Supporting Information

Can Time-Dependent Density Functional Theory Predict Intersystem Crossing in Organic Chromophores? A Case Study on Benzo(bis)-X-diazole Based Donor-Acceptor-Donor Type Molecules

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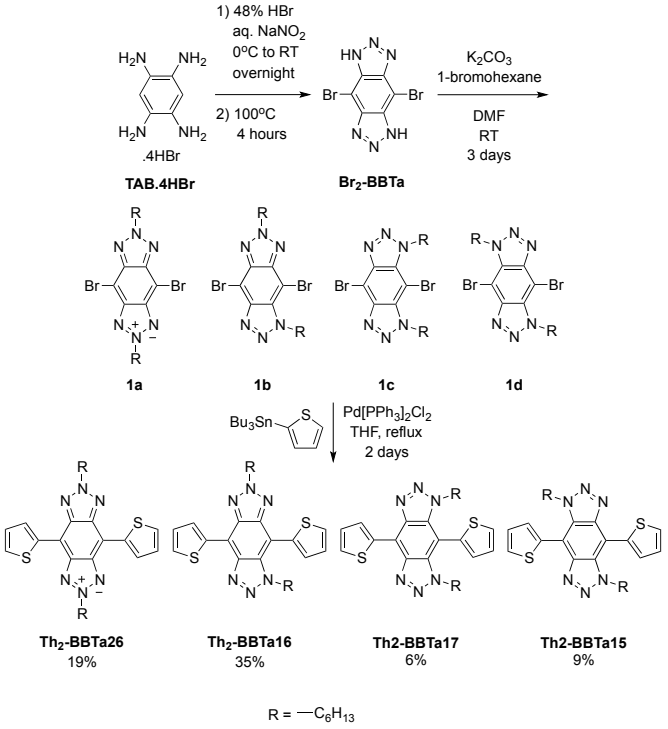
Experimental Details & Procedures

All reagents were purchased from Sigma Aldrich unless otherwise stated. TAB.4HBr (Hangzhou Trylead Chemical Technology Co. Ltd.), $Pd[PPh_3]Cl_2$ (Strem Chemicals Inc.). The Th_2-BBTa isomers,[1] Th_2-SBTa[2] and Th_2-BBT[3] were synthesized using literature procedures. ^1H and ^{13}C NMR were performed on JEOL 500MHz NMR system with chemical shifts referenced to the deuterated solvent. Matrix assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectra were obtained on a Bruker Daltonics Autoflex II TOF/TOF system. Elemental analysis was carried out using CHNS FlashEA 1112 Elemental Analyzer from Thermo Fisher Scientific. UV-Vis absorption spectra were recorded on a Shimadzu UV-3101PC UV-VIS-NIR Spectrophotometer. Cyclic voltammetry (CV) experiments were performed using Autolab potentiostat (model PGSTAT30) by Echochimie. All CV measurements of the Th_2-BBTa small molecules were recorded in dry chloroform with 0.1 M tetrabutylammonium hexafluorophosphate as supporting electrolyte (scan rate of 100 $mV \cdot s^{-1}$). Ferrocene was used as external standard (onset of oxidation was taken to be -4.8 eV). Fluorescence measurements were measured using Shimadzu RF-5301 PC spectrofluorophotometer and chloroform as solvent. Φ_f of the compounds were measured in chloroform using perylene (Φ_f = 0.94 in cyclohexane)[4] as actinometer for **Th_2-BBTa17** and **Th_2-BBTa15**, N,N′-bis(1-ethylpropyl)-3,4:9,10-perylene-bis(dicarboximide) (Φ_f = 0.98 in dichloromethane)[5] for **Th_2-BBTa26** and **Th_2-BBTa16**, and zinc phthalocyanine (Φ_f = 0.23 in THF) for **Th_2-SBTa**. For single crystal XRD, a suitable crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Bruker AXS SMART APEXII CCD diffractometer. The crystal was kept at about 100 K for **Th_2-BBTa17** and **Th_2-BBTa15** while 250 K for **Th_2-BBTa26** during data collection. Using Olex2[6], the structure was solved with the XM[7] structure solution program using Dual Space and refined with the ShelXL[7] refinement package using Least Squares minimization.

Synthesis of all four Th_2-BBTa isomers.



21 g of TAB.4HBr (45.5 mmol) was added to 300 mL of 48 % aq. HBr and allowed to cool down to 0° C. 31.38 g of $NaNO_2$ (454.7 mmol) was dissolved in 500 mL of deionized water and was added dropwisely to the reaction mixture using an additional funnel in air. Brown gas evolved upon addition of $NaNO_2$ solution. After addition of $NaNO_2$ solution, the reaction was allowed to warm up to room temperature overnight. The reaction mixture was heated to 100 °C for 4 hours and then cooled down to room temperature where the resulting precipitate of Br_2-BBTa was filtered, washed excessively with deionized water and dried. The crude Br_2-BBTa was used for the next step without further purification. The crude Br_2-BBTa, 15.06 g of anhydrous K_2CO_3 (109.0 mmol) and 14.04 mL of 1-bromohexane (100.0 mmol) was added to 90 mL of DMF and the reaction mixture was allowed to stir at room temperature for 3 days under N_2 environment. The reaction mixture was added to 500 mL of water and extracted using dichloromethane. The organic layer was collected, dried over anhydrous $MgSO_4$, and stripped from all volatiles. The residue was forced through a short silica column using dichloromethane as the eluent to yield the crude isomers **1a-d**. These isomers could not be well separated at this point of time. To the crude mixture under N_2 environment, 28.9 mL of 2-(tributylstannyl)thiophene (91.0 mmol), 958 mg of $Pd[PPh_3]Cl_2$ (1.36 mmol) and 200 mL of THF were added and the reaction was heated under reflux for 2 days. The reaction mixture was cooled to room temperature and most of the volatiles removed under vacuum. The residue was dry loaded into a silica column with hexane as the eluent. 4.2 g of **Th_2-BBTa26** (19 % yield, red crystalline solids, hexane to hexane: dichloromethane 80:20), 7.81 g of **Th_2-BBTa16** (35 % yield, orange waxy solids, hexane: dichloromethane 80:20 to hexane: dichloromethane 60:40), 1.40 g of **Th_2-BBTa17** (6 % yield, yellow solids, hexane: dichloromethane 60:40 to hexane: dichloromethane 30:70) and 2.35 g of **Th_2-BBTa15** (9 % yield, yellow solids, hexane: dichloromethane 30:70 to pure dichloromethane) were obtained.

Th_2-BBTa26. ^{1}H NMR ($CDCl_3$): δ, [ppm] 0.90 (t, 6 H, J = 7.3 Hz), 1.34-1.52 (m, 4 H), 2.30 (quintet, 4 H, J = 7.4 Hz), 4.94 (t, 4 H, J = 7.3 Hz), 7.29 (dd, 2H, J = 4.0, 5.0 Hz), 7.55 (dd, 2 H, J =1.0, 5.0 Hz), 8.72 (dd, 2 H, J = 1.0, 5.0 Hz). ^{13}C NMR ($CDCl_3$): δ, [ppm] 14.16, 22.64, 26.49, 30.15, 31.39, 31.22, 57.96, 109.94, 127,83, 128.05, 129.71, 137.26, 141.39. Anal. Calcd for $C_{26}H_{32}N_6S_2$: C, 63.38; H, 6.55; N, 17.06; S, 13.02. Found: C, 63.68; H, 6.71; N, 16.88. MALDI-TOF-MS m/z: 492.23 (M^+); calcd. for $C_{26}H_{32}N_6S_2$ = 492.70.

Th_2-BBTa16. ^{1}H NMR ($CDCl_3$): δ, [ppm] 0.80 (t, 3 H, J = 7.0 Hz), 0.87 (t, 3 H, J = 7.0 Hz), 1.06-1.20 (m, 6 H), 1.30-1.43 (m, 6 H), 1.57 (quintet, 2 H, J = 7.5 Hz), 2.18 (quintet, 2 H, J = 7.4), 4.50 (t, 2 H, J = 7.5 Hz), 4.82 (t, 2 H, J = 7.5 Hz), 7.25 (dd, 1H, J = 3.5, 5.0 Hz), 7.28-7.31 (m, 2 H), 7.60 (dd, 1 H, J = 1.0 Hz, 5.0 Hz), 7.63 (dd, 1 H, J = 1.0 Hz, 5.0 Hz), 8.93 (dd, 1 H, J = 1.0, 4.0 Hz). ^{13}C NMR ($CDCl_3$): δ, [ppm] 14.03, 14.06, 22.45, 22.52, 26.15, 26.30, 30.15, 30.22, 31.19, 31.24, 50.03, 57.80, 100.94, 114.80, 127.15, 127.73, 127.88, 129.74, 129,82, 131.36, 131.80, 133.39, 135.64, 139.09, 142.57, 145.66. Anal. Calcd for $C_{26}H_{32}N_6S_2$: C, 63.38; H, 6.55; N, 17.06; S, 13.02. Found: C, 63.57; H, 6.50; N, 16.66. MALDI-TOF-MS m/z: 493.18 ($M+H^+$); calcd. for $C_{26}H_{32}N_6S_2$ = 492.70.

Th_2-BBTa17. ^{1}H NMR ($CDCl_3$): δ, [ppm] 0.80 (t, 6 H, J = 7.3 Hz), 1.06-1.21 (m, 12 H), 1.64-1.69 (doublet of quintet, 4 H, J = 2.5, 7.6 Hz), 4.04 (doublet of multiplet, 2 H), 7.22-7.24 (m, 1H), 7.26-7.28 (m, 2 H), 7.61 (dd, 1 H, J = 1.3, 5.0 Hz), 7.63 (dd, 1 H, J = 1.5, 5.0 Hz), 9.12 (dd, 1 H, J = 1.0, 4.0 Hz). ^{13}C NMR ($CDCl_3$): δ, [ppm] 14.05, 22.52, 26.40, 30.88, 31.28, 49.49, 92.74, 117.69, 127.56, 127.81, 128.73, 130.78, 131.44, 131.96, 133.31, 133.39, 134.60, 140.72. Anal. Calcd for $C_{26}H_{32}N_6S_2$: C, 63.38; H, 6.55; N, 17.06; S, 13.02. Found: C, 63.56; H, 6.57; N, 17.07. MALDI-TOF-MS m/z: 493.20 ($M+H^+$); calcd. for $C_{26}H_{32}N_6S_2$ = 492.70.

Th_2-BBTa15. ^{1}H NMR ($CDCl_3$): δ, [ppm] 0.82 (t, 6 H, J = 7.3 Hz), 1.07-1.21 (m, 12 H), 1.58 (quintet, 4 H, J = 7.4 Hz), 4.56 (t, 4 H, J = 7.8), 7.30 (dd, 2H, J = 3.5, 5.5 Hz), 7.37 (dd, 2 H, J = 1.0, 3.5 Hz), 7.67 (dd, 2 H, J = 1.3, 5.3 Hz). ^{13}C NMR ($CDCl_3$): δ, [ppm] 14.08, 22.51, 26.22, 30.51, 31.23, 50.40, 107.14, 127.37, 128.59, 129.36, 130.50, 131.85, 146.97. Anal. Calcd for $C_{26}H_{32}N_6S_2$: C, 63.38; H, 6.55; N, 17.06; S, 13.02. Found: C, 63.58; H, 6.62; N, 16.98. MALDI-TOF-MS m/z: 492.68 (M^+); calcd. for $C_{26}H_{32}N_6S_2$ = 492.70.

