

SUPPORTING INFORMATION

Tetrasubstituted Thieno[3,2-*b*]thiophenes as Hole Transporting Materials for Perovskite Solar Cells

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1. Computational Details

Quantum-chemical calculations were carried out with the Gaussian 16 (revision A.03) software package.¹ All the calculations were performed within the density functional theory (DFT) framework using the B3LYP functional² and the 6-31G** basis set.³ Solvent effects were considered within the self-consistent reaction field (SCRF) theory by using the polarized continuum model (PCM) approach.⁴ C_2 -symmetry constraints were imposed during the optimization of the **TbT-1**, **TbT-2**, and **TbT-3** HTMs, whereas C_{2h} constraints were used to calculate the isolated TbT core. The TbT core extended with the four bridging thiophene rings (exTbT) present in **TbT-2** and **TbT-3**, the DPA and TPA substituent groups, and the spiro-OMeTAD reference molecule were also optimized under C_2 symmetry. Vertical electronic transition energies to the lowest-energy singlet excited states of **TbT-1**, **TbT-2**, and **TbT-3** were computed by using the time-dependent DFT (TDDFT) approach.⁵ The lowest 120 singlet excited states were calculated at the B3LYP/6-31G** level using the ground-state optimized geometries. Geometry optimizations in gas phase of the radical cations of **TbT-1**, **TbT-2**, and **TbT-3**, their cores, their DPA and TPA terminal groups, and spiro-OMeTAD were also performed to evaluate the reorganization energy (λ). The procedure used to evaluate λ is explained below. To investigate the oxidation processes, the ionization energies upon to the tetracation species were estimated in solution. Radical cations were treated as open-shell systems and computed within the spin-unrestricted DFT approximation at the UB3LYP/6-31G** level in the presence of CH₂Cl₂. Additionally, dication, trication and tetracation species were also computed in CH₂Cl₂. Molecular orbitals were plotted using the Chemcraft 1.6 software with isovalue contours of ± 0.03 a.u.⁶

Figure S1 shows the B3LYP/6-31G**-optimized values calculated for selected bond lengths of the TbT and exTbT cores and the **TbT-1**, **TbT-2**, and **TbT-3** HTMs. Figure S2 displays the optimized structures of the four-armed HTMs. Table S1 gathers the vertical excitation energies (E), the oscillator strengths (f), and the electronic descriptions in terms of one-electron molecular orbital excitations calculated for the most relevant S₀ → S_n electronic transitions of **TbT-1**, **TbT-2**, and **TbT-3** in CH₂Cl₂. Figure S3-S5 depict the topology and energy of the frontier molecular orbitals participating in the S₀ → S_n transitions quoted in Table S1.

