.77135100	-0.38639600	H	-3.22437600	6.82476100	-0.33712500
H	-2.65961600	8.64328000	1.17155700	H	-2.86760500	8.67374500	1.25872100
H	-1.69700000	8.21379300	3.42981300	H	-1.95270100	8.21746000	3.53237500

H	-1.16771500	5.87400000	4.10447500	H	-1.41525200	5.87134500	4.18105700
H	-1.60975100	3.99921800	2.55691300	H	-1.80268500	4.01831500	2.59477900
H	-5.86007400	-4.15005000	0.92228900	H	-5.93962300	-4.18255400	1.01745500
H	-7.84054400	-3.80227600	-0.51264100	H	-7.87649200	-3.94752700	-0.49463300
H	-7.56688100	-3.07950100	-2.88164400	H	-7.54294300	-3.29704300	-2.87786700
H	-5.27414600	-2.72501100	-3.79133100	H	-5.23064200	-2.89876300	-3.71983400
H	-3.29348300	-3.10348600	-2.36332200	H	-3.29150000	-3.16391500	-2.21379500
H	-4.20269000	-6.34581900	-0.19173900	H	-4.22642200	-6.35431900	0.10460000
H	-4.11908400	-8.21168200	1.42473500	H	-4.13659500	-8.12703400	1.81990500
H	-3.09501100	-7.88442500	3.67302900	H	-3.14905600	-7.66302700	4.06139500
H	-2.17044300	-5.65087700	4.27820400	H	-2.26602700	-5.38487100	4.55572500
H	-2.28431200	-3.77682400	2.67205100	H	-2.38511200	-3.60322200	2.84943700
O	2.03989986	-1.77625747	-2.18415036	O	1.97486000	-1.26768000	-2.22905200
C	2.81700636	-2.21991394	-3.29957603	C	2.52655100	-1.88628500	-3.38696400
H	3.39381713	-1.40289792	-3.67993659	H	3.16793300	-1.19194700	-3.94336700
H	3.47343975	-3.00504264	-2.98721707	H	3.09889400	-2.78501700	-3.12626100
H	2.16523320	-2.58376787	-4.06619332	H	1.67284700	-2.16640900	-4.00501600

Cartesian coordinates of molecule 3 for S₀ and S₁ geometry optimization

S ₀	B3LYP/6-31G(d)			S ₁	BMK/6-31G(d)		
C	9.30033300	-0.91079300	-0.71977400	C	9.24743000	-0.68468700	-0.71466500
C	8.67951100	0.16626400	-0.01476500	C	8.60644100	0.16015200	0.24378300
C	9.49365700	1.14692500	0.60931400	C	9.40181700	0.92758100	1.13406700
C	10.86526300	1.05475200	0.52689000	C	10.77554700	0.85523300	1.06441700
C	11.47932400	-0.01309900	-0.17666300	C	11.40988200	0.01910800	0.10972900
C	10.71337300	-0.98067800	-0.78941200	C	10.66226700	-0.73918300	-0.76489500
N	8.54301800	-1.87811200	-1.31575300	N	8.50707900	-1.44742100	-1.57240700
C	7.24030200	-1.75178600	-1.21941300	C	7.20122800	-1.34585600	-1.47862700
C	6.60073100	-0.66331500	-0.53888300	C	6.54370600	-0.48296200	-0.54124500
N	7.32557000	0.26962400	0.06045500	N	7.24996100	0.24528100	0.31020400
C	5.12489000	-0.55281100	-0.45875100	C	5.06408700	-0.39433200	-0.47221500
C	4.54200200	0.26920700	0.52153000	C	4.44926700	0.06252000	0.70427700
C	3.16276200	0.38747100	0.63283600	C	3.06467600	0.13884500	0.78390300
C	2.32005500	-0.30028300	-0.25364200	C	2.26729800	-0.22392100	-0.30831400
C	2.88850100	-1.10880400	-1.24645000	C	2.85549800	-0.65830000	-1.51163600
C	4.27120400	-1.23769500	-1.33948700	C	4.25111000	-0.74244600	-1.56215200
C	-2.19638700	-2.95482300	0.11193500	C	-2.18790000	-2.96075900	0.16541500
C	-0.88059900	-3.45973100	0.01494500	C	-0.86438500	-3.43908100	0.03967100
C	0.22188800	-2.61657000	-0.06955800	C	0.21733200	-2.57194500	-0.07263900
C	-0.00250700	-1.23715200	-0.08817300	C	-0.04141200	-1.19867000	-0.08880100
C	-1.31433400	-0.71074100	0.01108900	C	-1.36250000	-0.69660000	0.03341500
C	-2.40843900	-1.57318800	0.12147600	C	-2.43361300	-1.58460900	0.17255700
N	0.91358600	-0.17762200	-0.14777900	N	0.84871500	-0.12826600	-0.19081400
C	0.19453300	1.02427500	-0.08552300	C	0.11613900	1.05924900	-0.11648300

C	-1.18866200	0.73257600	0.00987600	C	-1.26165900	0.74897300	0.01426200
C	0.64855300	2.34467000	-0.14979900	C	0.56097600	2.38268800	-0.17408400
C	-0.29449500	3.36525900	-0.10071100	C	-0.39087800	3.39387000	-0.10079800
C	-1.67527100	3.09589100	0.02674200	C	-1.76690400	3.10823300	0.04731600
C	-2.12013900	1.77211400	0.08345000	C	-2.20046400	1.78100000	0.11053400
N	-2.60454500	4.17671600	0.08289600	N	-2.70758000	4.18063200	0.12318400
N	-3.29733800	-3.85716600	0.19963200	N	-3.26736000	-3.88863300	0.28402300
C	-3.76337000	4.15030700	-0.73749200	C	-3.85654200	4.16343200	-0.71011800
C	-5.00539700	4.58030400	-0.24067400	C	-5.10726900	4.57941100	-0.22175200
C	-6.13671900	4.55326300	-1.05384500	C	-6.22939100	4.55815500	-1.04826500
C	-6.05983700	4.08152200	-2.36589200	C	-6.13530000	4.10618500	-2.36661300
C	-4.82921900	3.64291100	-2.85923900	C	-4.89626500	3.68137000	-2.85198700
C	-3.68843100	3.68274400	-2.06030300	C	-3.76478800	3.71534300	-2.03909400
C	-2.37157100	5.25339100	0.97733900	C	-2.49039600	5.23440100	1.04750100
C	-2.66228500	6.57588700	0.60000200	C	-2.79970100	6.56374700	0.70914300
C	-2.42824600	7.62777800	1.48291300	C	-2.57829700	7.59328800	1.62162600
C	-1.88456700	7.38978100	2.74734200	C	-2.02889700	7.32677100	2.87834900
C	-1.58489800	6.07849800	3.12168000	C	-1.71023600	6.00911900	3.21403900
C	-1.83167100	5.01710800	2.25291900	C	-1.94394000	4.96963300	2.31514800
C	-4.43807700	-3.65559400	-0.62182600	C	-4.40713600	-3.74652200	-0.54986800
C	-3.25206300	-4.92957300	1.12829100	C	-3.19326400	-4.92473300	1.25031600
C	-5.73337900	-3.84708700	-0.11208400	C	-5.70048400	-3.96893900	-0.04619100
C	-6.84693900	-3.64947400	-0.92623400	C	-6.81331500	-3.82705700	-0.87332400
C	-6.69593300	-3.24019300	-2.25271900	C	-6.66507400	-3.44345800	-2.20825300
C	-5.41033900	-3.03832600	-2.75938200	C	-5.38215300	-3.21028300	-2.70922400
C	-4.28981600	-3.25065900	-1.95902100	C	-4.26180600	-3.36664200	-1.89521600
C	-3.76621200	-6.19327200	0.79010400	C	-3.68134300	-6.21193400	0.96387700
C	-3.71612700	-7.24198400	1.70584400	C	-3.59965500	-7.22516800	1.91697100
C	-3.13865400	-7.06192200	2.96484100	C	-3.01581900	-6.98627400	3.16366700
C	-2.61758000	-5.81079800	3.30036000	C	-2.52011100	-5.71193000	3.44793400
C	-2.67881300	-4.75009600	2.39846700	C	-2.61268700	-4.68667700	2.50799900
H	2.72825400	0.99755600	1.41825500	H	2.58320600	0.47030900	1.69905100
H	9.00170500	1.95624200	1.14000300	H	8.89600600	1.56243200	1.85502900
H	11.48839300	1.80637200	1.00366700	H	11.38440800	1.44346700	1.74512500
H	12.56326700	-0.06410300	-0.22874300	H	12.49474600	-0.02068700	0.07295500
H	11.15713500	-1.81003300	-1.33153900	H	11.12443000	-1.38868400	-1.50197600
H	6.64470800	-2.54200000	-1.67103400	H	6.61656700	-1.97786500	-2.14301700
H	5.19411800	0.80155300	1.20503600	H	5.06820500	0.34226300	1.54922500
H	4.67960000	-1.85040100	-2.13683200	H	4.70547200	-1.05244100	-2.49848000
H	-0.73291500	-4.53483700	0.01355000	H	-0.69445800	-4.51101900	0.03861300
H	1.22385200	-3.02819200	-0.12650900	H	1.22974300	-2.95599700	-0.15008900
H	-3.41723500	-1.18256400	0.21249900	H	-3.44977300	-1.21831200	0.28268000
H	1.70250500	2.57688700	-0.25821500	H	1.61418400	2.61936900	-0.28621500

H	0.03173800	4.39849500	-0.16187800	H	-0.07635600	4.43116900	-0.15662400
H	-3.18168900	1.56226900	0.17086200	H	-3.25799100	1.56311600	0.22450800
H	-5.07702100	4.93386900	0.78286700	H	-5.19419300	4.91679600	0.80604900
H	-7.08839400	4.88977000	-0.65042200	H	-7.18733800	4.88330800	-0.65045300
H	-6.94575700	4.05464500	-2.99386700	H	-7.01387200	4.08378200	-3.00497000
H	-4.75004000	3.27767600	-3.88000600	H	-4.80317100	3.33128100	-3.87687000
H	-2.73308300	3.35163200	-2.45463200	H	-2.80376500	3.39441100	-2.42796000
H	-3.07041600	6.77135100	-0.38639600	H	-3.21165800	6.78337900	-0.27054700
H	-2.65961600	8.64328000	1.17155700	H	-2.82401000	8.61392800	1.33949300
H	-1.69700000	8.21379300	3.42981300	H	-1.85121800	8.13336400	3.58385500
H	-1.16771500	5.87400000	4.10447500	H	-1.28768600	5.78197200	4.18950700
H	-1.60975100	3.99921800	2.55691300	H	-1.70610100	3.94709100	2.59000800
H	-5.86007400	-4.15005000	0.92228900	H	-5.82743800	-4.25136300	0.99392600
H	-7.84054400	-3.80227600	-0.51264100	H	-7.80461500	-4.00309800	-0.46349700
H	-7.56688100	-3.07950100	-2.88164400	H	-7.53552100	-3.32630800	-2.84737400
H	-5.27414600	-2.72501100	-3.79133100	H	-5.24729000	-2.91584600	-3.74687900
H	-3.29348300	-3.10348600	-2.36332200	H	-3.26805200	-3.19478200	-2.29606300
H	-4.20269000	-6.34581900	-0.19173900	H	-4.12203100	-6.41200000	-0.00747400
H	-4.11908400	-8.21168200	1.42473500	H	-3.98271900	-8.21324000	1.67480200
H	-3.09501100	-7.88442500	3.67302900	H	-2.94759400	-7.78097600	3.90102100
H	-2.17044300	-5.65087700	4.27820400	H	-2.06795500	-5.50594400	4.41477000
H	-2.28431200	-3.77682400	2.67205100	H	-2.23695000	-3.69601800	2.74278700
C	1.97462285	-1.82760004	-2.25628116	C	2.02069900	-0.99720400	-2.72277900
H	1.69706884	-2.78505344	-1.86750520	H	1.45704200	-1.92684400	-2.58105700
H	1.09504511	-1.24116549	-2.42162180	H	1.28756100	-0.21043000	-2.93091300
H	2.49678760	-1.95600419	-3.18135216	H	2.65357700	-1.11953400	-3.60633500