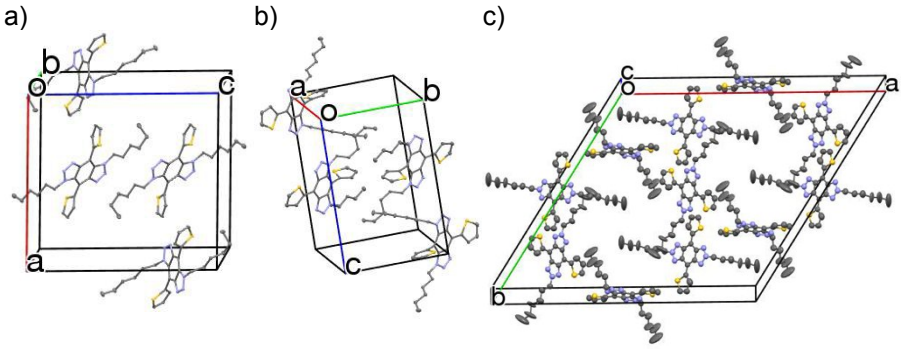
Single crystal growth of **Th_2-BBT**, **Th_2-BBTa26**, **Th_2-BBTa17** and **Th_2-BBTa15**. For **Th_2-BBTa17** and **Th_2-BBTa15**, the solids were separately heated in hot hexane and dichloromethane was added until all solids were dissolved. For **Th_2-BBTa26**, the solids were heated in hot ethanol and toluene was added until all solids were dissolved. The solutions were allowed to crystallize upon standing. **Th_2-BBTa26** red needles. **Th_2-BBTa17** yellow platelets. **Th_2-BBTa15** light yellow needles. No crystals of **Th_2-BBTa16** could be grown as it is a waxy solid.

Crystal Data for **Th_2-BBTa26** (*M* = 492.69): trigonal, space group R-3 (no. 148), *a* = 37.196(3) Å, *c* = 5.4457(9) Å, *V* = 6525.1(15) Å^3, *Z* = 9, *T* = 250(2) K, μ(CuKα) = 1.839 mm^{-1}, *Dcalc* = 1.128 g/mm^3, 4864 reflections measured (16.508 ≤ 2θ ≤ 110.09), 1791

unique (R_{int} = 0.0326, R_{sigma} = 0.0372) which were used in all calculations. The final R_1 was 0.0400 (I > 2σ(I)) and wR_2 was 0.1155 (all data).

Crystal Data for **Th_2-BBTa17** (M = 492.69): triclinic, space group P-1 (no. 2), a = 9.6442(3) Å, b = 13.9072(4) Å, c = 19.3218(6) Å, α = 80.5235(16)°, β = 89.0924(16)°, γ = 79.1833(15)°, V = 2510.43(13) Å^3, Z = 4, T = 100.07 K, μ(MoKα) = 0.239 mm^{-1}, $Dcalc$ = 1.304 g/mm^3, 189236 reflections measured (2.138 ≤ 2θ ≤ 70.03), 22113 unique (R_{int} = 0.0729, R_{sigma} = 0.0335) which were used in all calculations. The final R_1 was 0.0499 (I > 2σ(I)) and wR_2 was 0.1292 (all data). Refinement Details. The sulfur and disordered carbon atoms were refined with group anisotropic displacement parameters. Distance restraints were imposed on the disorder. 3 reflections were removed because they were behind the beam stop.

Crystal Data for **Th_2-BBTa15** (M = 492.69): monoclinic, space group $P2_1/n$ (no. 14), a = 20.6046(8) Å, b = 5.8783(2) Å, c = 20.9113(8) Å, β = 97.134(2)°, V = 2513.17(16) Å^3, Z = 4, T = 100.03 K, μ(MoKα) = 0.239 mm^{-1}, $Dcalc$ = 1.302 g/mm^3, 121995 reflections measured (5.98 ≤ 2θ ≤ 73.05), 12190 unique (R_{int} = 0.0634, R_{sigma} = 0.0330) which were used in all calculations. The final R_1 was 0.0498 (I > 2σ(I)) and wR_2 was 0.1270 (all data).



S1. XRD single crystal structure of a) **Th_2-BBTa15**, b) **Th_2-BBTa17** and c) **Th_2-BBTa26**. Blue – Nitrogen, Grey – Carbon, Yellow – Sulphur. Hydrogens are omitted for clarity. Disordered thiophene and hexyl groups are omitted for clarity. Thermal ellipsoids drawn at 50% probability.

DFT Calculations

All calculations were carried using Gaussian 09, Revision A.02 package. The ground states were geometry optimized to the global minimum using DFT RB3LYP 6-31G (d,p) level of theory. TDDFT calculations were performed on these structures to calculate the energies of S_1^{GS} and T_1^{GS}. The SES geometries were optimized from the ground state geometry using TDDFT. The energies of S_1^{SES} and T_1^{SES}, as well as the NPA atomic charges of the excited states (using keyword density=current) were also calculated in this step. Wavefunction stability checks were performed on all calculated geometries. When there is RHF→UHF instability, the geometries were re-optimized using UB3LYP. TDDFT calculations were performed on these re-optimized structures (using keyword

guess=mix). Single-point calculations using solvation model (IEFPCM, solvent = chloroform) were performed on the optimized geometries.

Note, TDDFT geometry optimization of the SES geometries for Th_2-SBTA and Th_2-BBT do not converge when guess=mix is used. To ensure convergence, TDDFT geometry optimization were carried out without the using the keyword guess=mix. A subsequent single-point energy TDDFT calculation on the optimized SES geometry with the keyword guess=mix was carried out to obtain the electronic transitions. Wavefunction stability check on the optimized SES geometry also includes the keyword guess=mix. Without it, there is an internal instability and wavefunction optimization automatically initiates orbital mixing to give the same solution (total energy) as single-point energy TDDFT calculation with guess=mix.

Excitation energies and oscillator strengths for **Th_2-SBTa** SES geometry (restricted):

Excited State 1: Triplet-A" -0.4603 eV -2693.62 nm f=-0.0000 <S**2>=2.000
91 -> 92 0.73334
91 <- 92 0.22435
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.
Excited State 2: Singlet-A" 1.2922 eV 959.50 nm f=0.3673 <S**2>=0.000
91 -> 92 0.71530
91 <- 92 -0.13968
Excited State 3: Triplet-A' 2.3168 eV 535.15 nm f=0.0000 <S**2>=2.000
88 -> 92 -0.10271
90 -> 92 0.66979
91 -> 96 0.16078

Excitation energies and oscillator strengths for **Th_2-SBTa** SES geometry (unrestricted, guess=mix):

Excited state symmetry could not be determined.
Excited State 1: 2.368-?Sym 0.6962 eV 1780.82 nm f=0.0005 <S**2>=1.152
91A -> 92A 0.71797
91B -> 92B 0.71797
91A <- 92A 0.16234
91B <- 92B 0.16234
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.
Excited state symmetry could not be determined.
Excited State 2: 0.969-?Sym 1.3799 eV 898.50 nm f=0.3205 <S**2>=-0.015
91A -> 92A 0.70418
91B -> 92B -0.70418
Excited state symmetry could not be determined.
Excited State 3: 2.795-?Sym 2.4637 eV 503.24 nm f=0.0116 <S**2>=1.704
90A -> 92A 0.65124
91A -> 95A 0.16892
90B -> 92B -0.65124
91B -> 95B -0.16892

Excitation energies and oscillator strengths for **Th_2-BBT** GS geometry (restricted):

Excited State 1: Triplet-BU -0.2429 eV -5104.87 nm f=-0.0000 <S**2>=2.000
87 -> 92 -0.15261
91 -> 92 0.86105
87 <- 92 -0.12303
91 <- 92 0.50785
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.
Excited State 2: Singlet-BU 1.3796 eV 898.70 nm f=0.2776 <S**2>=0.000
91 -> 92 0.71427
91 <- 92 -0.13193
Excited State 3: Triplet-AG 2.2405 eV 553.38 nm f=0.0000 <S**2>=2.000
88 -> 92 -0.18156
90 -> 92 0.66254
91 -> 95 0.11013

Excitation energies and oscillator strengths for **Th_2-BBT** GS geometry (unrestricted, guess=mix):

Excited state symmetry could not be determined.
Excited State 1: 2.638-?Sym 0.4837 eV 2563.47 nm f=0.0000 <S**2>=1.489
87A -> 92A 0.10544
91A -> 92A 0.74477
87B -> 92B 0.10544
91B -> 92B 0.74477
91A <- 92A 0.26250
91B <- 92B 0.26250
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.
Excited state symmetry could not be determined.
Excited State 2: 0.955-?Sym 1.3738 eV 902.49 nm f=0.2545 <S**2>=-0.022
91A -> 92A 0.70908
91B -> 92B -0.70908
91A <- 92A -0.10622
91B <- 92B 0.10622
Excited state symmetry could not be determined.
Excited State 3: 2.908-?Sym 2.2995 eV 539.18 nm f=0.0123 <S**2>=1.865
88A -> 92A -0.12700
89A -> 92A -0.11567
90A -> 92A 0.66060
91A -> 95A 0.11561
88B -> 92B 0.12700
89B -> 92B 0.11567
90B -> 92B -0.66060
91B -> 95B -0.11561

Excitation energies and oscillator strengths for **Th_2-BBT** SES geometry (restricted):