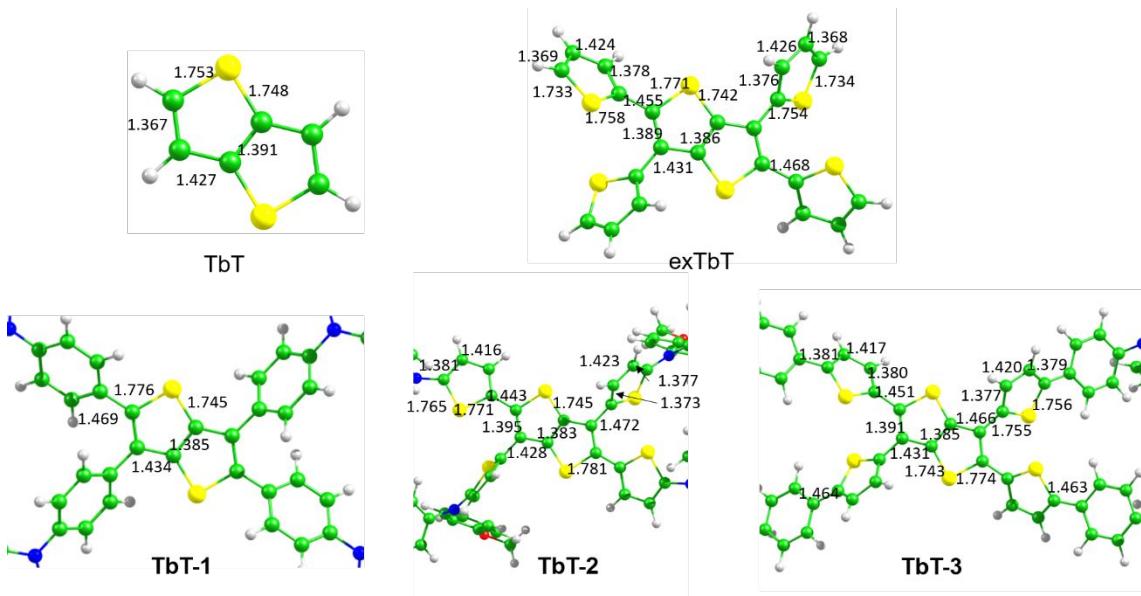


Figure S1. Optimized bond lengths (in Å) calculated at the B3LYP/6-31G** level, in CH₂Cl₂ solution, for the TbT and exTbT cores and for the TbT-1, TbT-2, and TbT-3 compounds. For the latter, the terminal DPA and TPA groups have been partially omitted and only the bond lengths calculated for the cores are shown.

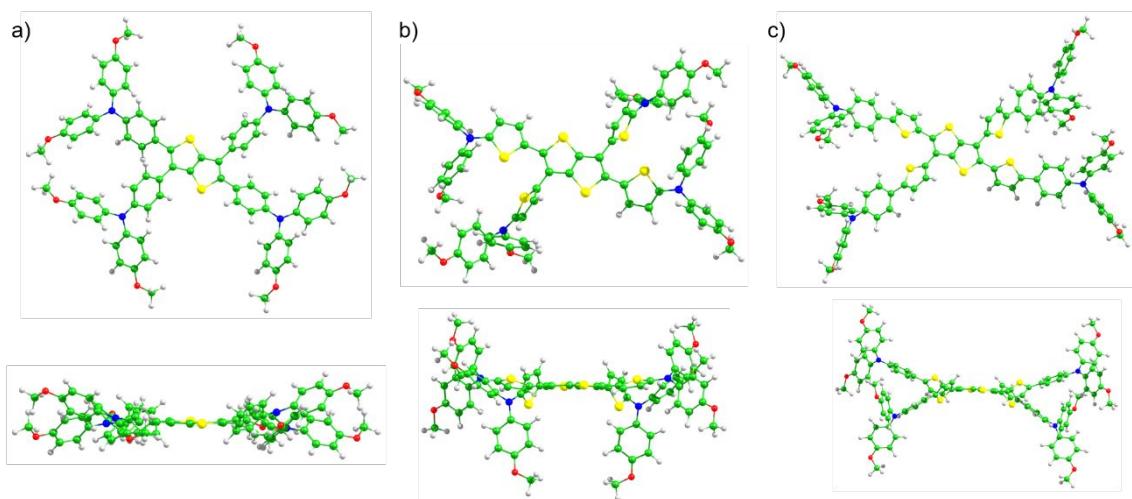


Figure S2. Top and side views of the minimum-energy optimized geometries calculated at the B3LYP/6-31G** level in CH₂Cl₂ for TbT-1 (a), TbT-2 (b), and TbT-3 (c).

Table S1. Lowest singlet excited states calculated at the TDDFT B3LYP/6-31G** level for **TbT-1**, **TbT-2**, and **TbT-3** in CH₂Cl₂ solution. Vertical excitation energies (*E*), oscillator strengths (*f*) and dominant monoexcitations with contributions (within parentheses) greater than 10%.

Compound	State	<i>E</i> (eV/nm)	<i>f</i>	Description ^a
TbT-1	S ₁	2.70 / 458	1.273	H → L (97)
	S ₃	3.04 / 407	0.460	H-1 → L (97)
	S ₈	3.52 / 352	0.651	H-2 → L (87)