Cartesian coordinates of molecule 4 for S₀ and S₁ geometry optimization

S ₀	B3LYP/6-31G(d)			S ₁	BMK/6-31G(d)		
C	9.29714200	-0.92175200	-0.71765000	C	9.15379500	-0.34231200	-0.35600200
C	8.67953800	0.16552900	-0.02531400	C	8.42903100	0.13572400	0.78032300
C	9.49649800	1.15330600	0.58379100	C	9.14252900	0.57660800	1.92514400
C	10.86812000	1.05822100	0.49975100	C	10.51925900	0.54363800	1.92957400
C	11.47902400	-0.01986200	-0.19100700	C	11.23709500	0.07233300	0.79974500
C	10.71007700	-0.99449000	-0.78939000	C	10.57008700	-0.36422300	-0.32403200
N	8.53584400	-1.89534000	-1.29967700	N	8.49265900	-0.78682000	-1.46446900
C	7.23295700	-1.76622900	-1.20202900	C	7.18058800	-0.73413200	-1.43446000
C	6.59746600	-0.66832600	-0.53301800	C	6.44255400	-0.23545800	-0.31287600
N	7.32527100	0.27172500	0.05174800	N	7.06967000	0.17945500	0.77658200
C	5.12172900	-0.55753900	-0.45010300	C	4.95799000	-0.18645000	-0.31287600
C	4.53928700	0.25328400	0.53978600	C	4.26503900	-0.11415800	0.90487400
C	3.15976100	0.37206700	0.65114600	C	2.87530300	-0.07085800	0.92795100
C	2.31861500	-0.30436100	-0.24508800	C	2.14001800	-0.09241300	-0.26066100
C	2.88601100	-1.10273200	-1.24647300	C	2.82382700	-0.15208700	-1.48772400

C	4.26885800	-1.23251900	-1.33957700	C	4.21744400	-0.19835600	-1.50432500
C	-2.20207700	-2.95269000	0.11439800	C	-2.18298100	-3.00502900	0.27114000
C	-0.88677000	-3.45935500	0.01813400	C	-0.84943300	-3.42951500	0.07665400
C	0.21709800	-2.61762500	-0.06462700	C	0.19075500	-2.51959700	-0.07818300
C	-0.00615000	-1.23769000	-0.08149200	C	-0.12321100	-1.15950100	-0.05849700
C	-1.31789600	-0.70965400	0.01631100	C	-1.45431200	-0.70943200	0.12531000
C	-2.41348600	-1.57109000	0.12473400	C	-2.48295500	-1.64016100	0.30163000
N	0.91093100	-0.17987000	-0.13984700	N	0.71646400	-0.05088500	-0.20314000
C	0.19415500	1.02266100	-0.07855200	C	-0.05767600	1.10748000	-0.08642900
C	-1.19011000	0.73344700	0.01499400	C	-1.41242900	0.73970100	0.10722400
C	0.65140300	2.34235600	-0.14081700	C	0.33406000	2.44622900	-0.14287000
C	-0.29001900	3.36470300	-0.09321000	C	-0.65191700	3.41829800	-0.01254500
C	-1.67168500	3.09756900	0.03097000	C	-2.00744600	3.07648800	0.19255400
C	-2.11995100	1.77502900	0.08715500	C	-2.38556100	1.73242700	0.25821900
N	-2.59978600	4.18060900	0.08446900	N	-2.98521300	4.10946000	0.32360400
N	-3.30453600	-3.85470800	0.20034000	N	-3.21864200	-3.97618200	0.42745600
C	-3.74675200	4.16331900	-0.75243100	C	-4.17006800	4.05379300	-0.45665100
C	-4.99503300	4.59406400	-0.27126700	C	-5.41242700	4.41294000	0.09395600
C	-6.11496200	4.57452800	-1.10086200	C	-6.56990500	4.35445800	-0.68039000
C	-6.02050200	4.10964200	-2.41466600	C	-6.51862500	3.92041900	-2.00708800
C	-4.78366200	3.67033000	-2.89274800	C	-5.28732500	3.55156700	-2.55400900
C	-3.65424700	3.70267200	-2.07688900	C	-4.12157800	3.62346800	-1.79366300
C	-2.37537500	5.24860700	0.99118400	C	-2.76723300	5.16312500	1.24756900
C	-2.66104700	6.57533100	0.62375800	C	-3.14505800	6.48176600	0.93797300
C	-2.43429100	7.61889600	1.51888000	C	-2.92312000	7.51145000	1.85015400
C	-1.90293300	7.36828000	2.78657800	C	-2.30571000	7.25668000	3.07740900
C	-1.60810800	6.05277700	3.15130800	C	-1.91905200	5.95018900	3.38406700
C	-1.84763300	4.99978000	2.26981000	C	-2.15228500	4.90994500	2.48594500
C	-4.43517700	-3.66321000	-0.63693300	C	-4.39732600	-3.87401500	-0.35741200
C	-3.26669400	-4.91721700	1.14053100	C	-3.06015800	-5.01867400	1.37587300
C	-5.73671700	-3.85796100	-0.14356000	C	-5.65855900	-4.14869400	0.19887700
C	-6.84060000	-3.66954700	-0.97346300	C	-6.80994500	-4.04564800	-0.57987000
C	-6.67394300	-3.26619300	-2.30034600	C	-6.73270600	-3.64971000	-1.91720400
C	-5.38224600	-3.06082500	-2.79091000	C	-5.48199000	-3.36452400	-2.47004200
C	-4.27127300	-3.26393500	-1.97436800	C	-4.32306400	-3.48176500	-1.70489500
C	-3.77588200	-6.18571400	0.81167500	C	-3.51105600	-6.32096600	1.09638200
C	-3.73145900	-7.22497200	1.73893000	C	-3.34721800	-7.34000700	2.03250400
C	-3.16464400	-7.03050700	3.00109500	C	-2.71672100	-7.09170700	3.25440800
C	-2.64840100	-5.77455400	3.32762600	C	-2.25772600	-5.80206600	3.53129300
C	-2.70402500	-4.72344000	2.41366400	C	-2.43226600	-4.77153100	2.60897200
H	2.72592700	0.97382300	1.44325700	H	2.34044500	-0.02348600	1.87129400
H	9.00847200	1.97088700	1.10541500	H	8.57365600	0.93524600	2.77737300
H	11.49324100	1.81502900	0.96514900	H	11.06662300	0.88180800	2.80474100

H	12.56259100	-0.07324400	-0.24486900	H	12.32279400	0.05702300	0.82695900
H	11.15404400	-1.83051300	-1.32114800	H	11.09709400	-0.73136900	-1.19923100
H	6.63382300	-2.55986400	-1.64218200	H	6.66065800	-1.11530600	-2.31020700
H	5.18908900	0.77640400	1.23251500	H	4.83139000	-0.09450000	1.82900300
H	4.67713000	-1.83691600	-2.14308700	H	4.71874400	-0.22098100	-2.46357600
H	-0.73976800	-4.53458400	0.01469100	H	-0.63924200	-4.49389500	0.04839000
H	1.21831400	-3.03067200	-0.12314600	H	1.20904900	-2.86279500	-0.23019700
H	-3.42175500	-1.17890400	0.21519200	H	-3.50741300	-1.31522100	0.45566500
H	1.70609800	2.57281400	-0.24512200	H	1.37024600	2.72599000	-0.30375000
H	0.03909500	4.39711500	-0.15362000	H	-0.38096500	4.46772300	-0.06891400
H	-3.18195500	1.56689300	0.17350600	H	-3.42694800	1.47112800	0.41924300
H	-5.08165700	4.94179400	0.75312800	H	-5.46506700	4.73569200	1.12877800
H	-7.07135300	4.91133500	-0.70910900	H	-7.52078400	4.63599500	-0.23516000
H	-6.89735200	4.08862100	-3.05543000	H	-7.42419900	3.86866000	-2.60472200
H	-4.69054800	3.31039800	-3.91418100	H	-5.22768400	3.21582400	-3.58611100
H	-2.69457900	3.37091400	-2.46005100	H	-3.16762100	3.34564000	-2.23017700
H	-3.05896200	6.78174700	-0.36459300	H	-3.61049500	6.69301900	-0.01934000
H	-2.66147500	8.63747500	1.21472100	H	-3.22258300	8.52364500	1.59041500
H	-1.72097900	8.18557400	3.47854300	H	-2.12816100	8.06366700	3.78250100
H	-1.20034100	5.83830800	4.13587600	H	-1.44299400	5.73191800	4.33667300
H	-1.62916200	3.97913200	2.56702400	H	-1.86120700	3.89552000	2.73880100
H	-5.87694400	-4.15572800	0.89057500	H	-5.73045300	-4.44111000	1.24153900
H	-7.83876400	-3.82480800	-0.57204000	H	-7.77566800	-4.26196000	-0.13015100
H	-7.53717400	-3.11276300	-2.94156800	H	-7.63317500	-3.56289800	-2.51847800
H	-5.23351100	-2.75196700	-3.82243100	H	-5.40231300	-3.05947500	-3.51028900
H	-3.27076400	-3.11392900	-2.36715700	H	-3.35450300	-3.26917100	-2.14586200
H	-4.20367400	-6.35068500	-0.17198600	H	-3.98745100	-6.52805200	0.14356600
H	-4.13030200	-8.19825100	1.46457200	H	-3.70276700	-8.33963500	1.79584500
H	-3.12537500	-7.84538500	3.71825900	H	-2.58468500	-7.89075400	3.97828400
H	-2.20944100	-5.60331300	4.30720700	H	-1.77042600	-5.58868400	4.47931300
H	-2.31310400	-3.74694500	2.68091000	H	-2.08502200	-3.76933000	2.83866300
C	1.97360927	-1.81015100	-2.26563022	C	2.06148500	-0.15294900	-2.79190100
F	2.63617385	-1.96439963	-3.43169862	F	2.89140600	-0.20103800	-3.85785200
F	1.61789216	-3.02113210	-1.78657895	F	1.23369100	-1.21630200	-2.88875600
F	0.86692947	-1.06506104	-2.47202979	F	1.30442200	0.95714000	-2.93093000

Cartesian coordinates of molecule 5 for S₀ and S₁ geometry optimization

S ₀	B3LYP/6-31G(d)			S ₁	BMK/6-31G(d)		
C	-7.12762696	-0.80537963	1.40398627	C	-7.69982600	-1.49743500	1.79948700
C	-7.21220404	-1.34920190	0.08976809	C	-7.81335600	-1.98054900	0.45903900
C	-8.48521087	-1.57170826	-0.49056276	C	-9.09999700	-2.25420400	-0.07356500
C	-9.63504191	-1.26022108	0.21131945	C	-10.22122300	-2.04903200	0.69970200
C	-9.54685325	-0.70872793	1.53655328	C	-10.10673400	-1.56572000	2.02873900
C	-8.30819902	-0.49005342	2.11359936	C	-8.86985200	-1.29469800	2.57228700