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 Excited State   1:      Triplet-BU     -0.5076 eV    -2442.70 nm  f=-0.0000  <S**2>=2.000
     91 -> 92         0.70355
 This state for optimization and/or second-order correction.
 Copying the excited state density for this state as the 1-particle RhoCI density.
 Excited State   2:      Singlet-BU     1.0200 eV 1215.57 nm  f=0.2487  <S**2>=0.000
     91 -> 92         0.72170
     91 <- 92        -0.16071
 Excited State   3:      Triplet-AG     2.0632 eV  600.93 nm  f=0.0000  <S**2>=2.000
     88 -> 92        -0.15922
     90 -> 92         0.66994
```

Excitation energies and oscillator strengths for **Th_2-BBT** SES geometry (unrestricted, guess=mix):

Excited state symmetry could not be determined.
Excited State 1: 2.016-?Sym 0.8750 eV 1416.92 nm f=0.0000 <S**2>=0.766
91A -> 92A 0.70460
91B -> 92B 0.70460
This state for optimization and/or second-order correction.
Copying the excited state density for this state as the 1-particle RhoCI density.
Excited state symmetry could not be determined.
Excited State 2: 1.046-?Sym 1.2008 eV 1032.48 nm f=0.2036 <S**2>=0.023
91A -> 92A -0.70191
91B -> 92B 0.70191
Excited state symmetry could not be determined.
Excited State 3: 2.657-?Sym 2.3616 eV 525.00 nm f=0.0517 <S**2>=1.515
89A -> 92A 0.10729
90A -> 92A -0.65391
91A -> 94A 0.11706
91A -> 96A -0.12029
89B -> 92B -0.10729
90B -> 92B 0.65391
91B -> 94B -0.11706
91B -> 96B 0.12029

Th_2-BBTa15 GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.745704	-1.154082	0.044613
2	6	0	1.494572	0.035255	0.092686
3	6	0	0.680512	1.184984	0.057630
4	6	0	-0.745705	1.154080	0.044655
5	6	0	-1.494573	-0.035259	0.092658
6	6	0	-0.680513	-1.184987	0.057562
7	7	0	1.087956	2.501341	0.010659
8	7	0	1.083205	-2.485829	-0.032108
9	7	0	-1.087956	-2.501342	0.010522
10	7	0	-0.043604	-3.253273	-0.057333
11	6	0	2.956751	0.105726	0.197403
12	6	0	3.765624	-0.506682	1.129913
13	6	0	5.149918	-0.221813	0.958217
14	6	0	5.387252	0.607842	-0.104234
15	6	0	-2.956754	-0.105736	0.197346
16	6	0	2.361276	-3.143376	-0.244814
17	16	0	3.922903	1.069833	-0.900675
18	1	0	2.876870	-2.708474	-1.104005
19	1	0	2.138427	-4.192339	-0.439412
20	1	0	3.005820	-3.058184	0.631849
21	1	0	3.369400	-1.108846	1.939640
22	1	0	5.930587	-0.607632	1.603425
23	1	0	6.335758	0.989234	-0.456411
24	7	0	0.043605	3.253276	-0.057177
25	7	0	-1.083204	2.485830	-0.032009
26	6	0	-2.361272	3.143387	-0.244702
27	1	0	-2.138421	4.192359	-0.439250
28	1	0	-2.876855	2.708524	-1.103919
29	1	0	-3.005828	3.058156	0.631949
30	6	0	-3.765645	0.506621	1.129874
31	6	0	-5.149936	0.221763	0.958136
32	16	0	-3.922887	-1.069785	-0.900802
33	6	0	-5.387250	-0.607835	-0.104365
34	1	0	-6.335750	-0.989206	-0.456580
35	1	0	-5.930618	0.607548	1.603350
36	1	0	-3.369437	1.108741	1.939641

Th_2-BBTa15 SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.689731	-1.207316	-0.224236
2	6	0	1.498585	-0.038141	-0.069261
3	6	0	0.729422	1.169789	-0.211701
4	6	0	-0.689770	1.207379	-0.224049
5	6	0	-1.498613	0.038180	-0.069134
6	6	0	-0.729457	-1.169731	-0.211783
7	7	0	1.207954	2.427858	-0.368508
8	7	0	0.959390	-2.530330	-0.434452
9	7	0	-1.207986	-2.427788	-0.368707
10	7	0	-0.209993	-3.259473	-0.524819
11	6	0	2.894275	-0.014914	0.251783
12	6	0	3.643874	-0.990779	0.920956
13	6	0	4.992388	-0.639576	1.118220
14	6	0	5.295450	0.606922	0.610723
15	6	0	-2.894268	0.014885	0.252070
16	6	0	2.188729	-3.227868	-0.770421
17	16	0	3.925927	1.388620	-0.091437
18	1	0	2.869515	-2.553800	-1.290516
19	1	0	1.913688	-4.057394	-1.422028
20	1	0	2.687818	-3.626341	0.117309
21	1	0	3.196804	-1.893900	1.313776
22	1	0	5.711592	-1.267827	1.631099
23	1	0	6.249049	1.117173	0.639410
24	7	0	0.209957	3.259569	-0.524442
25	7	0	-0.959425	2.530415	-0.434164
26	6	0	-2.188746	3.227996	-0.770112
27	1	0	-1.913678	4.057553	-1.421669
28	1	0	-2.869543	2.553976	-1.290252
29	1	0	-2.687832	3.626435	0.117634
30	6	0	-3.643781	0.990562	0.921611
31	6	0	-4.992321	0.639396	1.118767
32	16	0	-3.925894	-1.388683	-0.091088
33	6	0	-5.295486	-0.606898	0.610832
34	1	0	-6.249135	-1.117066	0.639309
35	1	0	-5.711498	1.267569	1.631780
36	1	0	-3.196665	1.893562	1.314652

Th_2-BBTa17 GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.429186	-1.111943	0.090177
2	6	0	1.273649	0.012921	0.115792
3	6	0	0.537416	1.213629	0.088191
4	6	0	-0.886661	1.294731	0.046231
5	6	0	-1.728611	0.156053	0.023628
6	6	0	-0.993781	-1.048416	0.048781
7	7	0	-1.236631	2.629398	0.036765
8	7	0	0.925623	2.527232	0.101433
9	7	0	-1.481551	-2.336707	0.039276
10	7	0	0.680115	-2.458573	0.102257
11	7	0	-0.495279	-3.161121	0.069906
12	7	0	-0.168727	3.346095	0.068601
13	6	0	2.748093	-0.058541	0.173174
14	6	0	-3.177232	0.225052	-0.019782
15	6	0	3.561372	-0.114470	1.278545
16	6	0	4.953689	-0.179153	0.966828
17	6	0	5.194904	-0.172892	-0.378596
18	6	0	-3.961224	1.368404	-0.045616
19	6	0	-5.351428	1.101373	-0.086993
20	6	0	-5.628922	-0.241682	-0.092837
21	6	0	2.244494	3.134202	0.133297
22	6	0	1.929754	-3.197352	0.128447
23	16	0	3.722658	-0.088424	-1.290665
24	16	0	-4.201217	-1.211062	-0.048000
25	1	0	2.523838	-2.991709	-0.765401
26	1	0	1.664498	-4.254139	0.157211
27	1	0	2.516104	-2.938382	1.012682
28	1	0	3.166454	-0.107975	2.288506
29	1	0	5.737736	-0.227762	1.713660
30	1	0	6.147539	-0.213093	-0.888668
31	1	0	-6.598783	-0.720126	-0.121283
32	1	0	-6.112032	1.872968	-0.111452
33	1	0	-3.525152	2.358254	-0.034254
34	1	0	2.088265	4.212060	0.175360
35	1	0	2.801642	2.805789	1.013120
36	1	0	2.813788	2.880128	-0.764137

Th_2-BBTa17 SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.408269	-1.160222	-0.115723
2	6	0	-1.275099	-0.023916	-0.126839
3	6	0	-0.551494	1.209613	-0.100194
4	6	0	0.865308	1.313287	-0.047898
5	6	0	1.727155	0.161238	-0.022565
6	6	0	1.007813	-1.078062	-0.065375
7	7	0	1.207624	2.627861	-0.095212
8	7	0	-0.955294	2.508129	-0.207882
9	7	0	1.519250	-2.332833	-0.003390
10	7	0	-0.643243	-2.502517	-0.058435
11	7	0	0.540755	-3.204979	-0.000651
12	7	0	0.123612	3.359189	-0.191729
13	6	0	-2.726432	-0.131096	-0.142800
14	6	0	3.143871	0.247800	0.033604
15	6	0	-3.537936	-0.732701	-1.090574
16	6	0	-4.921875	-0.691328	-0.776848
17	6	0	-5.180029	-0.067598	0.417251