	S ₁₄	3.77 / 329	0.559	H-4 → L (26) H-3 → L+1 (46) H → L+6 (15)
	S ₂₅	4.01 / 309	0.406	H → L+10 (56)
	S ₃₀	4.05 / 306	0.470	H-2 → L+9 (24) H-1 → L+8 (15) H → L+12 (33) H → L+14 (16)
	S ₃₇	4.12 / 301	0.256	H-5 → L (52) H-2 → L+6 (20)
	S ₁	2.31 / 634	1.511	H → L (98)
	S ₃	2.65 / 467	0.166	H-2 → L (98)
TbT-2	S ₆	3.25 / 382	0.272	H-1 → L+1 (18) H → L+2 (76)
	S ₇	3.34 / 372	0.138	H-1 → L+1 (71) H → L+2 (19)
	S ₁₂	3.60 / 344	0.197	H-3 → L+2 (79)
	S ₁₅	3.66 / 338	0.121	H-4 → L (31) H → L+6 (50)
	S ₁₈	3.71 / 334	0.186	H → L+9 (81)
	S ₂₈	3.92 / 316	0.139	H-1 → L+12 (10) H → L+13 (67)
	S ₃₅	4.05 / 306	0.124	H → L+15 (44) H → L+17 (10)
	S ₃₈	4.06 / 305	0.255	H-2 → L+13 (26) H-1 → L+12 (21) H → L+13 (14)
	S ₁	2.32 / 535	1.268	H → L (95)
	S ₃	2.51 / 494	0.572	H-2 → L (96)
TbT-3	S ₆	2.93 / 422	0.791	H-1 → L+1 (87)
	S ₈	3.06 / 405	0.766	H-4 → L (45) H-3 → L+1 (44)
	S ₁₀	3.15 / 393	0.582	H-4 → L (17) H → L+2 (69)
	S ₄₉	4.07 / 304	0.379	H-2 → L+13 (21) H-1 → L+14 (29) H → L+13 (17)
	S ₅₀	4.07 / 304	0.460	H-2 → L+14 (16) H-1 → L+13 (29) H → L+14 (20)