N	-5.91405107	-0.59499770	1.99422911	N	-6.47353100	-1.24192600	2.34351400
C	-4.85537507	-0.90078509	1.28428567	C	-5.42956800	-1.44323200	1.57268000
C	-4.92294347	-1.42653899	-0.05439386	C	-5.52875000	-1.90188700	0.21815400
N	-6.09627410	-1.65272723	-0.62419952	N	-6.71021200	-2.17438200	-0.31378500
H	-8.53570121	-1.98606975	-1.49119930	H	-9.16493300	-2.62115900	-1.09327200
H	-8.22138130	-0.07777500	3.11269117	H	-8.75626900	-0.92704800	3.58747300
H	-3.89288337	-0.75867775	1.76828490	H	-4.45490600	-1.26647300	2.02150200
C	-3.70047808	-1.75296852	-0.82514842	C	-4.32336900	-2.11185200	-0.62390000
C	-3.78391308	-2.64487657	-1.90825565	C	-4.38987800	-2.97881300	-1.72755100
C	-2.45564342	-1.19383419	-0.49681785	C	-3.10953500	-1.46720400	-0.34206800
C	-2.64499570	-2.96808007	-2.63940776	C	-3.26814300	-3.19522100	-2.52270500
H	-4.74560035	-3.07638514	-2.16068631	H	-5.32878900	-3.47479500	-1.94587000
C	-1.31640204	-1.50524252	-1.24653720	C	-1.98804800	-1.67459200	-1.15215100
H	-2.35235046	-0.50008068	0.32974637	H	-3.02082300	-0.78614000	0.49708200
C	-1.41216935	-2.39638883	-2.32264866	C	-2.06611100	-2.54166000	-2.24799400
H	-2.71682713	-3.65972815	-3.47350422	H	-3.33003700	-3.86898000	-3.37245400
H	-0.52893531	-2.62359178	-2.91066601	H	-1.19688600	-2.68682200	-2.88139300
N	-0.07004808	-0.91269189	-0.91721363	N	-0.77147900	-0.99869900	-0.86161800
C	1.12014378	-1.60084049	-0.64833473	C	0.46749400	-1.60648300	-0.63111000
C	0.18273158	0.46053227	-0.80256433	C	-0.60745200	0.38628200	-0.74810400
C	1.36970742	-2.97548646	-0.60704875	C	0.80740600	-2.96222100	-0.60555000
C	2.14071430	-0.66286551	-0.35311422	C	1.43356800	-0.60411000	-0.36263400
C	1.54282218	0.65331472	-0.45343883	C	0.74723600	0.66932500	-0.43933800
C	-0.66796594	1.54892557	-1.01571564	C	-1.53732300	1.41491800	-0.92606500
C	2.65337475	-3.39807303	-0.27907139	C	2.12495600	-3.30095500	-0.31765700
H	0.58705868	-3.70068140	-0.80352465	H	0.06716800	-3.73484200	-0.78472100
C	3.43174534	-1.10643940	-0.05059862	C	2.75928500	-0.96378500	-0.10078700
C	2.05157545	1.94769467	-0.31112927	C	1.17089600	1.99499500	-0.30473800
C	-0.15050665	2.82835915	-0.84433631	C	-1.10240700	2.72563300	-0.76297500
H	-1.70601838	1.41106088	-1.29953542	H	-2.57259700	1.20588200	-1.17422200
C	3.69228620	-2.47909612	-0.00994977	C	3.10880500	-2.31657300	-0.07414800
H	2.86914299	-4.46036146	-0.22674569	H	2.41180900	-4.34691300	-0.27751700
H	4.22680831	-0.39856221	0.16228039	H	3.51301400	-0.20652400	0.09202900
C	1.20188444	3.04240102	-0.49535168	C	0.24295100	3.02902300	-0.45573000
H	3.09489711	2.10974873	-0.05875781	H	2.20789100	2.22749500	-0.08253600
H	-0.79607286	3.68891018	-0.98696095	H	-1.80880300	3.54144100	-0.87830400
N	4.99612417	-2.96043114	0.31252783	N	4.45108800	-2.71313700	0.20850600
N	1.68952112	4.37295480	-0.33362172	N	0.64459200	4.39014700	-0.29959300
C	5.67968323	-2.43348497	1.44053167	C	5.12221300	-2.16423500	1.33275200
C	5.60552983	-3.93786393	-0.51639068	C	5.10213700	-3.63407100	-0.65206100
C	2.46267489	4.70401488	0.81081464	C	1.39972500	4.77082900	0.84082000
C	1.41878004	5.34406827	-1.33311178	C	0.30216200	5.33843500	-1.29781400
C	7.05610453	-2.15613300	1.38231851	C	6.47884900	-1.80475800	1.25620300

C	4.98569742	-2.17026673	2.63373573	C	4.43526100	-1.95929600	2.54154300
C	6.37590707	-4.97308477	0.04167637	C	5.95548100	-4.62376400	-0.13303700
C	5.43718971	-3.89638206	-1.91105082	C	4.89173400	-3.58370600	-2.04084500
C	3.58530467	5.54223325	0.70160871	C	2.46104800	5.68546300	0.72890300
C	2.12198913	4.18969276	2.07339096	C	1.10484900	4.22792100	2.10310600
C	1.11339001	6.67023948	-0.98080310	C	-0.07239000	6.64768700	-0.94772300
C	1.43715279	4.99208341	-2.69342421	C	0.31516500	4.97964700	-2.65667500
C	7.71865862	-1.64108869	2.49527034	C	7.12941800	-1.26770600	2.36574300
H	7.60083900	-2.34526262	0.46291832	H	7.01759400	-1.94739000	0.32497400
C	5.65367914	-1.63833458	3.73519044	C	5.09024900	-1.40503300	3.63975500
H	3.92324057	-2.38441979	2.69084667	H	3.38830200	-2.23596100	2.61318800
C	6.96894819	-5.93086493	-0.77849957	C	6.58737900	-5.52726200	-0.98512000
H	6.50513597	-5.02175297	1.11811249	H	6.11800000	-4.68025800	0.93847600
C	6.02011348	-4.86964204	-2.72117729	C	5.51508000	-4.50334400	-2.88282300
H	4.85068879	-3.09780663	-2.35389227	H	4.24007500	-2.82045200	-2.45383800
C	4.33658123	5.86429576	1.83065685	C	3.19594200	6.05349100	1.85463900
H	3.86436010	5.93740932	-0.26985959	H	2.70584300	6.10346500	-0.24225100
C	2.89019370	4.50314124	3.19318430	C	1.85706000	4.58886200	3.21940100
H	1.25442359	3.54478469	2.16997646	H	0.28535000	3.52332700	2.20197100
C	0.84551830	7.61728462	-1.96732628	C	-0.41166800	7.57138300	-1.93432900
H	1.08669162	6.95167626	0.06701810	H	-0.09702300	6.93437800	0.09867700
C	1.15018133	5.94281889	-3.67172566	C	-0.04298700	5.90624500	-3.63457900
H	1.67824780	3.97270150	-2.97730616	H	0.60769800	3.97363100	-2.93964300
C	7.02417281	-1.37425686	3.67745705	C	6.44162900	-1.05966800	3.56356500
H	8.78349851	-1.43297791	2.42963018	H	8.17879900	-0.99582200	2.28524700
H	5.09864650	-1.44198837	4.64891648	H	4.54047800	-1.25486500	4.56536600
C	6.79329976	-5.89055306	-2.16405005	C	6.37031000	-5.47825800	-2.36450100
H	7.56056237	-6.72309180	-0.32692108	H	7.24278800	-6.28487100	-0.56308300
H	5.87862868	-4.81850957	-3.79774353	H	5.33941700	-4.44595100	-3.95405000
C	3.99905488	5.34549626	3.08284987	C	2.90399600	5.50673100	3.10642500
H	5.20158247	6.51396979	1.72480818	H	4.01329300	6.76188100	1.74629300
H	2.60971194	4.09504362	4.16081965	H	1.61234300	4.15726300	4.18656500
C	0.85703233	7.26184356	-3.31850397	C	-0.40421100	7.20888000	-3.28366100
H	0.61127333	8.63741188	-1.67405813	H	-0.69882800	8.57823100	-1.64200900
H	1.17027517	5.65024240	-4.71841200	H	-0.02564300	5.60799500	-4.67974800
H	7.54270925	-0.96556954	4.53997189	H	6.95028000	-0.63350600	4.42353200
H	7.25163086	-6.64325091	-2.79904852	H	6.85939900	-6.18909600	-3.02434700
H	4.59171896	5.59271792	3.95889651	H	3.48423400	5.79024100	3.97982900
H	0.64037836	8.00151281	-4.08387779	H	-0.67657000	7.93002000	-4.04895400
H	-10.43873373	-0.46754194	2.07625554	H	-11.00532600	-1.41072700	2.61897200
H	-10.59352392	-1.43004070	-0.23294798	H	-11.20630300	-2.25722500	0.29183600

Cartesian coordinates of molecule 6 for S₀ and S₁ geometry optimization

S ₀	B3LYP/6-31G(d)			S ₁	BMK/6-31G(d)		
C	-7.12762696	-0.80537963	1.40398627	C	-7.65995600	-1.02974700	2.18622900
C	-7.21220404	-1.34920190	0.08976809	C	-7.88063600	-1.29492500	0.79960400
C	-8.48521087	-1.57170826	-0.49056276	C	-9.21119400	-1.41184500	0.32006900
C	-9.63504191	-1.26022108	0.21131945	C	-10.27061200	-1.26597400	1.18860200
C	-9.54685325	-0.70872793	1.53655328	C	-10.04910600	-0.99958100	2.56415000
C	-8.30819902	-0.49005342	2.11359936	C	-8.76735000	-0.88384600	3.05731000
N	-5.91405107	-0.59499770	1.99422911	N	-6.38959300	-0.92712300	2.67857700
C	-4.85537507	-0.90078509	1.28428567	C	-5.40738400	-1.06691700	1.81913000
C	-4.92294347	-1.42653899	-0.05439386	C	-5.61163700	-1.30925600	0.41967500
N	-6.09627410	-1.65272723	-0.62419952	N	-6.83888000	-1.42878000	-0.06554400
H	-8.53570121	-1.98606975	-1.49119930	H	-9.35893700	-1.61388200	-0.73644200
H	-8.22138130	-0.07777500	3.11269117	H	-8.57107200	-0.68300800	4.10610300
H	-3.89288337	-0.75867775	1.76828490	H	-4.40002900	-1.01119200	2.22496300
C	-3.70047808	-1.75296852	-0.82514842	C	-4.47604000	-1.45697800	-0.51966300
C	-3.78391308	-2.64487657	-1.90825565	C	-4.67552200	-2.06176300	-1.77002000
C	-2.45564342	-1.19383419	-0.49681785	C	-3.18121400	-1.00873700	-0.20937900
C	-2.64499570	-2.96808007	-2.63940776	C	-3.63317400	-2.22011400	-2.67719300
H	-4.74560035	-3.07638514	-2.16068631	H	-5.66950900	-2.41227600	-2.02471300
C	-1.31640204	-1.50524252	-1.24653720	C	-2.12727500	-1.14942800	-1.10812700
H	-2.35235046	-0.50008068	0.32974637	H	-2.96680300	-0.51933700	0.73458200
C	-1.41216935	-2.39638883	-2.32264866	C	-2.34617300	-1.76015300	-2.36437300
H	-2.71682713	-3.65972815	-3.47350422	H	-3.82820400	-2.69545500	-3.63122800
N	-0.07004808	-0.91269189	-0.91721363	N	-0.83718900	-0.65413900	-0.77339600
C	1.12014378	-1.60084049	-0.64833473	C	0.29578100	-1.42502700	-0.51052900
C	0.18273158	0.46053227	-0.80256433	C	-0.48506300	0.69372100	-0.67251700
C	1.36970742	-2.97548646	-0.60704875	C	0.43816400	-2.81422500	-0.48360500
C	2.14071430	-0.66286551	-0.35311422	C	1.38709500	-0.56609000	-0.22513300
C	1.54282218	0.65331472	-0.45343883	C	0.88803900	0.79041000	-0.33036100
C	-0.66796594	1.54892557	-1.01571564	C	-1.26742300	1.83481300	-0.86688900
C	2.65337475	-3.39807303	-0.27907139	C	1.68665700	-3.33576700	-0.16391400
H	0.58705868	-3.70068140	-0.80352465	H	-0.40127700	-3.47079200	-0.68843400
C	3.43174534	-1.10643940	-0.05059862	C	2.64147900	-1.10997400	0.06967300
C	2.05157545	1.94769467	-0.31112927	C	1.48238600	2.04835600	-0.18988600
C	-0.15050665	2.82835915	-0.84433631	C	-0.66326800	3.07622800	-0.69891900
H	-1.70601838	1.41106088	-1.29953542	H	-2.31809800	1.76059900	-1.12843800
C	3.69228620	-2.47909612	-0.00994977	C	2.79255900	-2.49857000	0.10616400
H	2.86914299	-4.46036146	-0.22674569	H	1.82423900	-4.41160400	-0.12049100
H	4.22680831	-0.39856221	0.16228039	H	3.49216100	-0.46831800	0.27844200
C	1.20188444	3.04240102	-0.49535168	C	0.70464900	3.19597400	-0.36682900
H	3.09489711	2.10974873	-0.05875781	H	2.53544000	2.14263700	0.05747500