18	6	0	3.932085	1.414863	0.078362
19	6	0	5.309104	1.151834	0.127015
20	6	0	5.602318	-0.201309	0.120380
21	6	0	-2.264390	3.101687	-0.409695
22	6	0	-1.870793	-3.272086	0.024222
23	16	0	-3.726517	0.475624	1.187323
24	16	0	4.192387	-1.194997	0.055894
25	1	0	-2.517494	-2.882293	0.812973
26	1	0	-1.573900	-4.294109	0.258791
27	1	0	-2.417905	-3.258458	-0.921323
28	1	0	-3.138805	-1.146644	-2.009535
29	1	0	-5.698088	-1.091877	-1.418711
30	1	0	-6.138547	0.104940	0.887385
31	1	0	6.581326	-0.661449	0.153761
32	1	0	6.069602	1.923520	0.165164
33	1	0	3.478438	2.397137	0.069288
34	1	0	-2.092551	4.107427	-0.792848
35	1	0	-2.835144	2.517886	-1.134323
36	1	0	-2.827804	3.157904	0.525062

Th_2-BBTa16 GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.696806	-1.315932	-0.000870
2	6	0	1.404090	-0.108229	0.065935
3	6	0	0.534496	1.010862	0.052609
4	6	0	-0.898611	0.912924	0.030098
5	6	0	-1.608539	-0.316989	0.012763
6	6	0	-0.734348	-1.422507	-0.013308
7	7	0	-1.399744	2.172762	0.051200
8	7	0	0.862906	2.325912	0.090952
9	7	0	1.104609	-2.626952	-0.091360
10	7	0	-1.058819	-2.764127	-0.092978
11	7	0	-0.317328	2.929594	0.087689
12	7	0	0.022672	-3.456590	-0.148149
13	6	0	2.860117	0.024164	0.185960
14	6	0	3.687963	-0.510867	1.147707
15	6	0	5.061221	-0.171668	0.975378
16	6	0	5.274282	0.626622	-0.114837
17	6	0	-3.055243	-0.426791	0.012278
18	6	0	-3.816199	-1.585152	-0.008690
19	6	0	-5.213222	-1.347443	-0.000769
20	6	0	-5.523232	-0.012594	0.026602
21	6	0	-0.414113	4.380523	0.056118
22	6	0	2.421885	-3.208206	-0.278217
23	16	0	3.798030	0.982074	-0.947343
24	16	0	-4.113113	0.985536	0.043103
25	1	0	-3.358868	-2.565041	-0.031405
26	1	0	-5.956870	-2.135783	-0.014932
27	1	0	-6.503278	0.444851	0.037867
28	1	0	0.405108	4.791301	0.645103
29	1	0	-1.377693	4.663677	0.476535
30	1	0	-0.339586	4.736783	-0.974898
31	1	0	2.929708	-2.742484	-1.126086
32	1	0	2.265655	-4.268234	-0.478163
33	1	0	3.042240	-3.085914	0.611681
34	1	0	3.310921	-1.098639	1.977061
35	1	0	5.851334	-0.496849	1.642382
36	1	0	6.208468	1.038084	-0.471329

Th_2-BBTa16 SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.678507	-1.390402	-0.151500
2	6	0	1.415701	-0.165855	-0.074046
3	6	0	0.563013	0.988597	-0.156485
4	6	0	-0.866203	0.916481	-0.079337
5	6	0	-1.588668	-0.312606	0.013345
6	6	0	-0.740777	-1.469769	-0.066373
7	7	0	-1.357227	2.167487	-0.085027
8	7	0	0.927014	2.275080	-0.218536
9	7	0	1.051343	-2.688419	-0.346083
10	7	0	-1.109971	-2.776386	-0.167838
11	7	0	-0.252046	2.938254	-0.150893
12	7	0	-0.053225	-3.518597	-0.348528
13	6	0	2.820693	-0.054252	0.187110
14	6	0	3.653394	-0.952890	0.863276
15	6	0	4.988009	-0.518684	0.981345
16	6	0	5.197355	0.716496	0.406382
17	6	0	-3.007945	-0.392340	0.124623
18	6	0	-3.798657	-1.547560	0.210737
19	6	0	-5.174295	-1.276985	0.322549
20	6	0	-5.457044	0.073521	0.321982
21	6	0	-0.334329	4.356527	-0.403167
22	6	0	2.309145	-3.280265	-0.770230
23	16	0	3.753000	1.384187	-0.261979
24	16	0	-4.041679	1.050253	0.182733
25	1	0	-3.355205	-2.534002	0.182993
26	1	0	-5.935413	-2.044905	0.400108
27	1	0	-6.428446	0.544433	0.396568
28	1	0	0.568818	4.827448	-0.013609
29	1	0	-1.215415	4.745971	0.108298
30	1	0	-0.418184	4.567538	-1.477070
31	1	0	2.875165	-2.565147	-1.367751
32	1	0	2.058984	-4.154095	-1.371934
33	1	0	2.919617	-3.597923	0.079066
34	1	0	3.276542	-1.861046	1.314083
35	1	0	5.764053	-1.081546	1.487116
36	1	0	6.119734	1.280209	0.367149

Th_2-BBTa26 GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.573824	1.252793	-0.005155
2	6	0	-1.511988	0.190113	-0.000856
3	6	0	-0.857956	-1.064690	0.004190
4	6	0	0.573823	-1.252792	0.005155
5	6	0	1.511987	-0.190113	0.000855
6	6	0	0.857956	1.064691	-0.004190
7	7	0	0.809514	-2.592421	0.015525
8	7	0	-1.435333	-2.293973	0.013637
9	7	0	1.435332	2.293974	-0.013637
10	7	0	-0.809515	2.592421	-0.015524
11	7	0	-0.403649	-3.117585	0.023305
12	7	0	0.403649	3.117585	-0.023305
13	6	0	-2.948410	0.375749	-0.001177
14	6	0	-3.647548	1.573303	-0.004094
15	16	0	-4.083189	-0.976695	0.002423
16	6	0	-5.056165	1.412097	-0.003582
17	1	0	-3.143552	2.529762	-0.006491
18	6	0	-5.439782	0.096948	-0.000338
19	1	0	-5.755565	2.240352	-0.005497
20	1	0	-6.443081	-0.306796	0.000832
21	6	0	2.948410	-0.375749	0.001177
22	6	0	3.647548	-1.573303	0.004094
23	16	0	4.083190	0.976695	-0.002423
24	6	0	5.056166	-1.412098	0.003582
25	1	0	3.143552	-2.529763	0.006491
26	6	0	5.439783	-0.096948	0.000338
27	1	0	5.755565	-2.240352	0.005497
28	1	0	6.443082	0.306796	-0.000832
29	6	0	-0.595770	-4.558534	-0.025362
30	6	0	0.595769	4.558534	0.025363
31	1	0	-1.561662	-4.785545	0.422931
32	1	0	0.213189	-5.031377	0.530197
33	1	0	-0.579165	-4.901250	-1.063492
34	1	0	-0.213189	5.031378	-0.530198
35	1	0	1.561661	4.785545	-0.422929
36	1	0	0.579163	4.901251	1.063493

Th_2-BBTa26 SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.560723	-1.282088	-0.012629
2	6	0	1.497887	-0.196582	-0.001837
3	6	0	0.863148	1.085147	0.010421
4	6	0	-0.560724	1.282088	0.012629
5	6	0	-1.497887	0.196582	0.001837
6	6	0	-0.863148	-1.085147	-0.010421
7	7	0	-0.803796	2.604297	0.032755
8	7	0	1.460528	2.287156	0.028966
9	7	0	-1.460528	-2.287156	-0.028964
10	7	0	0.803796	-2.604297	-0.032756
11	7	0	0.428156	3.150681	0.065031
12	7	0	-0.428157	-3.150681	-0.065032
13	6	0	2.911727	-0.384512	-0.002803
14	6	0	3.611666	-1.598739	-0.017115
15	16	0	4.059823	0.968273	0.015662
16	6	0	5.010175	-1.441587	-0.013338
17	1	0	3.093068	-2.547460	-0.030695
18	6	0	5.400050	-0.119181	0.003702
19	1	0	5.710238	-2.269176	-0.022839
20	1	0	6.408798	0.272132	0.009920
21	6	0	-2.911726	0.384512	0.002803
22	6	0	-3.611665	1.598738	0.017115
23	16	0	-4.059823	-0.968273	-0.015661
24	6	0	-5.010175	1.441587	0.013337
25	1	0	-3.093068	2.547460	0.030696
26	6	0	-5.400049	0.119181	-0.003704
27	1	0	-5.710238	2.269176	0.022838
28	1	0	-6.408797	-0.272132	-0.009924
29	6	0	0.627847	4.573997	-0.070741
30	6	0	-0.627847	-4.573996	0.070741
31	1	0	1.577260	4.833264	0.398486
32	1	0	-0.194475	5.087324	0.428905
33	1	0	0.652447	4.872266	-1.126284
34	1	0	0.194474	-5.087324	-0.428906
35	1	0	-1.577262	-4.833263	-0.398484
36	1	0	-0.652445	-4.872266	1.126285

Th_2-SBTa GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.083474	-0.001695	1.525463