^a H and L denotes HOMO and LUMO, respectively.

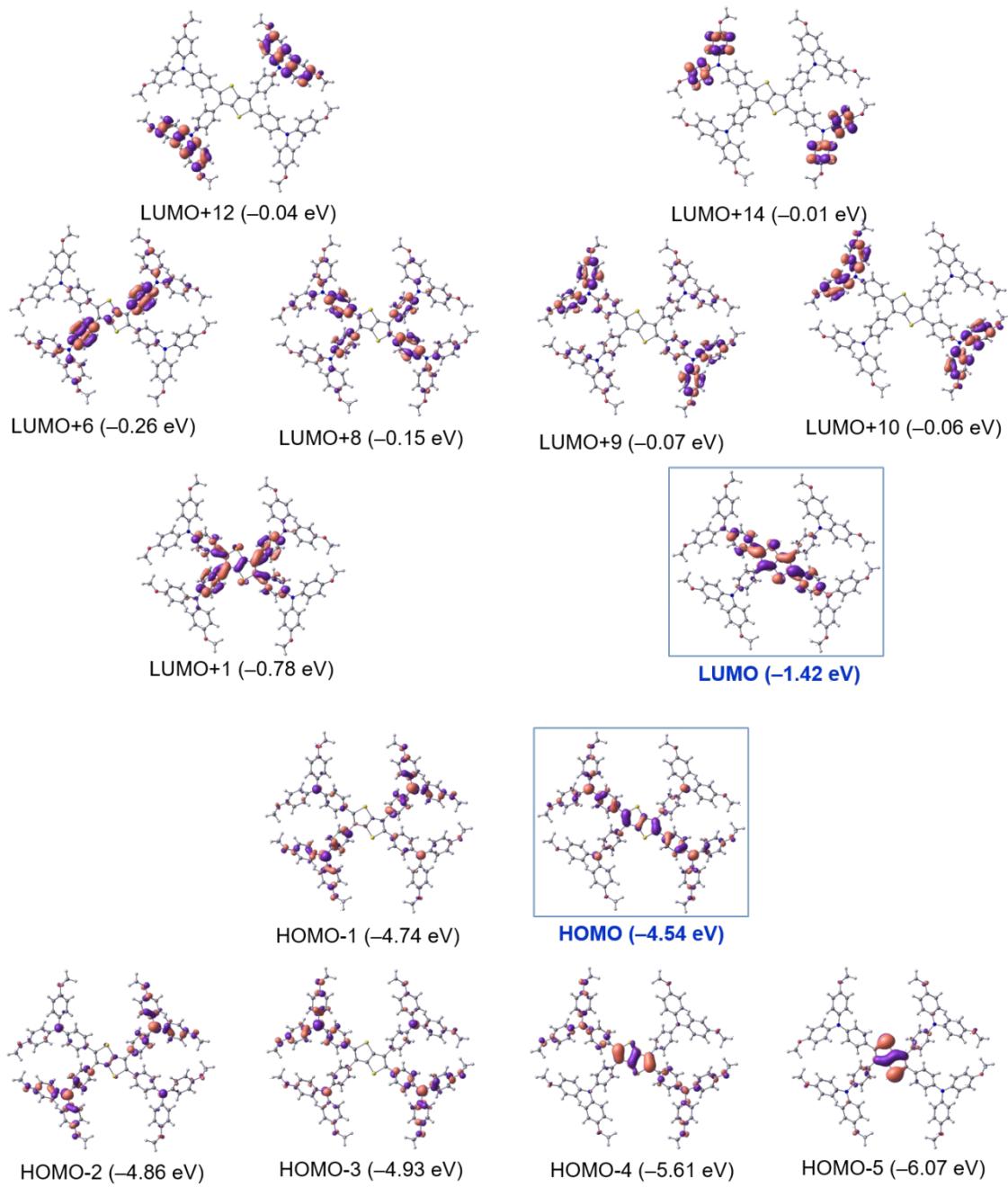


Figure S3. Isovalue contours (± 0.03 a.u.) and energies calculated at the B3LYP/6-31G** level in CH_2Cl_2 for selected molecular orbitals of **TbT-1**.

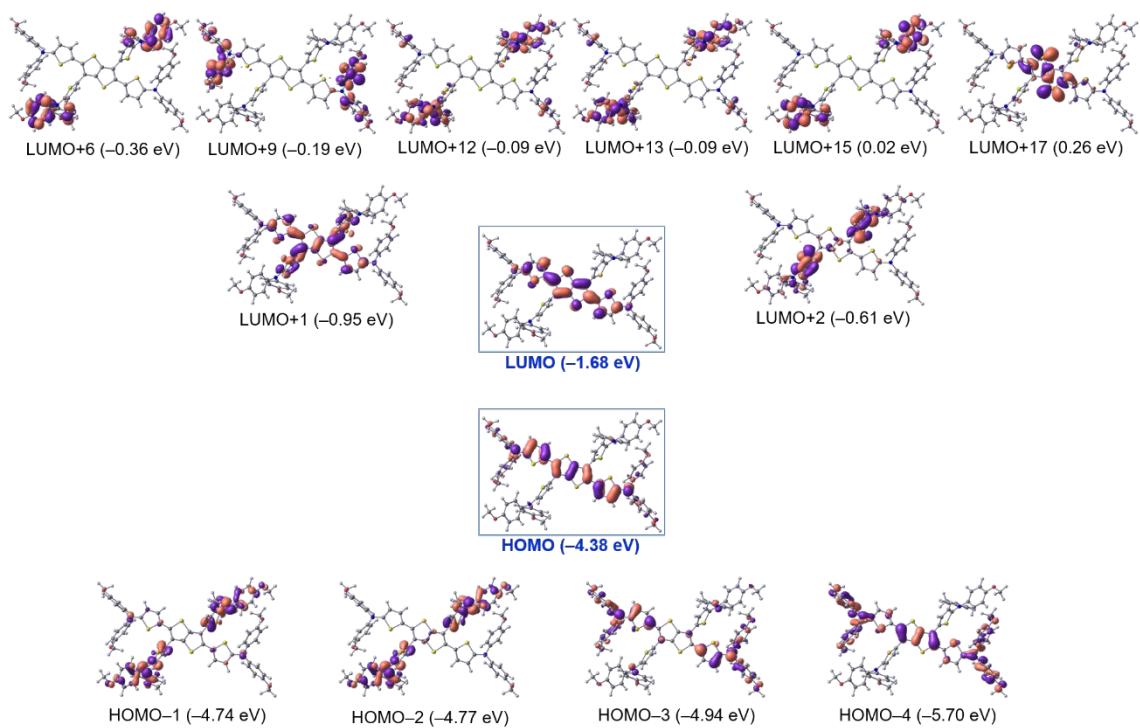


Figure S4. Isovalue contours (± 0.03 a.u.) and energies calculated at the B3LYP/6-31G** level in CH_2Cl_2 for selected molecular orbitals of **TbT-2**.