H	-0.79607286	3.68891018	-0.98696095	H	-1.24987100	3.98021900	-0.82865400
N	4.99612417	-2.96043114	0.31252783	N	4.05882100	-3.08069600	0.42418200
N	1.68952112	4.37295480	-0.33362172	N	1.28388600	4.49327000	-0.21074500
C	5.67968323	-2.43348497	1.44053167	C	4.75351300	-2.65014100	1.58441200
C	5.60552983	-3.93786393	-0.51639068	C	4.61047900	-4.06063400	-0.43921500
C	2.46267489	4.70401488	0.81081464	C	2.03101300	4.78805700	0.95919300
C	1.41878004	5.34406827	-1.33311178	C	1.12376300	5.45504500	-1.24045700
C	7.05610453	-2.15613300	1.38231851	C	6.14895400	-2.48095100	1.56849100
C	4.98569742	-2.17026673	2.63373573	C	4.05238100	-2.36956700	2.76984500
C	6.37590707	-4.97308477	0.04167637	C	5.31770300	-5.16098100	0.07762400
C	5.43718971	-3.89638206	-1.91105082	C	4.44314000	-3.95966900	-1.83136200
C	3.58530467	5.54223325	0.70160871	C	3.20783900	5.55389900	0.89000900
C	2.12198913	4.18969276	2.07339096	C	1.61273600	4.30386400	2.21067300
C	1.11339001	6.67023948	-0.98080310	C	0.93238800	6.81416100	-0.93391300
C	1.43715279	4.99208341	-2.69342421	C	1.13414800	5.06256300	-2.59022800
C	7.71865862	-1.64108869	2.49527034	C	6.82090000	-2.05587700	2.71325400
H	7.60083900	-2.34526262	0.46291832	H	6.70115700	-2.68216900	0.65616900
C	5.65367914	-1.63833458	3.73519044	C	4.73166800	-1.92835300	3.90389700
H	3.92324057	-2.38441979	2.69084667	H	2.97508600	-2.49823500	2.79475100
C	6.96894819	-5.93086493	-0.77849957	C	5.85084100	-6.12217100	-0.77875600
H	6.50513597	-5.02175297	1.11811249	H	5.44444700	-5.25790100	1.15104000
C	6.02011348	-4.86964204	-2.72117729	C	4.96608300	-4.93579300	-2.67798000
H	4.85068879	-3.09780663	-2.35389227	H	3.90362600	-3.11279500	-2.24285900
C	4.33658123	5.86429576	1.83065685	C	3.93455800	5.83595600	2.04542400
H	3.86436010	5.93740932	-0.26985959	H	3.54882700	5.92383500	-0.07154900
C	2.89019370	4.50314124	3.19318430	C	2.35603900	4.57687000	3.35747000
H	1.25442359	3.54478469	2.16997646	H	0.70464600	3.71335000	2.27698400
C	0.84551830	7.61728462	-1.96732628	C	0.76975000	7.75077700	-1.95268100
H	1.08669162	6.95167626	0.06701810	H	0.91043700	7.12955600	0.10422300
C	1.15018133	5.94281889	-3.67172566	C	0.95324600	6.00524600	-3.60100400
H	1.67824780	3.97270150	-2.97730616	H	1.28550600	4.01746800	-2.84014000
C	7.02417281	-1.37425686	3.67745705	C	6.11975500	-1.77261200	3.88770300
H	8.78349851	-1.43297791	2.42963018	H	7.90016000	-1.93057900	2.67889300
H	5.09864650	-1.44198837	4.64891648	H	4.16991200	-1.71699300	4.81019500
C	6.79329976	-5.89055306	-2.16405005	C	5.67718800	-6.02119100	-2.16147800
H	7.56056237	-6.72309180	-0.32692108	H	6.39347400	-6.96479000	-0.35770400
H	5.87862868	-4.81850957	-3.79774353	H	4.82621400	-4.83691200	-3.75151700
C	3.99905488	5.34549626	3.08284987	C	3.51859600	5.34801500	3.28642500
H	5.20158247	6.51396979	1.72480818	H	4.84223200	6.42928000	1.96930300
H	2.60971194	4.09504362	4.16081965	H	2.01438100	4.19258100	4.31518600
C	0.85703233	7.26184356	-3.31850397	C	0.77458200	7.35563800	-3.29284500
H	0.61127333	8.63741188	-1.67405813	H	0.62259900	8.79612400	-1.69319500
H	1.17027517	5.65024240	-4.71841200	H	0.96562400	5.67966300	-4.63810800

H	7.54270925	-0.96556954	4.53997189	H	6.64635300	-1.43390400	4.77532700
H	7.25163086	-6.64325091	-2.79904852	H	6.08872400	-6.77651100	-2.82485900
H	4.59171896	5.59271792	3.95889651	H	4.09220000	5.56362600	4.18330500
H	0.64037836	8.00151281	-4.08387779	H	0.64008200	8.08822300	-4.08351800
H	-10.43873373	-0.46754194	2.07625554	H	-10.90007400	-0.88764800	3.22989800
H	-10.59352392	-1.43004070	-0.23294798	H	-11.28891900	-1.35430600	0.82049200
O	-0.24822129	-2.69580260	-3.09755273	O	-1.27220500	-1.85090300	-3.18262400
C	-0.63193713	-3.39419277	-4.28495044	C	-1.43839200	-2.45094500	-4.46561500
H	-1.02441716	-4.35448392	-4.02284296	H	-1.75663900	-3.49647400	-4.37764900
H	-1.38066189	-2.83218997	-4.80308564	H	-2.16289900	-1.89568300	-5.07290700
H	0.22215178	-3.51847585	-4.91739478	H	-0.45679700	-2.40765400	-4.93837800

Cartesian coordinates of molecule 7 for S_0 and S_1 geometry optimization

S_0	B3LYP/6-31G(d)			S_1	BMK/6-31G(d)		
C	-7.12762696	-0.80537963	1.40398627	C	-7.63748000	-1.14170400	2.04131200
C	-7.21220404	-1.34920190	0.08976809	C	-7.90183000	-1.18658600	0.63748200
C	-8.48521087	-1.57170826	-0.49056276	C	-9.24657100	-1.17529000	0.18407200
C	-9.63504191	-1.26022108	0.21131945	C	-10.27829700	-1.11762200	1.09492700
C	-9.54685325	-0.70872793	1.53655328	C	-10.01366100	-1.06939900	2.48790200
C	-8.30819902	-0.49005342	2.11359936	C	-8.71759500	-1.08186000	2.95598900
N	-5.91405107	-0.59499770	1.99422911	N	-6.35351000	-1.16703500	2.50661300
C	-4.85537507	-0.90078509	1.28428567	C	-5.39803200	-1.21620600	1.60732400
C	-4.92294347	-1.42653899	-0.05439386	C	-5.64599200	-1.23694100	0.19511800
N	-6.09627410	-1.65272723	-0.62419952	N	-6.88689900	-1.23252600	-0.26766900
H	-8.53570121	-1.98606975	-1.49119930	H	-9.42668100	-1.21054100	-0.88601400
H	-8.22138130	-0.07777500	3.11269117	H	-8.48935300	-1.04821200	4.01684200
H	-3.89288337	-0.75867775	1.76828490	H	-4.37975800	-1.26359000	1.98605800
C	-3.70047808	-1.75296852	-0.82514842	C	-4.53849400	-1.28641300	-0.79075100
C	-3.78391308	-2.64487657	-1.90825565	C	-4.78801500	-1.71646000	-2.10395000
C	-2.45564342	-1.19383419	-0.49681785	C	-3.22888400	-0.90917800	-0.46024900
C	-2.64499570	-2.96808007	-2.63940776	C	-3.76399600	-1.76588300	-3.04293500
H	-4.74560035	-3.07638514	-2.16068631	H	-5.79684300	-2.00761100	-2.37477000
C	-1.31640204	-1.50524252	-1.24653720	C	-2.20544800	-0.95814100	-1.40921300
H	-2.35235046	-0.50008068	0.32974637	H	-2.98029700	-0.55140600	0.53320700
C	-1.41216935	-2.39638883	-2.32264866	C	-2.45211800	-1.38418000	-2.72796900
H	-2.71682713	-3.65972815	-3.47350422	H	-3.98407000	-2.10088200	-4.05335200
N	-0.07004808	-0.91269189	-0.91721363	N	-0.89284600	-0.54739400	-1.02069900
C	1.12014378	-1.60084049	-0.64833473	C	0.18102000	-1.39320000	-0.74268800
C	0.18273158	0.46053227	-0.80256433	C	-0.47371200	0.77098700	-0.83154000
C	1.36970742	-2.97548646	-0.60704875	C	0.24355000	-2.78901600	-0.77416900
C	2.14071430	-0.66286551	-0.35311422	C	1.30704100	-0.61207000	-0.37555300
C	1.54282218	0.65331472	-0.45343883	C	0.88779300	0.77399200	-0.43272000
C	-0.66796594	1.54892557	-1.01571564	C	-1.18703100	1.96166300	-0.99342900
C	2.65337475	-3.39807303	-0.27907139	C	1.44841500	-3.39570000	-0.43558000