2	6	0	-1.103602	0.002231	0.735899
3	6	0	-1.103602	0.002231	-0.735899
4	6	0	0.083474	-0.001695	-1.525463
5	6	0	1.247856	-0.003467	-0.723169
6	6	0	1.247856	-0.003467	0.723169
7	7	0	2.547137	-0.010146	1.131912
8	7	0	3.224326	-0.016807	0.000000
9	7	0	2.547137	-0.010146	-1.131912
10	7	0	-2.345724	0.006063	-1.250256
11	16	0	-3.392773	0.009103	0.000000
12	7	0	-2.345724	0.006063	1.250256
13	6	0	0.100028	-0.002422	-2.973314
14	6	0	0.100028	-0.002422	2.973314
15	6	0	1.212871	-0.004043	-3.804220
16	6	0	0.897042	-0.005025	-5.184716
17	6	0	-0.453623	-0.004160	-5.417609
18	16	0	-1.370807	-0.001523	-3.952555
19	16	0	-1.370807	-0.001523	3.952555
20	6	0	-0.453623	-0.004160	5.417609
21	6	0	0.897042	-0.005025	5.184716
22	6	0	1.212871	-0.004043	3.804220
23	6	0	4.678812	0.032834	0.000000
24	1	0	2.220016	-0.004447	-3.412552
25	1	0	1.642618	-0.006348	-5.971517
26	1	0	-0.966312	-0.004608	-6.370058
27	1	0	-0.966312	-0.004608	6.370058
28	1	0	1.642618	-0.006348	5.971517
29	1	0	2.220016	-0.004447	3.412552
30	1	0	5.036244	-0.469454	0.897616
31	1	0	5.013566	1.073585	0.000000
32	1	0	5.036244	-0.469454	-0.897616

Th_2-SBTa SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.082235	-0.003045	1.524800
2	6	0	-1.129614	0.002998	0.731189
3	6	0	-1.129614	0.002998	-0.731189
4	6	0	0.082235	-0.003045	-1.524800
5	6	0	1.293660	-0.005215	-0.713417
6	6	0	1.293660	-0.005215	0.713417
7	7	0	2.563247	-0.017055	1.131696
8	7	0	3.276077	-0.038011	0.000000
9	7	0	2.563247	-0.017055	-1.131696
10	7	0	-2.342939	0.009112	-1.261003
11	16	0	-3.451247	0.014758	0.000000
12	7	0	-2.342939	0.009112	1.261003
13	6	0	0.091691	-0.004950	-2.941365
14	6	0	0.091691	-0.004950	2.941365
15	6	0	1.219696	-0.010716	-3.784148
16	6	0	0.904359	-0.010800	-5.154682
17	6	0	-0.452794	-0.005274	-5.387934
18	16	0	-1.384242	0.000168	-3.926796
19	16	0	-1.384242	0.000168	3.926796
20	6	0	-0.452794	-0.005274	5.387934
21	6	0	0.904359	-0.010800	5.154682
22	6	0	1.219696	-0.010716	3.784148
23	6	0	4.720735	0.065577	0.000000
24	1	0	2.223856	-0.015189	-3.385066
25	1	0	1.647764	-0.014901	-5.943381
26	1	0	-0.959446	-0.004140	-6.343954
27	1	0	-0.959446	-0.004140	6.343954
28	1	0	1.647764	-0.014901	5.943381
29	1	0	2.223856	-0.015189	3.385066
30	1	0	5.100102	-0.429285	0.893968
31	1	0	5.039086	1.113383	0.000000
32	1	0	5.100102	-0.429285	-0.893968

Th_2-SBTa SES geometry (unrestricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.082157	-0.002930	1.524752
2	6	0	-1.129623	0.003013	0.731165
3	6	0	-1.129623	0.003013	-0.731165
4	6	0	0.082157	-0.002930	-1.524752
5	6	0	1.293628	-0.005089	-0.713283
6	6	0	1.293628	-0.005089	0.713283
7	7	0	2.563363	-0.017012	1.131521
8	7	0	3.276052	-0.037990	0.000000
9	7	0	2.563363	-0.017012	-1.131521
10	7	0	-2.342953	0.008997	-1.260964
11	16	0	-3.451486	0.014425	0.000000
12	7	0	-2.342953	0.008997	1.260964
13	6	0	0.091637	-0.004789	-2.941375
14	6	0	0.091637	-0.004789	2.941375
15	6	0	1.219660	-0.010343	-3.784110
16	6	0	0.904395	-0.010531	-5.154728
17	6	0	-0.452687	-0.005311	-5.388100
18	16	0	-1.384162	0.000184	-3.926959
19	16	0	-1.384162	0.000184	3.926959
20	6	0	-0.452687	-0.005311	5.388100
21	6	0	0.904395	-0.010531	5.154728
22	6	0	1.219660	-0.010343	3.784110
23	6	0	4.720744	0.064746	0.000000
24	1	0	2.223841	-0.014652	-3.385127
25	1	0	1.647872	-0.014542	-5.943347
26	1	0	-0.959243	-0.004337	-6.344176
27	1	0	-0.959243	-0.004337	6.344176
28	1	0	1.647872	-0.014542	5.943347
29	1	0	2.223841	-0.014652	3.385127
30	1	0	5.099870	-0.430279	0.893973
31	1	0	5.039684	1.112369	0.000000
32	1	0	5.099870	-0.430279	-0.893973

Th_2-BBT GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.018671	1.388207	0.000000
2	6	0	1.287141	0.822668	0.000000
3	6	0	1.265484	-0.602869	0.000000
4	6	0	0.018671	-1.388207	0.000000
5	6	0	-1.287141	-0.822668	0.000000
6	6	0	-1.265484	0.602869	0.000000
7	6	0	2.503425	1.608492	0.000000
8	6	0	-2.503425	-1.608492	0.000000
9	6	0	-3.816136	-1.147635	0.000000
10	6	0	-4.787067	-2.176145	0.000000
11	6	0	-4.229701	-3.428825	0.000000
12	6	0	3.816136	1.147635	0.000000
13	6	0	4.787067	2.176145	0.000000
14	6	0	4.229701	3.428825	0.000000
15	16	0	-2.503425	-3.378896	0.000000
16	16	0	2.503425	3.378896	0.000000
17	16	0	1.856624	-2.935224	0.000000
18	16	0	-1.856624	2.935224	0.000000
19	7	0	2.361640	-1.389044	0.000000
20	7	0	0.245885	-2.715631	0.000000
21	7	0	-0.245885	2.715631	0.000000
22	7	0	-2.361640	1.389044	0.000000
23	1	0	4.052023	0.094142	0.000000
24	1	0	5.855247	1.992708	0.000000
25	1	0	4.736828	4.384366	0.000000
26	1	0	-4.052023	-0.094142	0.000000
27	1	0	-5.855247	-1.992708	0.000000
28	1	0	-4.736828	-4.384366	0.000000

Th_2-BBT GS geometry (unrestricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.021356	1.390998	0.000000
2	6	0	1.286983	0.822674	0.000000
3	6	0	1.267356	-0.606535	0.000000
4	6	0	0.021356	-1.390998	0.000000
5	6	0	-1.286983	-0.822674	0.000000
6	6	0	-1.267356	0.606535	0.000000
7	6	0	2.499932	1.607690	0.000000
8	6	0	-2.499932	-1.607690	0.000000
9	6	0	-3.814560	-1.146571	0.000000
10	6	0	-4.784527	-2.174565	0.000000
11	6	0	-4.226550	-3.427705	0.000000
12	6	0	3.814560	1.146571	0.000000
13	6	0	4.784527	2.174565	0.000000
14	6	0	4.226550	3.427705	0.000000
15	16	0	-2.499932	-3.378842	0.000000
16	16	0	2.499932	3.378842	0.000000
17	16	0	1.860290	-2.941719	0.000000
18	16	0	-1.860290	2.941719	0.000000
19	7	0	2.362205	-1.388937	0.000000
20	7	0	0.245010	-2.715791	0.000000
21	7	0	-0.245010	2.715791	0.000000
22	7	0	-2.362205	1.388937	0.000000
23	1	0	4.049594	0.092884	0.000000
24	1	0	5.852766	1.991588	0.000000
25	1	0	4.734142	4.383043	0.000000
26	1	0	-4.049594	-0.092884	0.000000
27	1	0	-5.852766	-1.991588	0.000000
28	1	0	-4.734142	-4.383043	0.000000

Th_2-BBT SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.034283	1.403695	0.000000
2	6	0	1.271668	0.804649	0.000000
3	6	0	1.271668	-0.635819	0.000000
4	6	0	0.034283	-1.403695	0.000000
5	6	0	-1.271668	-0.804649	0.000000
6	6	0	-1.271668	0.635819	0.000000
7	6	0	2.470393	1.579687	0.000000
8	6	0	-2.470393	-1.579687	0.000000
9	6	0	-3.793914	-1.108920	0.000000
10	6	0	-4.759030	-2.128694	0.000000
11	6	0	-4.197153	-3.388946	0.000000
12	6	0	3.793914	1.108920	0.000000