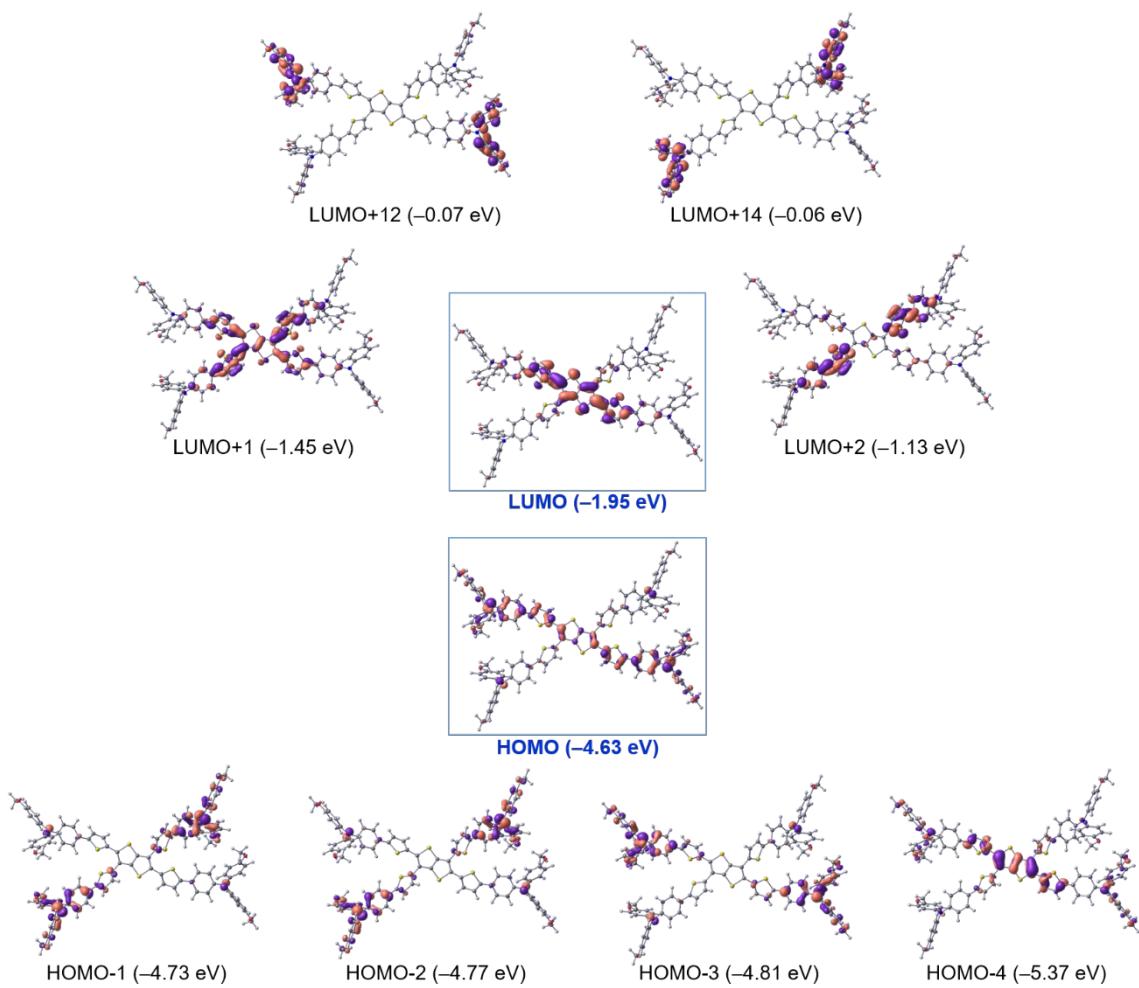


Figure S5. Isovalue contours (± 0.03 a.u.) and energies calculated at the B3LYP/6-31G** level in CH_2Cl_2 for selected molecular orbitals of **TbT-3**.

Oxidized species. B3LYP/6-31G** calculations in CH₂Cl₂ were used to investigate the molecular structure and charge distribution of the four-armed HTMs in different oxidation states, from the monocation to the tetracation. Cation species were computed as doublet open-shell species. Dications of **TbT-1**, **TbT-2**, and **TbT-3** were calculated as singlet closed-shell species, in which both electrons are extracted from the same orbital, and triplet open-shell species, in which the electrons are extracted from different orbitals. The triplet and the singlet states were found to be close in energy, being the triplet the most stable state (less than 0.090 eV) for [TbT-1]²⁺ and [TbT-3]²⁺, whereas for [TbT-2]²⁺ the singlet state is more stable by 0.087 eV. In the case of trications, doublet and quadruplet open-shell states were computed. For [TbT-1]³⁺ and [TbT-3]³⁺, the quadruplet states turned out to be the most stable states by approximately 0.2 eV, whereas for [TbT-2]³⁺ the doublet state was found to be slightly more stable by 0.072 eV. For [TbT-1]⁴⁺, the quintet state is predicted to be the most stable state followed by the triplet and singlet (0.309 and 0.551 eV). For [TbT-3]⁴⁺, the quintet state is also calculated to be the most stable state followed by the singlet by 0.597 eV. The triplet state for [TbT-3]⁴⁺ did not converge. Conversely, the triplet state was the most stable state for [TbT-2]⁴⁺ followed by the singlet (0.048 eV) and the quintet (0.181 eV). Table S1 gathers the Mulliken atomic charges computed for the cores and the DPA and TPA groups of the different oxidized species of **TbT-1**, **TbT-2**, and **TbT-3** in their most stable electronic states.