H	0.58705868	-3.70068140	-0.80352465	H	-0.62534500	-3.38646300	-1.03253100
C	3.43174534	-1.10643940	-0.05059862	C	2.51617700	-1.24112700	-0.06230200
C	2.05157545	1.94769467	-0.31112927	C	1.54199300	1.98887600	-0.20481800
C	-0.15050665	2.82835915	-0.84433631	C	-0.52536200	3.15746800	-0.73617700
H	-1.70601838	1.41106088	-1.29953542	H	-2.22994800	1.95779100	-1.29404000
C	3.69228620	-2.47909612	-0.00994977	C	2.58833600	-2.63681600	-0.08736800
H	2.86914299	-4.46036146	-0.22674569	H	1.52279000	-4.47852300	-0.43630300
H	4.22680831	-0.39856221	0.16228039	H	3.39270900	-0.66010800	0.20798500
C	1.20188444	3.04240102	-0.49535168	C	0.83336600	3.18502700	-0.34852100
H	3.09489711	2.10974873	-0.05875781	H	2.58743800	2.01234200	0.08734900
H	-0.79607286	3.68891018	-0.98696095	H	-1.05844700	4.09754200	-0.83660300
N	4.99612417	-2.96043114	0.31252783	N	3.80661600	-3.30426200	0.24666300
N	1.68952112	4.37295480	-0.33362172	N	1.47257400	4.43823600	-0.09992400
C	5.67968323	-2.43348497	1.44053167	C	4.48567600	-2.96157300	1.44515700
C	5.60552983	-3.93786393	-0.51639068	C	4.32947900	-4.28265100	-0.63692800
C	2.46267489	4.70401488	0.81081464	C	2.20204500	4.62457500	1.10345700
C	1.41878004	5.34406827	-1.33311178	C	1.38783200	5.46883500	-1.07072100
C	7.05610453	-2.15613300	1.38231851	C	5.88808300	-2.87226600	1.47850400
C	4.98569742	-2.17026673	2.63373573	C	3.76285500	-2.69101800	2.61971600
C	6.37590707	-4.97308477	0.04167637	C	4.94786300	-5.44418300	-0.14094300
C	5.43718971	-3.89638206	-1.91105082	C	4.22220900	-4.11661400	-2.02862600
C	3.58530467	5.54223325	0.70160871	C	3.41930800	5.32749600	1.10663000
C	2.12198913	4.18969276	2.07339096	C	1.72397200	4.09523900	2.31448200
C	1.11339001	6.67023948	-0.98080310	C	1.24999000	6.81347900	-0.68295900
C	1.43715279	4.99208341	-2.69342421	C	1.42227600	5.16158700	-2.44189800
C	7.71865862	-1.64108869	2.49527034	C	6.54506600	-2.53446000	2.66043500
H	7.60083900	-2.34526262	0.46291832	H	6.45748900	-3.06714300	0.57541800
C	5.65367914	-1.63833458	3.73519044	C	4.42838300	-2.33700200	3.79190300
H	3.92324057	-2.38441979	2.69084667	H	2.67983100	-2.75927700	2.60662500
C	6.96894819	-5.93086493	-0.77849957	C	5.45372000	-6.40255200	-1.01686200
H	6.50513597	-5.02175297	1.11811249	H	5.02743400	-5.59044200	0.93142200
C	6.02011348	-4.86964204	-2.72117729	C	4.71630000	-5.08967500	-2.89590400
H	4.85068879	-3.09780663	-2.35389227	H	3.75224900	-3.22182700	-2.42381200
C	4.33658123	5.86429576	1.83065685	C	4.12803100	5.50469200	2.29363800
H	3.86436010	5.93740932	-0.26985959	H	3.80541200	5.73139500	0.17628700
C	2.89019370	4.50314124	3.19318430	C	2.44901100	4.26284300	3.49281900
H	1.25442359	3.54478469	2.16997646	H	0.78391900	3.55306400	2.32485200
C	0.84551830	7.61728462	-1.96732628	C	1.16261300	7.81897400	-1.64365500
H	1.08669162	6.95167626	0.06701810	H	1.21058600	7.06357300	0.37231000
C	1.15018133	5.94281889	-3.67172566	C	1.31644600	6.17340600	-3.39488100
H	1.67824780	3.97270150	-2.97730616	H	1.53364900	4.12816800	-2.75384300
C	7.02417281	-1.37425686	3.67745705	C	5.82278900	-2.26056700	3.82425600
H	8.78349851	-1.43297791	2.42963018	H	7.63018300	-2.47014000	2.66435300

H	5.09864650	-1.44198837	4.64891648	H	3.85015900	-2.13194100	4.68922300
C	6.79329976	-5.89055306	-2.16405005	C	5.33939500	-6.23675200	-2.39949600
H	7.56056237	-6.72309180	-0.32692108	H	5.92747700	-7.29329400	-0.61212200
H	5.87862868	-4.81850957	-3.79774353	H	4.62385100	-4.94039400	-3.96870200
C	3.99905488	5.34549626	3.08284987	C	3.65260000	4.97181700	3.49412900
H	5.20158247	6.51396979	1.72480818	H	5.06769400	6.05085100	2.27384200
H	2.60971194	4.09504362	4.16081965	H	2.06112700	3.84542300	4.41850800
C	0.85703233	7.26184356	-3.31850397	C	1.19078100	7.50875900	-3.00569500
H	0.61127333	8.63741188	-1.67405813	H	1.05601500	8.85184400	-1.32195400
H	1.17027517	5.65024240	-4.71841200	H	1.34619600	5.91354200	-4.45000300
H	7.54270925	-0.96556954	4.53997189	H	6.33828600	-1.98999700	4.74128100
H	7.25163086	-6.64325091	-2.79904852	H	5.72891300	-6.98984200	-3.07848600
H	4.59171896	5.59271792	3.95889651	H	4.21198200	5.10544500	4.41560700
H	0.64037836	8.00151281	-4.08387779	H	1.11497500	8.29512200	-3.75120500
H	-10.43873373	-0.46754194	2.07625554	H	-10.84359100	-1.02316900	3.18716400
H	-10.59352392	-1.43004070	-0.23294798	H	-11.30762900	-1.10787900	0.74777300
C	-0.15868683	-2.71883443	-3.15716073	C	-1.35880600	-1.41749100	-3.76578300
H	0.47402700	-1.85691550	-3.19801384	H	-0.82139200	-0.46364100	-3.80640400
H	0.37231774	-3.52994211	-2.70434899	H	-0.61447900	-2.19151300	-3.54346200
H	-0.45147944	-2.99368246	-4.14894249	H	-1.77259200	-1.62211500	-4.75718700

Cartesian coordinates of molecule 8 for S_0 and S_1 geometry optimization

S_0	B3LYP/6-31G(d)			S_1	BMK/6-31G(d)		
C	-7.43465400	-0.54858500	2.52810800	C	-7.59089200	-0.32599200	2.24865200
C	-7.79414800	-0.23219600	1.18025500	C	-7.88889900	-0.28389100	0.84186700
C	-9.14911800	0.05485000	0.87035200	C	-9.26173200	-0.28733000	0.45585300
C	-10.09970600	0.02976300	1.86630500	C	-10.27155100	-0.32121400	1.40911600
C	-9.74088900	-0.28090400	3.20383800	C	-9.96716000	-0.35681700	2.78766400
C	-8.43378000	-0.56620200	3.53271600	C	-8.63199800	-0.36105800	3.19372500
N	-6.14181000	-0.84273400	2.85079700	N	-6.27422900	-0.34850900	2.68462000
C	-5.26154700	-0.80232000	1.87632100	C	-5.36261200	-0.31085000	1.74802800
C	-5.60349200	-0.46510400	0.52786300	C	-5.63204400	-0.24410400	0.33897100
N	-6.85665800	-0.19718000	0.19596700	N	-6.92192700	-0.24235200	-0.10467600
H	-9.40082100	0.29181800	-0.15867600	H	-9.48680500	-0.26053700	-0.60903300
H	-8.13633500	-0.80890100	4.54812100	H	-8.35707500	-0.39493400	4.24708100
H	-4.23868300	-1.06300000	2.13739100	H	-4.33055900	-0.33984400	2.10044200
C	-4.58325800	-0.42385200	-0.55260700	C	-4.56819500	-0.20080000	-0.63825700
C	-4.98581300	-0.50149900	-1.89394500	C	-4.87497200	-0.19752600	-2.04337900
C	-3.21361500	-0.30055000	-0.27412500	C	-3.18041400	-0.13432800	-0.30111600
C	-4.04932200	-0.46375200	-2.92222700	C	-3.88875400	-0.16326500	-3.01007100
H	-6.04217800	-0.59200700	-2.11844900	H	-5.92106500	-0.22621100	-2.32913600
C	-2.26477800	-0.26166500	-1.29759400	C	-2.20611500	-0.10415200	-1.28013000
H	-2.85284600	-0.21226300	0.74468600	H	-2.85617100	-0.09195700	0.73516900
C	-2.68845500	-0.34286600	-2.63388900	C	-2.51553400	-0.12068500	-2.66964900

H	-4.37314300	-0.52734500	-3.95332700	H	-4.16535100	-0.17348300	-4.06169600
N	-0.88821300	-0.13986900	-0.95446500	N	-0.83459600	-0.03873800	-0.85261400
C	-0.01792400	-1.19865000	-0.67566100	C	-0.04059900	-1.12546900	-0.59294700
C	-0.22043300	1.06139700	-0.69854300	C	-0.13793100	1.11353400	-0.60166800
C	-0.23596800	-2.57438200	-0.76335700	C	-0.34818100	-2.49093400	-0.72014500
C	1.22509800	-0.67111400	-0.24680500	C	1.23939600	-0.68306200	-0.14759100
C	1.09621200	0.77287400	-0.26152700	C	1.17605000	0.78361400	-0.15128600
C	-0.67693300	2.37436100	-0.82340600	C	-0.56052200	2.44759900	-0.73739200
C	0.80788400	-3.42145700	-0.40774200	C	0.64088100	-3.40909500	-0.39979200
H	-1.18633300	-2.97692400	-1.09859200	H	-1.33628200	-2.80789900	-1.04155000
C	2.27145200	-1.53984800	0.07957400	C	2.22126600	-1.60549200	0.17585900
C	1.97279900	1.82057300	0.03700400	C	2.07198200	1.78884100	0.17263200
C	0.20089100	3.40166200	-0.49401600	C	0.34389800	3.44842000	-0.41624500
H	-1.68584500	2.59398200	-1.15789900	H	-1.57063100	2.67894200	-1.06339400
C	2.06202400	-2.91983700	0.00742100	C	1.92741700	-2.99197100	0.04770700
H	0.66511500	-4.49634200	-0.45353800	H	0.43165100	-4.47220100	-0.47006700
H	3.23661700	-1.15503200	0.39420500	H	3.21040800	-1.29359300	0.49966600
C	1.52331200	3.13988300	-0.07092700	C	1.65966300	3.14481800	0.03982000
H	2.99079600	1.62111000	0.35727200	H	3.08121400	1.56299600	0.50458600
H	-0.12945100	4.43285600	-0.56701600	H	0.04460800	4.48937400	-0.49012500
N	3.10728000	-3.82956500	0.35420400	N	2.90964300	-3.93850000	0.36311500
N	2.39215600	4.22763200	0.24809400	N	2.54935000	4.17487000	0.36368800
C	3.80808100	-3.65600400	1.57619500	C	3.82909300	-3.68700400	1.41463600
C	3.45099400	-4.87206900	-0.54472500	C	3.00491300	-5.15347600	-0.36720600
C	3.11300200	4.21177300	1.47064500	C	3.48374600	4.00447800	1.41821800
C	2.54647000	5.29192800	-0.67747300	C	2.52382200	5.40464400	-0.34727200
C	5.19876000	-3.84941400	1.64348800	C	5.18967000	-4.01663600	1.26071300
C	3.12198100	-3.27268000	2.74139700	C	3.38542300	-3.11922200	2.62531700
C	3.80976500	-6.14478900	-0.06651800	C	3.26719400	-6.36217900	0.30586000
C	3.42151100	-4.65555700	-1.93322300	C	2.86339500	-5.15439700	-1.76805600
C	4.44810600	4.64801100	1.52567700	C	4.80761500	4.46278200	1.27268800
C	2.50501500	3.74582200	2.64901100	C	3.09004600	3.38849600	2.62276700
C	2.66859600	6.61993800	-0.23198300	C	2.64480900	6.62142600	0.35047900
C	2.56275100	5.03838700	-2.05984500	C	2.40041700	5.41626800	-1.75001900
C	5.87733400	-3.67568800	2.84845900	C	6.08763500	-3.77553400	2.30287500
H	5.74228800	-4.13405100	0.74838000	H	5.53254300	-4.45333600	0.32588700
C	3.81236900	-3.08440800	3.93729600	C	4.29598800	-2.87301100	3.65617400
H	2.04776000	-3.12325300	2.70215800	H	2.33063900	-2.89024000	2.75586000
C	4.14132000	-7.16461100	-0.95635200	C	3.38245400	-7.55165200	-0.41742400
H	3.82540400	-6.32877600	1.00288700	H	3.37092500	-6.36104400	1.38812900
C	3.73824000	-5.68770800	-2.81499400	C	2.97008200	-6.35228100	-2.47861000
H	3.15034700	-3.67676200	-2.31525000	H	2.67947200	-4.21878300	-2.29054600
C	5.14705600	4.62868400	2.73138100	C	5.72035900	4.29804600	2.31684600