13	6	0	4.759030	2.128694	0.000000
14	6	0	4.197153	3.388946	0.000000
15	16	0	-2.476727	-3.358578	0.000000
16	16	0	2.476727	3.358578	0.000000
17	16	0	1.865524	-2.986749	0.000000
18	16	0	-1.865524	2.986749	0.000000
19	7	0	2.368784	-1.399521	0.000000
20	7	0	0.221649	-2.724732	0.000000
21	7	0	-0.221649	2.724732	0.000000
22	7	0	-2.368784	1.399521	0.000000
23	1	0	4.012126	0.051285	0.000000
24	1	0	5.827494	1.948040	0.000000
25	1	0	4.714963	4.339488	0.000000
26	1	0	-4.012126	-0.051285	0.000000
27	1	0	-5.827494	-1.948040	0.000000
28	1	0	-4.714963	-4.339488	0.000000

Th_2-BBT SES geometry (unrestricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.039788	1.408779	0.000000
2	6	0	1.281276	0.820409	0.000000
3	6	0	1.279236	-0.630195	0.000000
4	6	0	0.039788	-1.408779	0.000000
5	6	0	-1.281276	-0.820409	0.000000
6	6	0	-1.279236	0.630195	0.000000
7	6	0	2.474030	1.600656	0.000000
8	6	0	-2.474030	-1.600656	0.000000
9	6	0	-3.800771	-1.136764	0.000000
10	6	0	-4.764380	-2.161440	0.000000
11	6	0	-4.202133	-3.417656	0.000000
12	6	0	3.800771	1.136764	0.000000
13	6	0	4.764380	2.161440	0.000000
14	6	0	4.202133	3.417656	0.000000
15	16	0	-2.474030	-3.376808	0.000000
16	16	0	2.474030	3.376808	0.000000
17	16	0	1.884097	-2.981323	0.000000
18	16	0	-1.884097	2.981323	0.000000
19	7	0	2.368747	-1.389139	0.000000
20	7	0	0.241145	-2.719510	0.000000
21	7	0	-0.241145	2.719510	0.000000
22	7	0	-2.368747	1.389139	0.000000
23	1	0	4.029480	0.081654	0.000000
24	1	0	5.833025	1.981623	0.000000
25	1	0	4.713294	4.371391	0.000000
26	1	0	-4.029480	-0.081654	0.000000
27	1	0	-5.833025	-1.981623	0.000000
28	1	0	-4.713294	-4.371391	0.000000

Th_2-BBT TES geometry (unrestricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.022079	1.402755	0.000000
2	6	0	1.276732	0.802643	0.000000
3	6	0	1.275413	-0.624812	0.000000
4	6	0	0.022079	-1.402755	0.000000
5	6	0	-1.276732	-0.802643	0.000000
6	6	0	-1.275413	0.624812	0.000000
7	6	0	2.491901	1.584228	0.000000
8	6	0	-2.491901	-1.584228	0.000000
9	6	0	-3.828489	-1.102901	0.000000
10	6	0	-4.800396	-2.121341	0.000000
11	6	0	-4.254603	-3.380169	0.000000
12	6	0	3.828489	1.102901	0.000000
13	6	0	4.800396	2.121341	0.000000
14	6	0	4.254603	3.380169	0.000000
15	16	0	-2.491901	-3.333410	0.000000
16	16	0	2.491901	3.333410	0.000000
17	16	0	1.862131	-2.978262	0.000000
18	16	0	-1.862131	2.978262	0.000000
19	7	0	2.368173	-1.402926	0.000000
20	7	0	0.220121	-2.718967	0.000000
21	7	0	-0.220121	2.718967	0.000000
22	7	0	-2.368173	1.402926	0.000000
23	1	0	4.037864	0.043546	0.000000
24	1	0	5.867291	1.930392	0.000000
25	1	0	4.761175	4.335846	0.000000
26	1	0	-4.037864	-0.043546	0.000000
27	1	0	-5.867291	-1.930392	0.000000
28	1	0	-4.761175	-4.335846	0.000000

Th_2-BTa GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.714135	0.790590	-0.002930
2	6	0	-1.478642	-0.417811	0.002146
3	6	0	-0.705607	-1.575136	0.010049
4	6	0	0.705607	-1.575136	0.010047
5	6	0	1.478643	-0.417811	0.002142
6	6	0	0.714135	0.790590	-0.002932
7	7	0	1.132841	2.076165	-0.014916
8	7	0	-1.132842	2.076165	-0.014912
9	7	0	-0.000001	2.764746	-0.026137
10	6	0	-2.935833	-0.428546	0.000999
11	6	0	-3.811683	0.638276	0.001570
12	16	0	-3.837583	-1.941772	-0.001379
13	6	0	-5.181188	0.252672	0.000488
14	1	0	-3.467054	1.663379	0.002682
15	6	0	-5.354379	-1.103920	-0.001049
16	1	0	-6.004193	0.958166	0.000886
17	1	0	-6.278108	-1.665470	-0.002231
18	6	0	2.935833	-0.428545	0.000993
19	6	0	3.811683	0.638276	0.001524
20	16	0	3.837584	-1.941772	-0.001335
21	6	0	5.181188	0.252672	0.000449
22	1	0	3.467054	1.663380	0.002603
23	6	0	5.354379	-1.103919	-0.001040
24	1	0	6.004193	0.958166	0.000818
25	1	0	6.278108	-1.665469	-0.002206
26	6	0	-0.000001	4.217122	0.025755
27	1	0	-0.896357	4.576650	-0.477971
28	1	0	0.896351	4.576650	-0.477979
29	1	0	0.000004	4.557732	1.065043
30	1	0	-1.201328	-2.541125	0.017144
31	1	0	1.201329	-2.541124	0.017139

Th_2-BTa SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.713181	0.807974	-0.026299
2	6	0	-1.460478	-0.413386	-0.005883
3	6	0	-0.689022	-1.619295	0.017128
4	6	0	0.689022	-1.619295	0.017128
5	6	0	1.460478	-0.413386	-0.005882
6	6	0	0.713181	0.807974	-0.026300
7	7	0	1.154609	2.079194	-0.051693
8	7	0	-1.154609	2.079194	-0.051694
9	7	0	0.000000	2.800311	-0.117557
10	6	0	-2.888027	-0.429132	-0.006852
11	6	0	-3.776785	0.652578	-0.031662
12	16	0	-3.802298	-1.952223	0.026269
13	6	0	-5.131067	0.264906	-0.023560
14	1	0	-3.415455	1.671827	-0.056133
15	6	0	-5.306949	-1.102958	0.006987
16	1	0	-5.958839	0.964651	-0.039995
17	1	0	-6.237078	-1.654568	0.018835
18	6	0	2.888027	-0.429132	-0.006852
19	6	0	3.776785	0.652578	-0.031661
20	16	0	3.802298	-1.952223	0.026270
21	6	0	5.131067	0.264906	-0.023560
22	1	0	3.415454	1.671827	-0.056131
23	6	0	5.306950	-1.102958	0.006985
24	1	0	5.958839	0.964651	-0.039996
25	1	0	6.237078	-1.654567	0.018832
26	6	0	0.000000	4.214544	0.160378
27	1	0	-0.894013	4.654095	-0.284381
28	1	0	0.894012	4.654095	-0.284383
29	1	0	0.000000	4.417469	1.240974
30	1	0	-1.207889	-2.572378	0.033901
31	1	0	1.207890	-2.572378	0.033901

Th_2-BT GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000002	3.195477	-0.000007
2	6	0	1.482297	-0.326198	0.000004
3	6	0	0.730539	0.905635	0.000000
4	6	0	-1.482297	-0.326197	0.000002
5	6	0	-0.730539	0.905637	-0.000001
6	6	0	0.706704	-1.474806	0.000007
7	1	0	1.197515	-2.443126	0.000011
8	6	0	-0.706705	-1.474805	0.000006
9	1	0	-1.197516	-2.443125	0.000010
10	7	0	1.252927	2.135725	-0.000003
11	7	0	-1.252927	2.135726	-0.000005
12	6	0	-2.940081	-0.361532	0.000001
13	6	0	-3.848461	0.678653	-0.000009
14	16	0	-3.800361	-1.901492	0.000006
15	6	0	-5.205540	0.253046	-0.000006
16	1	0	-3.536512	1.713219	-0.000014
17	6	0	-5.339310	-1.107938	0.000009
18	1	0	-6.048109	0.934859	-0.000010
19	1	0	-6.246352	-1.696147	0.000012
20	6	0	2.940081	-0.361533	0.000004
21	6	0	3.848460	0.678653	0.000025
22	16	0	3.800360	-1.901493	-0.000025
23	6	0	5.205539	0.253046	0.000024
24	1	0	3.536512	1.713218	0.000041
25	6	0	5.339310	-1.107938	-0.000002
26	1	0	6.048108	0.934859	0.000040
27	1	0	6.246351	-1.696147	-0.000005

Th_2-BT SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	3.233125	0.000000
2	6	0	1.445030	-0.329153	0.000002