Table S2. Mulliken atomic charges (in e) computed for the central TbT cores and the terminal DPA and TPA groups of **TbT-1**, **TbT-2**, and **TbT-3** in different oxidized states.

Compound	Neutral	Cation	Dication	Trication	Tetracation
TbT-1					
TbT	-0.305	-0.142	-0.120	-0.078	-0.081
TPA-1	0.047	0.168	0.533	0.808	1.003
TPA-2	0.105	0.403	0.528	0.731	1.038
TPA-3	0.047	0.168	0.533	0.808	1.003
TPA-4	0.105	0.403	0.528	0.731	1.038
TbT-2					
exTbT	0.342	0.930	1.436	1.694	2.042
DPA1	-0.121	-0.083	0.061	0.384	0.613
DPA2	-0.050	0.118	0.220	0.267	0.366
DPA3	-0.121	-0.083	0.061	0.387	0.613
DPA4	-0.050	0.119	0.220	0.267	0.366
TbT-3					
exTbT	-0.493	-0.104	0.033	0.052	0.089
TPA-1	0.119	0.151	0.530	0.956	0.991
TPA-2	0.128	0.401	0.455	0.519	0.965
TPA-3	0.119	0.151	0.528	0.956	0.991
TPA-4	0.128	0.401	0.454	0.519	0.965

Figure S6 represents the potential energy surfaces for the neutral and cation states of two molecules (labelled as 1 and 2) involved in an intermolecular charge transfer process. The intramolecular reorganization energy (λ) consists of two terms related to the geometry relaxation energies of one molecule going from the fully relaxed ground state of the neutral species to the cation state (Figure S6, left) and a neighbouring molecule evolving in the opposite way (Figure S6, right),

$$\lambda = \lambda_1 + \lambda_2 \quad (1)$$

$$\lambda_1 = E(M1) - E(M1^+) \quad (2)$$

$$\lambda_2 = E(M2^+) - E(M2) \quad (3)$$

Here, $E(M1)$ and $E(M1^+)$ for molecule 1 are the energies of the positively charged molecule (the cation) at the equilibrium geometry of the neutral molecule and the relaxed cation, respectively, and $E(M2^+)$ and $E(M2)$ for molecule 2 are, accordingly, the energies of the neutral molecule at the equilibrium geometry of the cation and the neutral molecule, respectively.

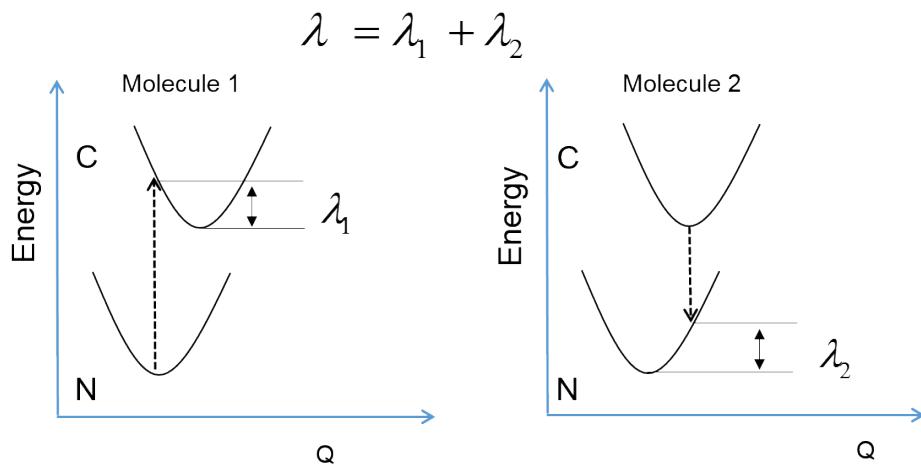


Figure S6. Scheme of the potential energy surfaces of the neutral state (N) and the cation state (C) for two molecules (1 and 2) involved in a charge (hole) transfer process. λ_1 and λ_2 are the two contributions to the total intramolecular reorganization energy (λ).