H	4.93293000	4.99923300	0.62052000	H	5.11151500	4.93641700	0.34249300
C	3.21802300	3.71444600	3.84602800	C	4.01591100	3.22062200	3.65557600
H	1.47364800	3.40929600	2.61926000	H	2.06038300	3.06252500	2.74738500
C	2.81518400	7.65998900	-1.14773800	C	2.63532700	7.83030300	-0.34952300
H	2.64659600	6.83044600	0.83244300	H	2.73280400	6.61104000	1.43410900
C	2.69240500	6.08803800	-2.96792300	C	2.38327700	6.63222500	-2.43768400
H	2.47426200	4.01726200	-2.41630800	H	2.33005200	4.47623500	-2.29178700
C	5.19266500	-3.28862300	4.00285000	C	5.64896600	-3.20005600	3.50313100
H	6.95302500	-3.82938400	2.87830400	H	7.13685400	-4.03284000	2.17260600
H	3.26231200	-2.78779300	4.82672800	H	3.93987500	-2.44044600	4.58909200
C	4.10499800	-6.94727900	-2.33601200	C	3.23188000	-7.55516700	-1.81024900
H	4.41548900	-8.14115700	-0.56531500	H	3.58237300	-8.48074800	0.11267000
H	3.70951400	-5.49817700	-3.88495800	H	2.86191300	-6.34120300	-3.56119700
C	4.54113300	4.15916700	3.89912300	C	5.33289100	3.67374600	3.51039200
H	6.17908300	4.96946200	2.75171000	H	6.74233300	4.65041600	2.19253500
H	2.72872800	3.35045800	4.74587900	H	3.69938800	2.74853200	4.58348100
C	2.82422900	7.40475000	-2.52137500	C	2.50116500	7.84391500	-1.74422800
H	2.90771000	8.67949300	-0.78201900	H	2.72166900	8.76534600	0.20029100
H	2.70313100	5.86954000	-4.03268800	H	2.29102500	6.63005900	-3.52177300
H	5.72654900	-3.14665800	4.93810400	H	6.35276600	-3.01559600	4.31182400
H	4.35739100	-7.74713300	-3.02627600	H	3.32024600	-8.48422900	-2.36897800
H	5.09184500	4.13851000	4.83516400	H	6.04816400	3.54690500	4.32016800
H	2.93139200	8.21928000	-3.23199900	H	2.49151500	8.78771000	-2.28490600
H	-10.50889800	-0.29328800	3.97177900	H	-10.76501500	-0.38392100	3.52677000
H	-11.13706100	0.25004100	1.63142200	H	-11.31164400	-0.32173700	1.08477300
C	-1.68356800	-0.30921300	-3.76032200	C	-1.44369900	-0.09777100	-3.70548300
F	-0.93934800	0.81782100	-3.74020700	F	-0.65346700	0.99760000	-3.62870300
F	-2.28221900	-0.36455800	-4.97170700	F	-1.93707800	-0.12353700	-4.94637200
F	-0.82767500	-1.35585900	-3.69530600	F	-0.59169300	-1.14393400	-3.60680100

Cartesian coordinates of molecule 9 for S_0 and S_1 geometry optimization

S_0	B3LYP/6-31G(d)			S_1	BMK/6-31G(d)		
C	9.29714200	-0.92175200	-0.71765000	C	8.76465100	-1.03150000	-0.61017800
C	8.67953800	0.16552900	-0.02531400	C	8.09748400	-0.31536500	0.45155700
C	9.49649800	1.15330600	0.58379100	C	8.90026900	0.26157100	1.48042300
C	10.86812000	1.05822100	0.49975100	C	10.27809300	0.13059800	1.44246000
C	11.47902400	-0.01986200	-0.19100700	C	10.91660800	-0.56577500	0.40573100
C	10.71007700	-0.99449000	-0.78939000	C	10.16871300	-1.14390100	-0.61365400
N	8.53584400	-1.89534000	-1.29967700	N	8.03634000	-1.61374100	-1.62875700
C	7.23295700	-1.76622900	-1.20202900	C	6.72917900	-1.45960800	-1.55811300
C	6.59746600	-0.66832600	-0.53301800	C	6.05121100	-0.75494200	-0.52758400
N	7.32527100	0.27172500	0.05174800	N	6.75396400	-0.18111300	0.49363000
C	5.12172900	-0.55753900	-0.45010300	C	4.59450900	-0.62542500	-0.50676700
C	4.53928700	0.25328400	0.53978600	C	3.97106600	0.03714400	0.59104400

C	3.15976100	0.37206700	0.65114600	C	2.59205900	0.18064900	0.66846100
C	2.31861500	-0.30436100	-0.24508800	C	1.77438800	-0.32331300	-0.35904300
C	2.88601100	-1.10273200	-1.24647300	C	2.35904500	-0.97462300	-1.46361800
C	4.26885800	-1.23251900	-1.33957700	C	3.73880300	-1.12155000	-1.53088100
C	-2.20207700	-2.95269000	0.11439800	C	-2.73163000	-2.94129600	0.03594500
C	-0.88677000	-3.45935500	0.01813400	C	-1.40031600	-3.44455600	-0.02894000
C	0.21709800	-2.61762500	-0.06462700	C	-0.30652700	-2.59802100	-0.14225600
C	-0.00615000	-1.23769000	-0.08149200	C	-0.54662700	-1.21350700	-0.19703000
C	-1.31789600	-0.70965400	0.01631100	C	-1.87039200	-0.68781200	-0.12866200
C	-2.41348600	-1.57109000	0.12473400	C	-2.95874300	-1.53900000	-0.01586700
N	0.91093100	-0.17987000	-0.13984700	N	0.35599700	-0.17722000	-0.28638600
C	0.19415500	1.02266100	-0.07855200	C	-0.32319300	1.01779900	-0.27058800
C	-1.19011000	0.73344700	0.01499400	C	-1.72504200	0.76896500	-0.16919400
C	0.65140300	2.34235600	-0.14081700	C	0.18255900	2.32897400	-0.34065700
C	-0.29001900	3.36470300	-0.09321000	C	-0.72043200	3.37980400	-0.28590300
C	-1.67168500	3.09756900	0.03097000	C	-2.12400500	3.15478100	-0.16627200
C	-2.11995100	1.77502900	0.08715500	C	-2.62256800	1.82338700	-0.11508600
N	-2.59978600	4.18060900	0.08446900	N	-3.00374000	4.23236000	-0.09078200
N	-3.30453600	-3.85470800	0.20034000	N	-3.81045400	-3.81651300	0.16875700
C	-3.74675200	4.16331900	-0.75243100	C	-4.33459300	4.12286600	-0.58034000
C	-4.99503300	4.59406400	-0.27126700	C	-5.40488800	4.63089900	0.17787000
C	-6.11496200	4.57452800	-1.10086200	C	-6.70936400	4.53799900	-0.31249900
C	-6.02050200	4.10964200	-2.41466600	C	-6.96098100	3.93561100	-1.55258700
C	-4.78366200	3.67033000	-2.89274800	C	-5.89377200	3.42907700	-2.30555800
C	-3.65424700	3.70267200	-2.07688900	C	-4.58340000	3.52499300	-1.82947800
C	-2.37537500	5.24860700	0.99118400	C	-2.59567200	5.46723400	0.48874700
C	-2.66104700	6.57533100	0.62375800	C	-2.92109100	6.67992200	-0.14384300
C	-2.43429100	7.61889600	1.51888000	C	-2.53592900	7.89110300	0.43694700
C	-1.90293300	7.36828000	2.78657800	C	-1.82151100	7.90578000	1.64210200
C	-1.60810800	6.05277700	3.15130800	C	-1.49739600	6.69582800	2.26989100
C	-1.84763300	4.99978000	2.26981000	C	-1.88592100	5.47906800	1.70328300
C	-4.43517700	-3.66321000	-0.63693300	C	-5.07833000	-3.48807600	-0.38478000
C	-3.26669400	-4.91721700	1.14053100	C	-3.66975300	-5.04102100	0.87990600
C	-5.73671700	-3.85796100	-0.14356000	C	-6.24896800	-3.67980800	0.37084300
C	-6.84060000	-3.66954700	-0.97346300	C	-7.49263900	-3.36266600	-0.18118300
C	-6.67394300	-3.26619300	-2.30034600	C	-7.58303300	-2.84799600	-1.48144300
C	-5.38224600	-3.06082500	-2.79091000	C	-6.41616200	-2.65860600	-2.23293800
C	-4.27127300	-3.26393500	-1.97436800	C	-5.16755000	-2.98132200	-1.69446700
C	-3.77588200	-6.18571400	0.81167500	C	-4.24315600	-6.22005700	0.37127500
C	-3.73145900	-7.22497200	1.73893000	C	-4.11779600	-7.41650700	1.08252900
C	-3.16464400	-7.03050700	3.00109500	C	-3.41677200	-7.45281400	2.29478400
C	-2.64840100	-5.77455400	3.32762600	C	-2.84495900	-6.27710100	2.79853500
C	-2.70402500	-4.72344000	2.41366400	C	-2.97422300	-5.07295800	2.10229000