3	6	0	0.714043	0.914502	0.000000
4	6	0	-1.445030	-0.329153	-0.000001
5	6	0	-0.714043	0.914503	-0.000001
6	6	0	0.689335	-1.532347	0.000002
7	1	0	1.207505	-2.485600	0.000003
8	6	0	-0.689335	-1.532347	0.000000
9	1	0	-1.207506	-2.485600	0.000000
10	7	0	1.286405	2.140210	0.000002
11	7	0	-1.286405	2.140210	-0.000002
12	6	0	-2.877517	-0.370741	-0.000003
13	6	0	-3.790674	0.688763	-0.000005
14	16	0	-3.758925	-1.913766	-0.000004
15	6	0	-5.136075	0.272442	-0.000007
16	1	0	-3.443346	1.712774	-0.000004
17	6	0	-5.277652	-1.099256	-0.000007
18	1	0	-5.978897	0.953498	-0.000008
19	1	0	-6.195155	-1.672148	-0.000009
20	6	0	2.877517	-0.370741	0.000004
21	6	0	3.790674	0.688763	0.000005
22	16	0	3.758925	-1.913766	0.000003
23	6	0	5.136075	0.272442	0.000007
24	1	0	3.443346	1.712773	0.000005
25	6	0	5.277652	-1.099256	0.000007
26	1	0	5.978897	0.953498	0.000009
27	1	0	6.195155	-1.672148	0.000008

Th_2-ST GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.482297	-0.326198	0.000004
2	6	0	0.730539	0.905635	0.000000
3	6	0	-1.482297	-0.326197	0.000002
4	6	0	-0.730539	0.905637	-0.000001
5	6	0	0.706704	-1.474806	0.000007
6	1	0	1.197515	-2.443126	0.000011
7	6	0	-0.706705	-1.474805	0.000006
8	1	0	-1.197516	-2.443125	0.000010
9	7	0	1.252927	2.135725	-0.000003
10	7	0	-1.252927	2.135726	-0.000005
11	6	0	-2.940081	-0.361532	0.000001
12	6	0	-3.848461	0.678653	-0.000009
13	16	0	-3.800361	-1.901492	0.000006
14	6	0	-5.20554	0.253046	-0.000006
15	1	0	-3.536512	1.713219	-0.000014
16	6	0	-5.33931	-1.107938	0.000009
17	1	0	-6.048109	0.934859	-0.00001
18	1	0	-6.246352	-1.696147	0.000012
19	6	0	2.940081	-0.361533	0.000004
20	6	0	3.84846	0.678653	0.000025
21	16	0	3.80036	-1.901493	-0.000025
22	6	0	5.205539	0.253046	0.000024
23	1	0	3.536512	1.713218	0.000041
24	6	0	5.33931	-1.107938	-0.000002
25	1	0	6.048108	0.934859	0.00004
26	1	0	6.246351	-1.696147	-0.000005
27	34	0	0.000002	3.195477	-0.000007

Th_2-ST SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.442128	-0.677422	0.000003
2	6	0	0.717856	0.576435	0.000000
3	6	0	-1.442129	-0.677422	-0.000001
4	6	0	-0.717856	0.576436	-0.000001
5	6	0	0.688824	-1.880087	0.000002
6	1	0	1.206649	-2.833462	0.000004
7	6	0	-0.688824	-1.880087	0.000000
8	1	0	-1.206650	-2.833462	0.000000
9	7	0	1.342592	1.772167	0.000002
10	7	0	-1.342592	1.772167	-0.000003
11	6	0	-2.875113	-0.732206	-0.000003
12	6	0	-3.802563	0.314572	-0.000003
13	16	0	-3.739431	-2.286296	-0.000001
14	6	0	-5.142834	-0.117904	-0.000007
15	1	0	-3.464646	1.341334	-0.000002
16	6	0	-5.267620	-1.490936	-0.000010
17	1	0	-5.993716	0.553064	-0.000009
18	1	0	-6.177905	-2.075271	-0.000013
19	6	0	2.875113	-0.732205	0.000004
20	6	0	3.802563	0.314573	0.000007
21	16	0	3.739431	-2.286296	0.000004
22	6	0	5.142833	-0.117904	0.000007
23	1	0	3.464646	1.341335	0.000007
24	6	0	5.267620	-1.490935	0.000005
25	1	0	5.993716	0.553064	0.000009
26	1	0	6.177904	-2.075270	0.000005
27	34	0	0.000000	3.013834	-0.000001

Sh_2-BT GS geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.483636	-0.864299	0.000000
2	6	0	-0.726985	0.357989	0.000000
3	6	0	1.483636	-0.864299	0.000000
4	6	0	0.726985	0.357989	0.000001
5	6	0	-0.706658	-2.015441	0.000000
6	1	0	-1.196811	-2.982701	-0.000001
7	6	0	0.706658	-2.015441	0.000000
8	1	0	1.196811	-2.982701	-0.000001
9	7	0	-1.251860	1.585985	0.000001
10	7	0	1.251860	1.585985	0.000000
11	6	0	2.938917	-0.893257	0.000000
12	6	0	3.742421	-2.015572	0.000001
13	6	0	5.144321	-1.784146	0.000001
14	1	0	3.333736	-3.020147	0.000003
15	6	0	5.502893	-0.465070	0.000000
16	1	0	5.866337	-2.594046	0.000002
17	1	0	6.507495	-0.065025	-0.000001
18	6	0	-2.938917	-0.893257	0.000000
19	6	0	-3.742421	-2.015572	0.000000
20	6	0	-5.144321	-1.784146	0.000000
21	1	0	-3.333736	-3.020147	0.000000
22	6	0	-5.502893	-0.465070	0.000000
23	1	0	-5.866337	-2.594046	0.000000
24	1	0	-6.507496	-0.065025	0.000000
25	16	0	0.000000	2.649883	0.000001
26	34	0	4.018227	0.659992	-0.000001
27	34	0	-4.018227	0.659992	0.000000

Sh_2-BT SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.446347	-0.895636
2	6	0	0.000000	0.708481	0.335376
3	6	0	0.000000	-1.446347	-0.895636
4	6	0	0.000000	-0.708481	0.335376
5	6	0	0.000000	0.690789	-2.100660
6	1	0	0.000000	1.208426	-3.052611
7	6	0	0.000000	-0.690789	-2.100660
8	1	0	0.000000	-1.208426	-3.052611
9	7	0	0.000000	1.285304	1.556782
10	7	0	0.000000	-1.285304	1.556782
11	6	0	0.000000	-2.874387	-0.910911
12	6	0	0.000000	-3.713858	-2.029676
13	6	0	0.000000	-5.093049	-1.761597
14	1	0	0.000000	-3.324281	-3.040986
15	6	0	0.000000	-5.412739	-0.417253
16	1	0	0.000000	-5.841224	-2.547170
17	1	0	0.000000	-6.414344	-0.007271
18	6	0	0.000000	2.874387	-0.910911
19	6	0	0.000000	3.713858	-2.029676
20	6	0	0.000000	5.093049	-1.761597
21	1	0	0.000000	3.324281	-3.040986
22	6	0	0.000000	5.412739	-0.417253
23	1	0	0.000000	5.841224	-2.547170
24	1	0	0.000000	6.414344	-0.007271
25	16	0	0.000000	0.000000	2.657499
26	34	0	0.000000	-3.918156	0.681550
27	34	0	0.000000	3.918156	0.681550

Sh_2-ST GS geometry (restricted)

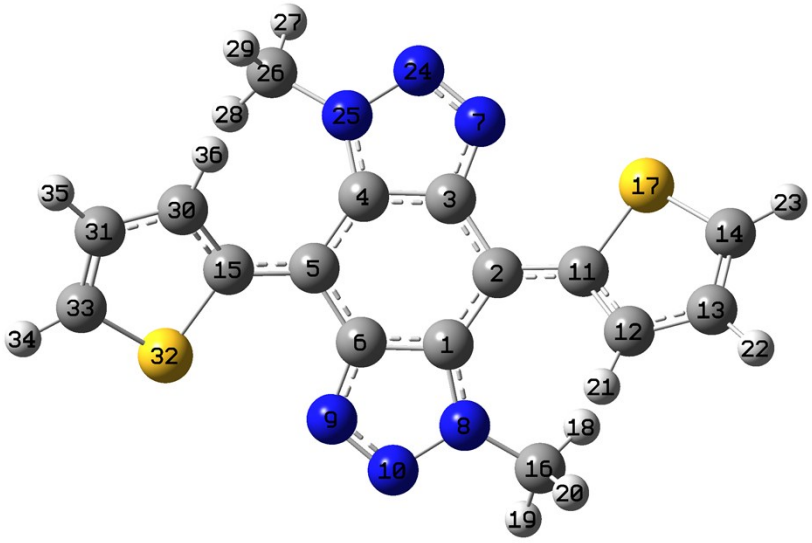
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.481673	-1.114411
2	6	0	0.000000	0.733531	0.120799
3	6	0	0.000000	-1.481673	-1.114411
4	6	0	0.000000	-0.733531	0.120799
5	6	0	0.000000	0.707494	-2.263536
6	1	0	0.000000	1.197955	-3.230684
7	6	0	0.000000	-0.707494	-2.263536
8	1	0	0.000000	-1.197955	-3.230684
9	7	0	0.000000	1.308631	1.314027
10	7	0	0.000000	-1.308631	1.314027
11	6	0	0.000000	-2.936759	-1.145191
12	6	0	0.000000	-3.739752	-2.268019
13	6	0	0.000000	-5.141919	-2.037836
14	1	0	0.000000	-3.330510	-3.272407
15	6	0	0.000000	-5.501334	-0.718994
16	1	0	0.000000	-5.862533	-2.849082
17	1	0	0.000000	-6.506881	-0.321039
18	6	0	0.000000	2.936759	-1.145191
19	6	0	0.000000	3.739752	-2.268019
20	6	0	0.000000	5.141919	-2.037836
21	1	0	0.000000	3.330510	-3.272407
22	6	0	0.000000	5.501334	-0.718994
23	1	0	0.000000	5.862533	-2.849082
24	1	0	0.000000	6.506881	-0.321039
25	34	0	0.000000	-4.016599	0.408015
26	34	0	0.000000	4.016599	0.408015
27	34	0	0.000000	0.000000	2.539156

Sh_2-ST SES geometry (restricted)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.441921	-1.142360
2	6	0	0.000000	0.711121	0.098527