2. Differential scan calorimetry (DSC)

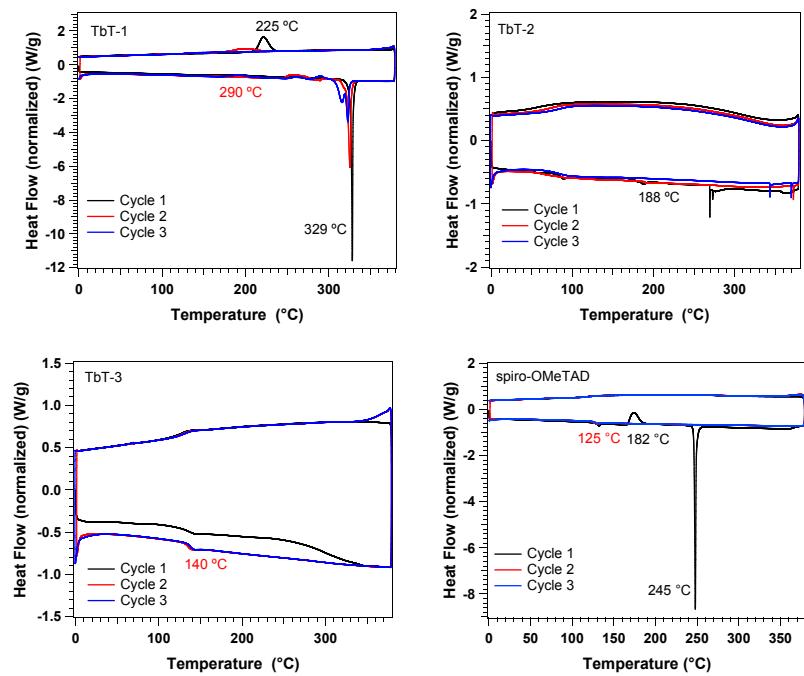


Figure S7. DSC of TbT-1, TbT-2, TbT-3 and spiro-OMeTAD at a scan rate of 20 °C min⁻¹.

3. Device characterization

3.1. External quantum efficiency

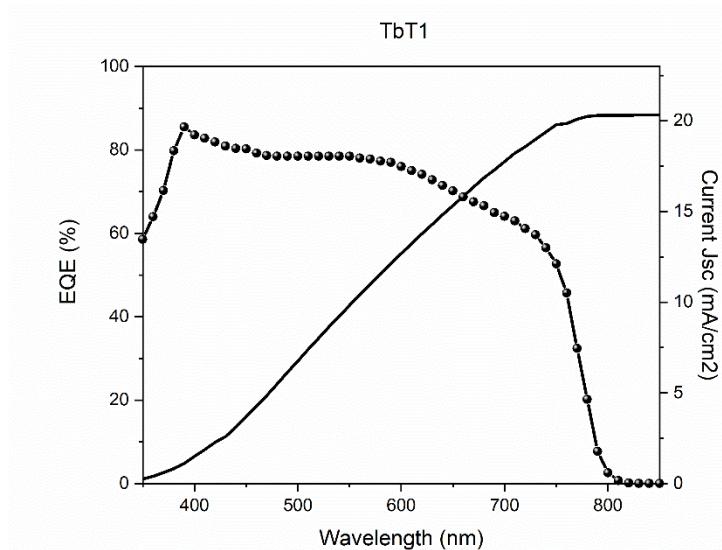


Figure S8. External quantum efficiency (EQE) plots of **TbT-1** with corresponding integrated current.

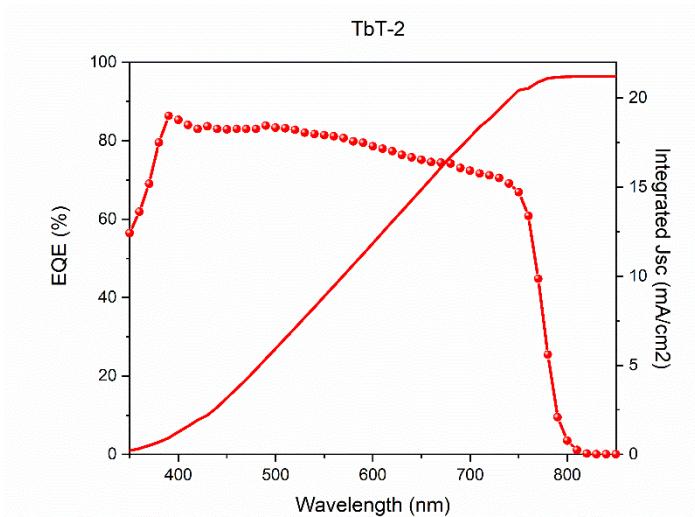


Figure S9. External quantum efficiency (EQE) plots of **TbT-2** with corresponding integrated current.