H	2.72592700	0.97382300	1.44325700	H	2.13601800	0.67254100	1.52677300
H	9.00847200	1.97088700	1.10541500	H	8.42486200	0.80585400	2.29134300
H	11.15404400	-1.83051300	-1.32114800	H	10.66232200	-1.68510000	-1.41646400
H	6.63382300	-2.55986400	-1.64218200	H	6.16249700	-1.92589700	-2.36418200
H	5.18908900	0.77640400	1.23251500	H	4.61138600	0.42290500	1.37824100
H	2.24313200	-1.60118000	-1.96457200	H	1.72705000	-1.34706900	-2.26823900
H	4.67713000	-1.83691600	-2.14308700	H	4.15481600	-1.62181200	-2.40133800
H	-0.73976800	-4.53458400	0.01469100	H	-1.24491400	-4.51891000	0.00406700
H	1.21831400	-3.03067200	-0.12314600	H	0.70435200	-2.99250900	-0.19593200
H	-3.42175500	-1.17890400	0.21519200	H	-3.97153300	-1.15284100	0.06176600
H	1.70609800	2.57281400	-0.24512200	H	1.24821700	2.51291400	-0.44707200
H	0.03909500	4.39711500	-0.15362000	H	-0.35651800	4.40076500	-0.34944200
H	-3.18195500	1.56689300	0.17350600	H	-3.68986600	1.64787300	-0.01083600
H	-5.08165700	4.94179400	0.75312800	H	-5.20682700	5.09037400	1.14342100
H	-7.07135300	4.91133500	-0.70910900	H	-7.53196900	4.93051900	0.28180600
H	-6.89735200	4.08862100	-3.05543000	H	-7.97910000	3.86594700	-1.92944400
H	-4.69054800	3.31039800	-3.91418100	H	-6.07752700	2.97141900	-3.27554400
H	-2.69457900	3.37091400	-2.46005100	H	-3.75012600	3.15007100	-2.41991700
H	-3.05896200	6.78174700	-0.36459300	H	-3.46941800	6.66560100	-1.08301800
H	-2.66147500	8.63747500	1.21472100	H	-2.78856500	8.82517800	-0.06074000
H	-1.72097900	8.18557400	3.47854300	H	-1.52088400	8.85135400	2.08795000
H	-1.20034100	5.83830800	4.13587600	H	-0.94949400	6.69599700	3.20996300
H	-1.62916200	3.97913200	2.56702400	H	-1.64637900	4.53906700	2.19563000
H	-5.87694400	-4.15572800	0.89057500	H	-6.17658600	-4.06877700	1.38386400
H	-7.83876400	-3.82480800	-0.57204000	H	-8.39214500	-3.50925700	0.41328200
H	-7.53717400	-3.11276300	-2.94156800	H	-8.55381900	-2.59973100	-1.90501000
H	-5.23351100	-2.75196700	-3.82243100	H	-6.47490200	-2.27408800	-3.24923800
H	-3.27076400	-3.11392900	-2.36715700	H	-4.26199400	-2.85378200	-2.28353900
H	-4.20367400	-6.35068500	-0.17198600	H	-4.78021300	-6.19166600	-0.57411900
H	-4.13030200	-8.19825100	1.46457200	H	-4.56216600	-8.32488800	0.68065000
H	-3.12537500	-7.84538500	3.71825900	H	-3.31858700	-8.38706200	2.84337700
H	-2.20944100	-5.60331300	4.30720700	H	-2.30558600	-6.29153800	3.74345900
H	-2.31310400	-3.74694500	2.68091000	H	-2.54365900	-4.15653900	2.49962300
F	11.64496245	1.99871185	1.07810451	F	11.03732200	0.67271300	2.40473900
F	12.82572999	-0.08620756	-0.25794913	F	12.25520500	-0.66129000	0.41736900

Cartesian coordinates of molecule 10 for S₀ and S₁ geometry optimization

S ₀	B3LYP/6-31G(d)			S ₁	BMK/6-31G(d)		
C	8.38562500	-1.10089600	-0.75747200	C	8.38562500	-1.10089600	-0.75747200
C	7.78427000	-0.01377000	-0.04974200	C	7.78427000	-0.01377000	-0.04974200
C	8.62060700	0.94949400	0.57082200	C	8.62060700	0.94949400	0.57082200
C	9.98897800	0.83591400	0.48456700	C	9.98897800	0.83591400	0.48456700
C	10.58101600	-0.23712000	-0.22013300	C	10.58101600	-0.23712000	-0.22013300
C	9.79680300	-1.18968800	-0.83002000	C	9.79680300	-1.18968800	-0.83002000

N	7.61327600	-2.05375400	-1.34679100	N	7.61327600	-2.05375400	-1.34679100
C	6.31348300	-1.90733800	-1.24511000	C	6.31348300	-1.90733800	-1.24511000
C	5.69263900	-0.80640600	-0.56359100	C	5.69263900	-0.80640600	-0.56359100
N	6.43837800	0.11478600	0.02975400	N	6.43837800	0.11478600	0.02975400
C	4.22220200	-0.67019700	-0.47721300	C	4.22220200	-0.67019700	-0.47721300
C	3.65908900	0.18797300	0.48452100	C	3.65908900	0.18797300	0.48452100
C	2.28297000	0.33167000	0.59943900	C	2.28297000	0.33167000	0.59943900
C	1.42464600	-0.36742300	-0.26384200	C	1.42464600	-0.36742300	-0.26384200
C	1.97413200	-1.21311600	-1.23713400	C	1.97413200	-1.21311600	-1.23713400
C	3.35337000	-1.36680300	-1.33481400	C	3.35337000	-1.36680300	-1.33481400
C	-3.13488200	-2.94057700	0.15059700	C	-3.13488200	-2.94057700	0.15059700
C	-1.82812600	-3.46929400	0.05755200	C	-1.82812600	-3.46929400	0.05755200
C	-0.71120700	-2.64661600	-0.04162200	C	-0.71120700	-2.64661600	-0.04162200
C	-0.91192000	-1.26377500	-0.07949100	C	-0.91192000	-1.26377500	-0.07949100
C	-2.21432000	-0.71390400	0.01626500	C	-2.21432000	-0.71390400	0.01626500
C	-3.32327600	-1.55535700	0.14144700	C	-3.32327600	-1.55535700	0.14144700
N	0.02213400	-0.21996200	-0.15408800	N	0.02213400	-0.21996200	-0.15408800
C	-0.67718200	0.99513700	-0.10538100	C	-0.67718200	0.99513700	-0.10538100
C	-2.06467100	0.72723500	-0.00415100	C	-2.06467100	0.72723500	-0.00415100
C	-0.20239700	2.30723400	-0.18966500	C	-0.20239700	2.30723400	-0.18966500
C	-1.12936700	3.34329800	-0.15406700	C	-1.12936700	3.34329800	-0.15406700
C	-2.51420600	3.09781700	-0.02114400	C	-2.51420600	3.09781700	-0.02114400
C	-2.97999800	1.78209100	0.05559500	C	-2.97999800	1.78209100	0.05559500
N	-3.42653300	4.19358700	0.01912800	N	-3.42653300	4.19358700	0.01912800
N	-4.25080500	-3.82265600	0.25386000	N	-4.25080500	-3.82265600	0.25386000
C	-4.58711600	4.17191200	-0.79930800	C	-4.58711600	4.17191200	-0.79930800
C	-5.82262500	4.62510600	-0.30638000	C	-5.82262500	4.62510600	-0.30638000
C	-6.95588500	4.60245600	-1.11763000	C	-6.95588500	4.60245600	-1.11763000
C	-6.88723000	4.11234000	-2.42383400	C	-6.88723000	4.11234000	-2.42383400
C	-5.66296300	3.65096600	-2.91338600	C	-5.66296300	3.65096600	-2.91338600
C	-4.52033200	3.68621300	-2.11622700	C	-4.52033200	3.68621300	-2.11622700
C	-3.17559200	5.28134000	0.89559400	C	-3.17559200	5.28134000	0.89559400
C	-3.44380400	6.60206900	0.49551000	C	-3.44380400	6.60206900	0.49551000
C	-3.19234900	7.66508700	1.36069700	C	-3.19234900	7.66508700	1.36069700
C	-2.65328800	7.43921800	2.62977700	C	-2.65328800	7.43921800	2.62977700
C	-2.37597700	6.12926200	3.02679600	C	-2.37597700	6.12926200	3.02679600
C	-2.64044800	5.05744100	2.17560400	C	-2.64044800	5.05744100	2.17560400
C	-5.38920400	-3.61568100	-0.56972800	C	-5.38920400	-3.61568100	-0.56972800
C	-4.22084900	-4.88219300	1.19824700	C	-4.22084900	-4.88219300	1.19824700
C	-6.68695900	-3.77993700	-0.05613000	C	-6.68695900	-3.77993700	-0.05613000
C	-7.79858000	-3.57759800	-0.87235400	C	-7.79858000	-3.57759800	-0.87235400
C	-7.64260100	-3.19039700	-2.20532400	C	-7.64260100	-3.19039700	-2.20532400
C	-6.35424800	-3.01561900	-2.71612200	C	-6.35424800	-3.01561900	-2.71612200

C	-5.23607100	-3.23302900	-1.91317000	C	-5.23607100	-3.23302900	-1.91317000
C	-4.75073300	-6.14413600	0.87760900	C	-4.75073300	-6.14413600	0.87760900
C	-4.71509100	-7.18041500	1.80861500	C	-4.71509100	-7.18041500	1.80861500
C	-4.13683200	-6.98922500	3.06607000	C	-4.13683200	-6.98922500	3.06607000
C	-3.60038200	-5.73965600	3.38444600	C	-3.60038200	-5.73965600	3.38444600
C	-3.64711900	-4.69133600	2.46675400	C	-3.64711900	-4.69133600	2.46675400
H	1.86469900	0.96944500	1.37113600	H	1.86469900	0.96944500	1.37113600
H	5.70683900	-2.68882800	-1.69431600	H	5.70683900	-2.68882800	-1.69431600
H	4.32012900	0.72728400	1.15370000	H	4.32012900	0.72728400	1.15370000
H	1.31970700	-1.72897800	-1.93174300	H	1.31970700	-1.72897800	-1.93174300
H	3.74425600	-2.00833000	-2.11766500	H	3.74425600	-2.00833000	-2.11766500
H	-1.69770300	-4.54653000	0.06992700	H	-1.69770300	-4.54653000	0.06992700
H	0.28239200	-3.07805200	-0.09553100	H	0.28239200	-3.07805200	-0.09553100
H	-4.32430900	-1.14500900	0.23090400	H	-4.32430900	-1.14500900	0.23090400
H	0.85439800	2.52302100	-0.30283200	H	0.85439800	2.52302100	-0.30283200
H	-0.78552700	4.36966800	-0.23160300	H	-0.78552700	4.36966800	-0.23160300
H	-4.04432900	1.58920400	0.14768400	H	-4.04432900	1.58920400	0.14768400
H	-5.88876300	4.99292000	0.71252600	H	-5.88876300	4.99292000	0.71252600
H	-7.90225600	4.95697100	-0.71732700	H	-7.90225600	4.95697100	-0.71732700
H	-7.77437700	4.08909300	-3.05017200	H	-7.77437700	4.08909300	-3.05017200
H	-5.59009900	3.27160900	-3.92940400	H	-5.59009900	3.27160900	-3.92940400
H	-3.57027600	3.33764500	-2.50840000	H	-3.57027600	3.33764500	-2.50840000
H	-3.84770800	6.78851000	-0.49440100	H	-3.84770800	6.78851000	-0.49440100
H	-3.40626300	8.67884500	1.03190100	H	-3.40626300	8.67884500	1.03190100
H	-2.45199200	8.27138800	3.29823300	H	-2.45199200	8.27138800	3.29823300
H	-1.96271600	5.93439600	4.01311900	H	-1.96271600	5.93439600	4.01311900
H	-2.43588200	4.04149200	2.49786600	H	-2.43588200	4.04149200	2.49786600
H	-6.81814600	-4.06521200	0.98271500	H	-6.81814600	-4.06521200	0.98271500
H	-8.79385900	-3.70924200	-0.45568800	H	-8.79385900	-3.70924200	-0.45568800
H	-8.51161500	-3.02605900	-2.83592600	H	-8.51161500	-3.02605900	-2.83592600
H	-6.21419700	-2.72002900	-3.75271500	H	-6.21419700	-2.72002900	-3.75271500
H	-4.23837200	-3.10732600	-2.32141700	H	-4.23837200	-3.10732600	-2.32141700
H	-5.18781000	-6.30629500	-0.10245000	H	-5.18781000	-6.30629500	-0.10245000
H	-5.12998800	-8.14881200	1.54096900	H	-5.12998800	-8.14881200	1.54096900
H	-4.10456200	-7.80180900	3.78616600	H	-4.10456200	-7.80180900	3.78616600
H	-3.15270600	-5.57108100	4.36052000	H	-3.15270600	-5.57108100	4.36052000
H	-3.24086600	-3.71935900	2.72764200	H	-3.24086600	-3.71935900	2.72764200
F	10.37490300	-2.19801000	-1.48925800	F	10.37490300	-2.19801000	-1.48925800
F	11.91422700	-0.30443300	-0.27822500	F	11.91422700	-0.30443300	-0.27822500
F	10.78892700	1.73641200	1.06251200	F	10.78892700	1.73641200	1.06251200
F	8.08358100	1.97345800	1.24158300	F	8.08358100	1.97345800	1.24158300