3	6	0	0.000000	-1.441921	-1.142360
4	6	0	0.000000	-0.711121	0.098527
5	6	0	0.000000	0.690766	-2.347730
6	1	0	0.000000	1.209440	-3.298963
7	6	0	0.000000	-0.690766	-2.347730
8	1	0	0.000000	-1.209440	-3.298963
9	7	0	0.000000	1.341004	1.288832
10	7	0	0.000000	-1.341004	1.288832
11	6	0	0.000000	-2.869690	-1.160412
12	6	0	0.000000	-3.706706	-2.281381
13	6	0	0.000000	-5.086638	-2.017313
14	1	0	0.000000	-3.315276	-3.291905
15	6	0	0.000000	-5.409044	-0.673939
16	1	0	0.000000	-5.831793	-2.805817
17	1	0	0.000000	-6.412202	-0.267311
18	6	0	0.000000	2.869690	-1.160412
19	6	0	0.000000	3.706706	-2.281381
20	6	0	0.000000	5.086638	-2.017313
21	1	0	0.000000	3.315276	-3.291905
22	6	0	0.000000	5.409044	-0.673939
23	1	0	0.000000	5.831793	-2.805817
24	1	0	0.000000	6.412202	-0.267311
25	34	0	0.000000	-3.915507	0.429578
26	34	0	0.000000	3.915507	0.429578
27	34	0	0.000000	0.000000	2.540245

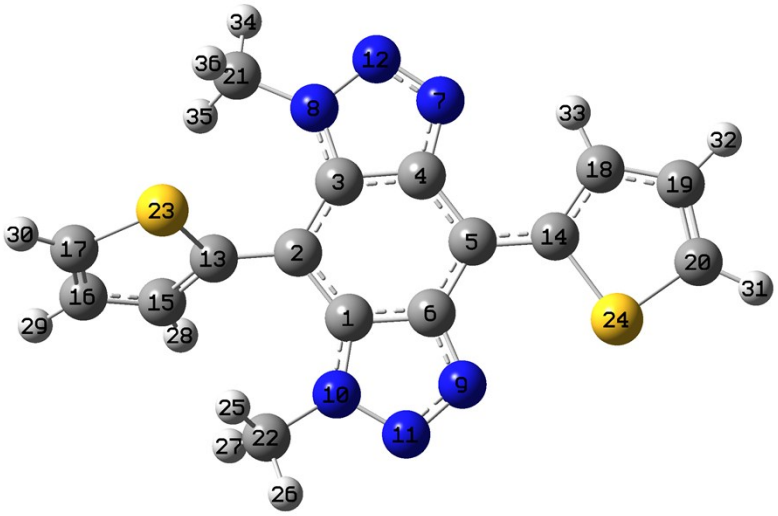
Th_2-BBTa15

Atom	No	PEC
C	1	0.00635
C	2	0.00951
C	3	-0.01736
C	4	0.00635
C	5	0.00951
C	6	-0.01736
N	7	-0.00524
N	8	0.01778
N	9	-0.00526
N	10	-0.06643
C	11	0.03199
C	12	0.01438
C	13	0.00181
C	14	0.02299
C	15	0.03199
C	16	-0.00406
S	17	-0.01427
H	18	0.00593
H	19	0.00278
H	20	-0.00036
H	21	-0.00598
H	22	0.00146
H	23	-0.00128
N	24	-0.06643
N	25	0.01778
C	26	-0.00406
H	27	0.00278
H	28	0.00593
H	29	-0.00036
C	30	0.01438
C	31	0.00182
S	32	-0.01427
C	33	0.02299
H	34	-0.00127
H	35	0.00146
H	36	-0.00597



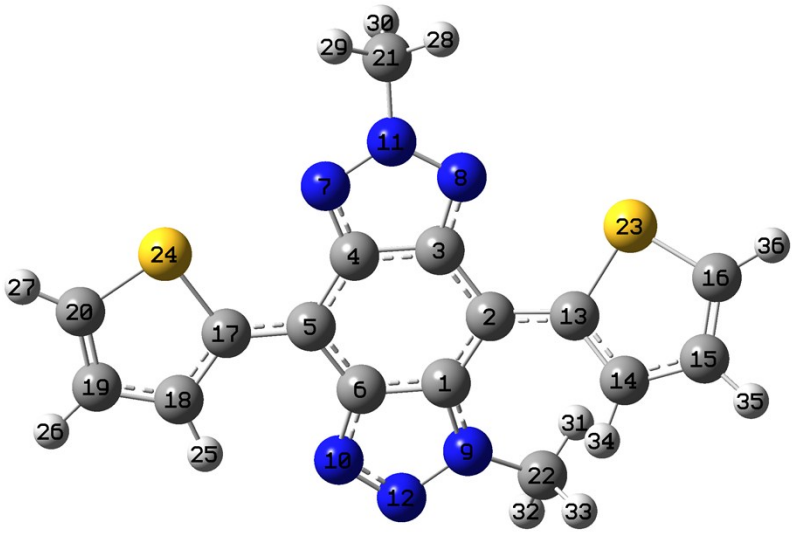
Th_2-BBTa17

Atom	No	PEC
C	1	-0.03003
C	2	0.08615
C	3	-0.03449
C	4	0.02919
C	5	-0.06416
C	6	0.02947
N	7	-0.0114
N	8	0.02218
N	9	-0.01102
N	10	0.02302
N	11	-0.05417
N	12	-0.05225
C	13	-0.00529
C	14	0.07464
C	15	0.00452
C	16	0.0018
C	17	0.01037
C	18	-0.0113
C	19	0.00694
C	20	0.02567
C	21	-0.00164
C	22	0.00234
S	23	0.00182
S	24	-0.05549
H	25	0.00472
H	26	0.00189
H	27	-0.0028
H	28	0.00096
H	29	0.00302
H	30	0.00274
H	31	-0.00431
H	32	0.00047
H	33	6E-05
H	34	0.00154
H	35	0.00283
H	36	0.00202



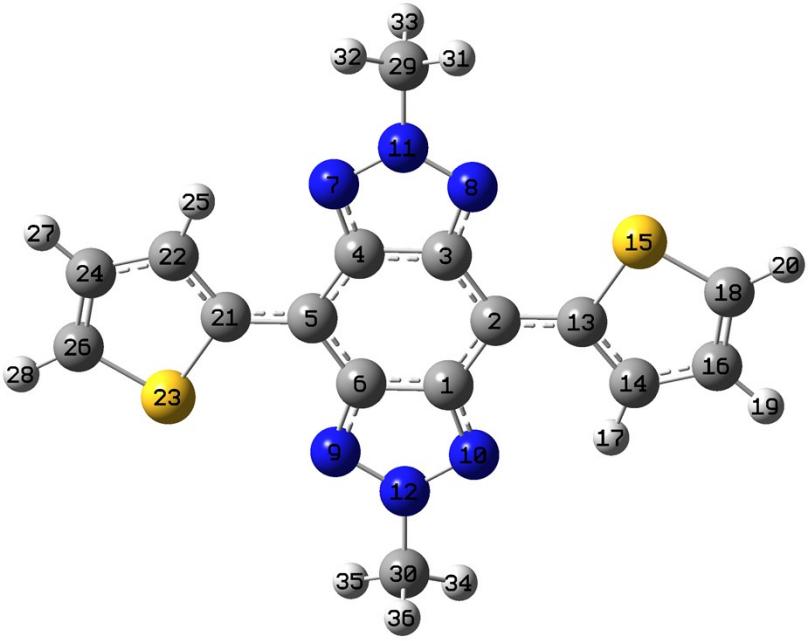
Th_2-BBTa16

Atom	No	PEC
C	1	-0.01122
C	2	0.05815
C	3	-0.01532
C	4	0.01308
C	5	-0.02228
C	6	0.00535
N	7	0.00323
N	8	0.00885
N	9	0.02061
N	10	-0.00039
N	11	-0.07241
N	12	-0.06633
C	13	0.0158
C	14	0.02506
C	15	0.00107
C	16	0.02685
C	17	0.03762
C	18	0.00022
C	19	0.001
C	20	0.01808
C	21	0.00056
C	22	-0.00382
S	23	0.00632
S	24	-0.03258
H	25	5E-05
H	26	0.00045
H	27	-0.00281
H	28	-0.00609
H	29	-0.00636
H	30	-0.0154
H	31	0.00619
H	32	0.00385
H	33	-0.00043
H	34	-0.00312
H	35	0.00412
H	36	0.00203



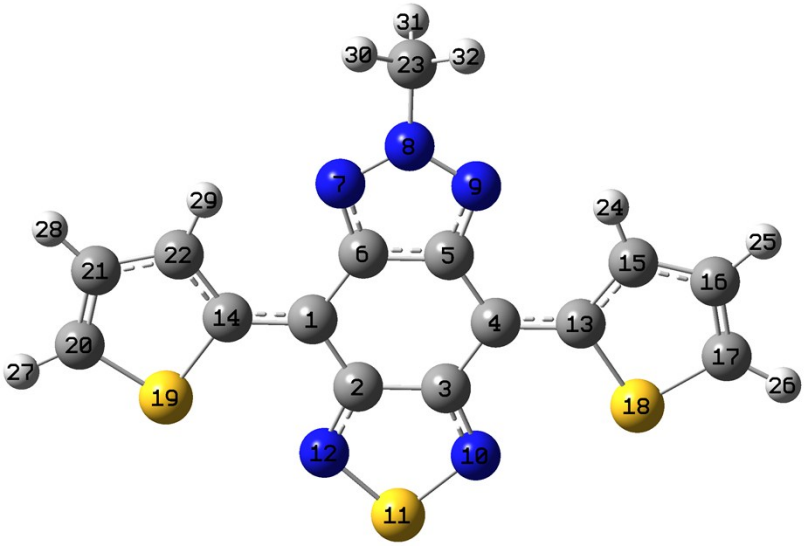
Th_2-BBTa26

Atom	No	PEC
C	1	-0.00042
C	2	0.03006
C	3	-0.00185
C	4	-0.00042
C	5	0.03006
C	6	-0.00185
N	7	0.01457
N	8	0.01339
N	9	0.01339
N	10	0.01457
N	11	-0.08693
N	12	-0.08693
C	13	0.02085
C	14	0.02302
S	15	-0.01761
C	16	-0.00048
H	17	0.00339
C	18	0.03026
H	19	0.00352
H	20	0.00049
C	21	0.02085
C	22	0.02302
S	23	-0.01761
C	24	-0.00048
H	25	0.00339
C	26	0.03026
H	27	0.00352
H	28	0.00049
C	29	0.00151
C	30	0.00151
H	31	-0.00768
H	32	-0.00767
H	33	-0.01842
H	34	-0.00767
H	35	-0.00768
H	36	-0.01842



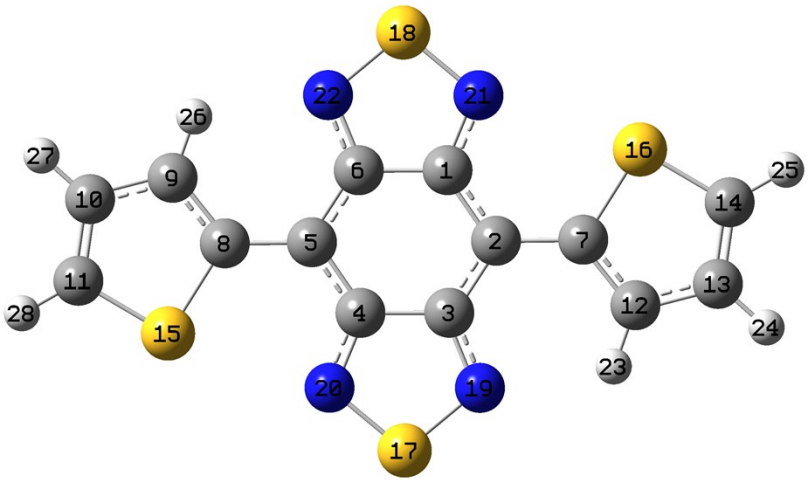
Th_2-SBTa

Atom	No	PEC
C	1	0.03512
C	2	-0.0002
C	3	-0.0002
C	4	0.03512
C	5	-0.0028
C	6	-0.0028
N	7	0.0093
N	8	-0.06831
N	9	0.0093
N	10	0.03417
S	11	-0.20098
N	12	0.03417
C	13	0.01305
C	14	0.01305
C	15	0.02636
C	16	-0.00344
C	17	0.03074
S	18	0.00136
S	19	0.00136
C	20	0.03074
C	21	-0.00344
C	22	0.02636
C	23	0.00063
H	24	-0.00031
H	25	0.00368
H	26	0.00059
H	27	0.00059
H	28	0.00368
H	29	-0.00031
H	30	-0.00637
H	31	-0.01383
H	32	-0.00637



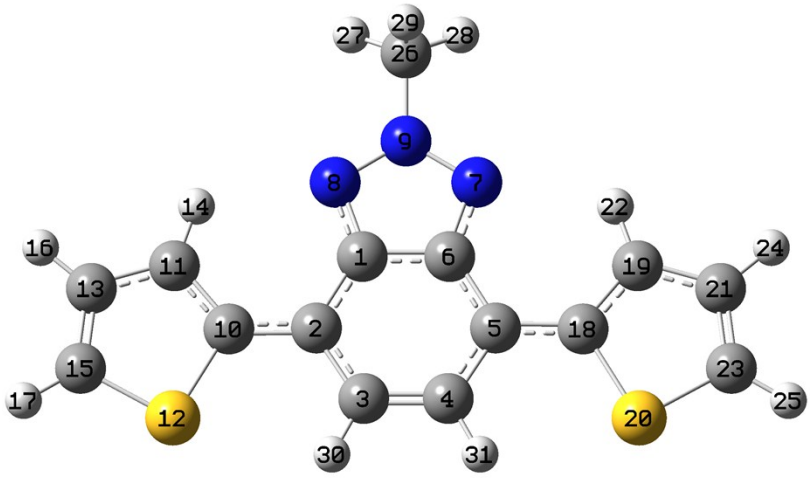
Th_2-BBT

Atom	No	PEC
C	1	0.00448
C	2	0.02291
C	3	0.00535
C	4	0.00448
C	5	0.02291
C	6	0.00535
C	7	0.01714
C	8	0.01714
C	9	0.02345
C	10	-0.0003
C	11	0.02262
C	12	0.02345
C	13	-0.0003
C	14	0.02262
S	15	0.00846
S	16	0.00846
S	17	-0.16721
S	18	-0.16721
N	19	0.02626
N	20	0.02531
N	21	0.02531
N	22	0.02626
H	23	0.00565
H	24	0.00392
H	25	0.00197
H	26	0.00565
H	27	0.00392
H	28	0.00197



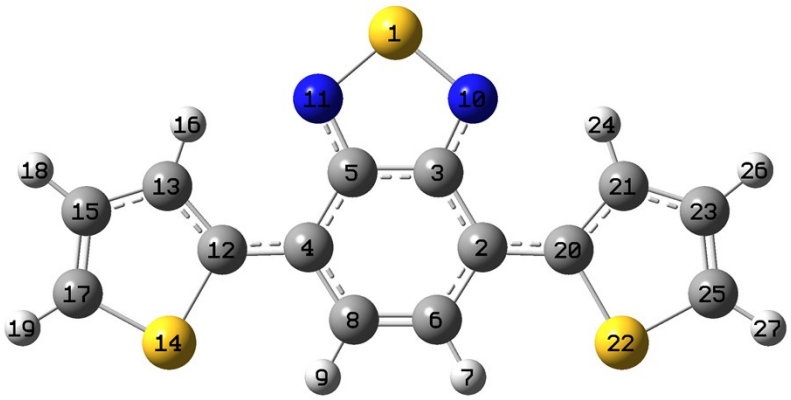
Th_2-BTa

Atom	No	PEC
C	1	0.0012
C	2	0.0069
C	3	0.00033
C	4	0.00033
C	5	0.0069
C	6	0.0012
N	7	-0.00446
N	8	-0.00446
N	9	-0.07139
C	10	0.03015
C	11	0.01082
S	12	-0.02719
C	13	0.00464
H	14	0.0037
C	15	0.02191
H	16	0.00272
H	17	-0.0003
C	18	0.03015
C	19	0.01082
S	20	-0.02719
C	21	0.00464
H	22	0.0037
C	23	0.02191
H	24	0.00272
H	25	-0.0003
C	26	0.00028
H	27	-0.00695
H	28	-0.00695
H	29	-0.01588
H	30	1E-05
H	31	1E-05



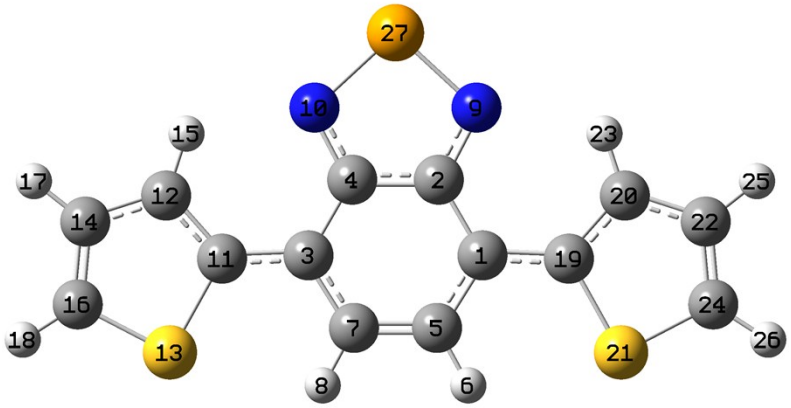
Th_2-BT

Atom	No	PEC
S	1	-0.20513
C	2	0.02582
C	3	-0.02252
C	4	0.02582
C	5	-0.02252
C	6	-0.00585
H	7	-0.00168
C	8	-0.00585
H	9	-0.00168
N	10	0.00723
N	11	0.00724
C	12	0.03011
C	13	0.02335
S	14	-0.00391
C	15	0.00535
H	16	0.00945
C	17	0.02758
H	18	0.00499
H	19	0.00265
C	20	0.03011
C	21	0.02335
S	22	-0.00391
C	23	0.00535
H	24	0.00945
C	25	0.02757
H	26	0.00499
H	27	0.00265



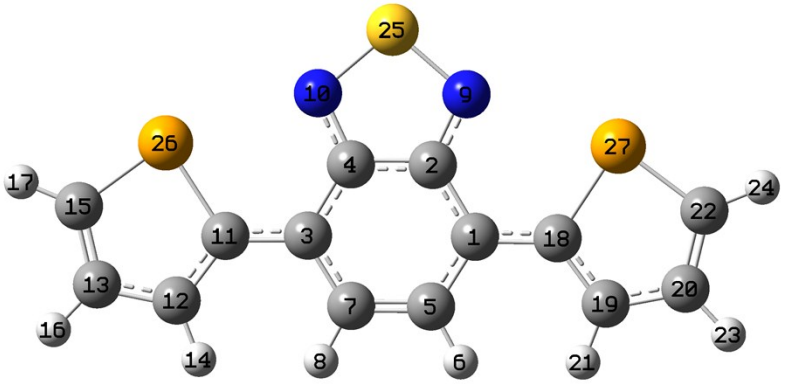
Th_2-ST

Atom	No	PEC
C	1	0.03538
C	2	-0.03347
C	3	0.03538
C	4	-0.03347
C	5	-0.00521
H	6	-0.00158
C	7	-0.00521
H	8	-0.00158
N	9	-0.00088
N	10	-0.00088
C	11	0.02614
C	12	0.02712
S	13	-9E-05
C	14	0.00505
H	15	0.01017
C	16	0.02799
H	17	0.00542
H	18	0.00324
C	19	0.02614
C	20	0.02712
S	21	-9E-05
C	22	0.00505
H	23	0.01017
C	24	0.02799
H	25	0.00542
H	26	0.00324
Se	27	-0.19855



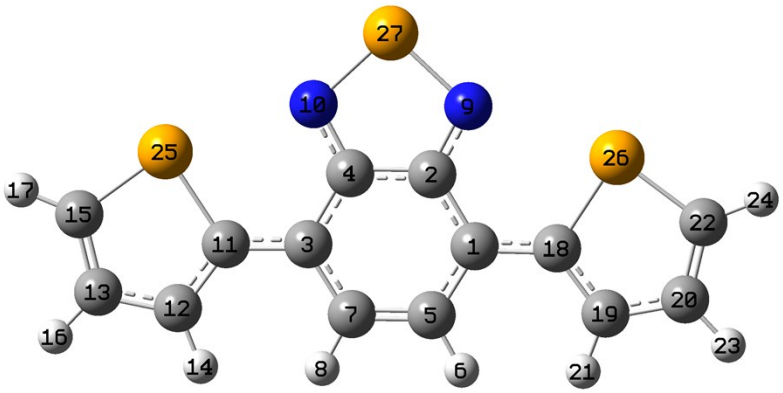
Sh_2-BT

Atom	No	PEC
C	1	0.02513
C	2	-0.02126
C	3	0.02513
C	4	-0.02126
C	5	-0.00981
H	6	-0.00204
C	7	-0.00981
H	8	-0.00204
N	9	0.00377
N	10	0.00377
C	11	0.03379
C	12	0.02506
C	13	-0.00063
H	14	0.00398
C	15	0.03133
H	16	0.00395
H	17	0.00024
C	18	0.03379
C	19	0.02506
C	20	-0.00063
H	21	0.00398
C	22	0.03133
H	23	0.00395
H	24	0.00024
S	25	-0.21402
Se	26	0.01353
Se	27	0.01353



Sh_2-ST

Atom	No	PEC
C	1	0.03596
C	2	-0.03322
C	3	0.03596
C	4	-0.03322
C	5	-0.0096
H	6	-0.00209
C	7	-0.0096
H	8	-0.00209
N	9	-0.00512
N	10	-0.00512
C	11	0.03003
C	12	0.03067
C	13	-0.0023
H	14	0.00441
C	15	0.0353
H	16	0.00439
H	17	0.00056
C	18	0.03003
C	19	0.03067
C	20	-0.0023
H	21	0.00441
C	22	0.0353
H	23	0.00439
H	24	0.00056
Se	25	0.01944
Se	26	0.01944
Se	27	-0.21689



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