Cartesian coordinates of molecule 11 for S₀ and S₁ geometry optimization

S ₀	B3LYP/6-31G(d)			S ₁	BMK/6-31G(d)		
C	8.87478800	-0.88886700	-0.67214400	C	8.87478800	-0.88886700	-0.67214400
C	8.25174200	0.19090400	0.02331000	C	8.25174200	0.19090400	0.02331000
C	9.06280300	1.17853700	0.64274000	C	9.06280300	1.17853700	0.64274000
C	10.43204600	1.09642900	0.56881700	C	10.43204600	1.09642900	0.56881700
C	11.05122700	0.01766200	-0.13038700	C	11.05122700	0.01766200	-0.13038700
C	10.28310500	-0.96243000	-0.74173300	C	10.28310500	-0.96243000	-0.74173300
N	8.12154200	-1.86359100	-1.26512200	N	8.12154200	-1.86359100	-1.26512200
C	6.81995100	-1.73993300	-1.17226500	C	6.81995100	-1.73993300	-1.17226500
C	6.17502600	-0.64577000	-0.49795700	C	6.17502600	-0.64577000	-0.49795700
N	6.89837200	0.29325300	0.09519900	N	6.89837200	0.29325300	0.09519900
C	4.70157500	-0.54110400	-0.42195100	C	4.70157500	-0.54110400	-0.42195100
C	4.11315000	0.29557600	0.54372300	C	4.11315000	0.29557600	0.54372300
C	2.73375100	0.41100100	0.64897200	C	2.73375100	0.41100100	0.64897200
C	1.89625900	-0.29540600	-0.22891200	C	1.89625900	-0.29540600	-0.22891200
C	2.47041700	-1.12035700	-1.20596500	C	2.47041700	-1.12035700	-1.20596500
C	3.85311400	-1.24621700	-1.29324200	C	3.85311400	-1.24621700	-1.29324200
C	-2.61944300	-2.95637300	0.11116700	C	-2.61944300	-2.95637300	0.11116700
C	-1.30261100	-3.46020700	0.02173600	C	-1.30261100	-3.46020700	0.02173600
C	-0.19989400	-2.61638800	-0.05687900	C	-0.19989400	-2.61638800	-0.05687900
C	-0.42507000	-1.23697200	-0.07759500	C	-0.42507000	-1.23697200	-0.07759500
C	-1.73784700	-0.71201800	0.01519400	C	-1.73784700	-0.71201800	0.01519400
C	-2.83249200	-1.57467600	0.11964400	C	-2.83249200	-1.57467600	0.11964400
N	0.49062700	-0.17538100	-0.12976000	N	0.49062700	-0.17538100	-0.12976000
C	-0.23115400	1.02613700	-0.06951700	C	-0.23115400	1.02613700	-0.06951700
C	-1.61425000	0.73175000	0.01647300	C	-1.61425000	0.73175000	0.01647300
C	0.22006200	2.34774800	-0.13169800	C	0.22006200	2.34774800	-0.13169800
C	-0.72594100	3.36618700	-0.08861800	C	-0.72594100	3.36618700	-0.08861800
C	-2.10701400	3.09373300	0.02994200	C	-2.10701400	3.09373300	0.02994200
C	-2.54920700	1.76872600	0.08380900	C	-2.54920700	1.76872600	0.08380900
N	-3.03926600	4.17211800	0.07915300	N	-3.03926600	4.17211800	0.07915300
N	-3.72004300	-3.85942500	0.19286100	N	-3.72004300	-3.85942500	0.19286100
C	-4.19339700	4.14167200	-0.74818500	C	-4.19339700	4.14167200	-0.74818500
C	-5.44029400	4.56562200	-0.25797900	C	-5.44029400	4.56562200	-0.25797900
C	-6.56708500	4.53466400	-1.07792300	C	-6.56708500	4.53466400	-1.07792300
C	-6.48024100	4.06487600	-2.39049700	C	-6.48024100	4.06487600	-2.39049700
C	-5.24444900	3.63247800	-2.87750700	C	-5.24444900	3.63247800	-2.87750700
C	-4.10839600	3.67644100	-2.07141100	C	-4.10839600	3.67644100	-2.07141100
C	-2.81432300	5.25127500	0.97312200	C	-2.81432300	5.25127500	0.97312200
C	-3.10256600	6.57277200	0.58987900	C	-3.10256600	6.57277200	0.58987900
C	-2.87680700	7.62735300	1.47230800	C	-2.87680700	7.62735300	1.47230800

C	-2.34400000	7.39252600	2.74241000	C	-2.34400000	7.39252600	2.74241000
C	-2.04688200	6.08198700	3.12284900	C	-2.04688200	6.08198700	3.12284900
C	-2.28556200	5.01818000	2.25415000	C	-2.28556200	5.01818000	2.25415000
C	-4.85743600	-3.65861200	-0.63379200	C	-4.85743600	-3.65861200	-0.63379200
C	-3.67744300	-4.93382600	1.11992700	C	-3.67744300	-4.93382600	1.11992700
C	-6.15487800	-3.85256300	-0.12993700	C	-6.15487800	-3.85256300	-0.12993700
C	-7.26543900	-3.65634700	-0.94911200	C	-7.26543900	-3.65634700	-0.94911200
C	-7.10894300	-3.24598100	-2.27506800	C	-7.10894300	-3.24598100	-2.27506800
C	-5.82105100	-3.04170100	-2.77600000	C	-5.82105100	-3.04170100	-2.77600000
C	-4.70362500	-3.25274200	-1.97030500	C	-4.70362500	-3.25274200	-1.97030500
C	-4.18200700	-6.19954700	0.77444800	C	-4.18200700	-6.19954700	0.77444800
C	-4.13458700	-7.25030500	1.68855900	C	-4.13458700	-7.25030500	1.68855900
C	-3.56922700	-7.06957600	2.95340500	C	-3.56922700	-7.06957600	2.95340500
C	-3.05777200	-5.81605200	3.29642500	C	-3.05777200	-5.81605200	3.29642500
C	-3.11668400	-4.75366700	2.39574800	C	-3.11668400	-4.75366700	2.39574800
H	2.29661500	1.03169100	1.42412900	H	2.29661500	1.03169100	1.42412900
H	8.57142500	1.99134000	1.16748900	H	8.57142500	1.99134000	1.16748900
H	10.73754200	-1.79070500	-1.27441300	H	10.73754200	-1.79070500	-1.27441300
H	6.22674300	-2.53262500	-1.62072800	H	6.22674300	-2.53262500	-1.62072800
H	4.75822300	0.84006100	1.22410500	H	4.75822300	0.84006100	1.22410500
H	1.83215600	-1.64128300	-1.91173600	H	1.83215600	-1.64128300	-1.91173600
H	4.26320400	-1.87148600	-2.07938000	H	4.26320400	-1.87148600	-2.07938000
H	-1.15280300	-4.53497700	0.02039300	H	-1.15280300	-4.53497700	0.02039300
H	0.80163300	-3.02937100	-0.10824400	H	0.80163300	-3.02937100	-0.10824400
H	-3.84130900	-1.18334100	0.20663100	H	-3.84130900	-1.18334100	0.20663100
H	1.27348700	2.58432900	-0.23403400	H	1.27348700	2.58432900	-0.23403400
H	-0.40044100	4.39966700	-0.14905300	H	-0.40044100	4.39966700	-0.14905300
H	-3.61049100	1.55506500	0.16439200	H	-3.61049100	1.55506500	0.16439200
H	-5.52038100	4.91732700	0.76560200	H	-5.52038100	4.91732700	0.76560200
H	-7.52249800	4.86646100	-0.67964800	H	-7.52249800	4.86646100	-0.67964800
H	-7.36228800	4.03498900	-3.02371000	H	-7.36228800	4.03498900	-3.02371000
H	-5.15751700	3.26926800	-3.89830200	H	-5.15751700	3.26926800	-3.89830200
H	-3.14946100	3.35054800	-2.46147400	H	-3.14946100	3.35054800	-2.46147400
H	-3.50192900	6.76642900	-0.40048900	H	-3.50192900	6.76642900	-0.40048900
H	-3.10601600	8.64187000	1.15643000	H	-3.10601600	8.64187000	1.15643000
H	-2.16292200	8.21828700	3.42446000	H	-2.16292200	8.21828700	3.42446000
H	-1.63841800	5.88006500	4.10976000	H	-1.63841800	5.88006500	4.10976000
H	-2.06598300	4.00134100	2.56348800	H	-2.06598300	4.00134100	2.56348800
H	-6.28669200	-4.15601500	0.90366800	H	-6.28669200	-4.15601500	0.90366800
H	-8.26054400	-3.81115900	-0.54007800	H	-8.26054400	-3.81115900	-0.54007800
H	-7.97725900	-3.08655000	-2.90788500	H	-7.97725900	-3.08655000	-2.90788500
H	-5.68055800	-2.72783400	-3.80714100	H	-5.68055800	-2.72783400	-3.80714100
H	-3.70603300	-3.10410900	-2.37105200	H	-3.70603300	-3.10410900	-2.37105200

H	-4.60881500	-6.35317400	-0.21149700	H	-4.60881500	-6.35317400	-0.21149700
H	-4.52996100	-8.22141600	1.40189700	H	-4.52996100	-8.22141600	1.40189700
H	-3.52764100	-7.89325800	3.66029000	H	-3.52764100	-7.89325800	3.66029000
H	-2.62050600	-5.65570200	4.27858100	H	-2.62050600	-5.65570200	4.27858100
H	-2.73013100	-3.77895800	2.67571000	H	-2.73013100	-3.77895800	2.67571000
H	11.05741700	1.84824100	1.03842600	H	11.05741700	1.84824100	1.03842600
C	12.48198100	-0.04786200	-0.19622500	C	12.48198100	-0.04786200	-0.19622500
N	13.64366300	-0.09232000	-0.24408600	N	13.64366300	-0.09232000	-0.24408600