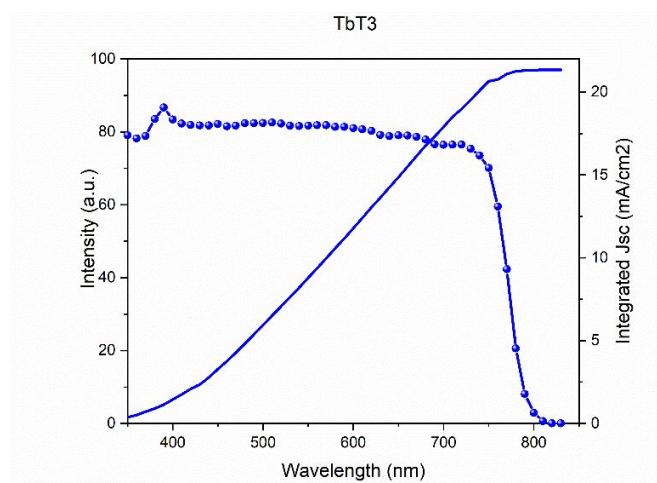


Figure S10. External quantum efficiency (EQE) plots of **TbT-3** with corresponding integrated current.

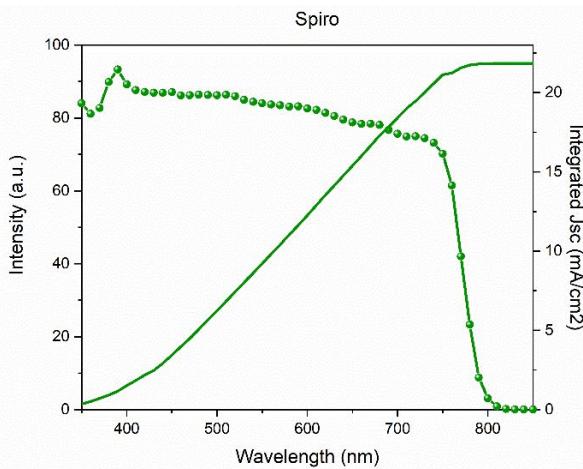


Figure S11. External quantum efficiency (EQE) plots of spiro-OMeTAD with corresponding integrated current.

3.2. Hysteresis curves

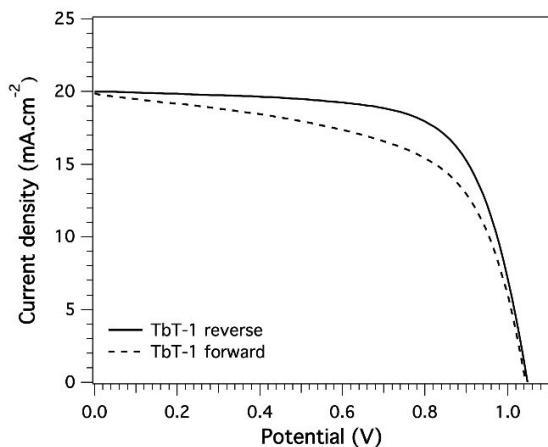


Figure S12. Hysteresis curve of a device with **TbT-1** on $(\text{FAPbI}_3)_{0.85}(\text{MAPbBr}_3)_{0.15}$ perovskite measured at 10 mVs^{-1} .

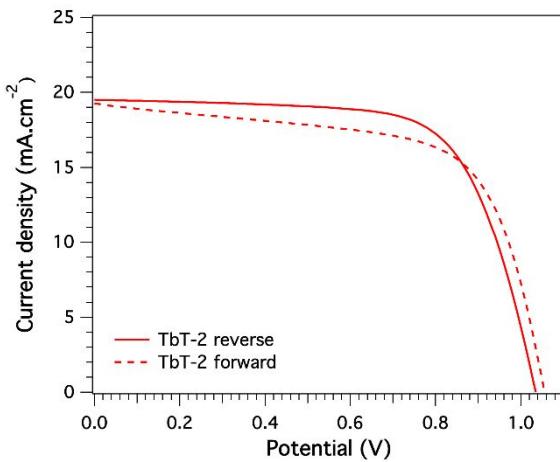


Figure S13. Hysteresis curve of a device with **TbT-2** on $(\text{FAPbI}_3)_{0.85}(\text{MAPbBr}_3)_{0.15}$ perovskite measured at 10 mVs^{-1} .

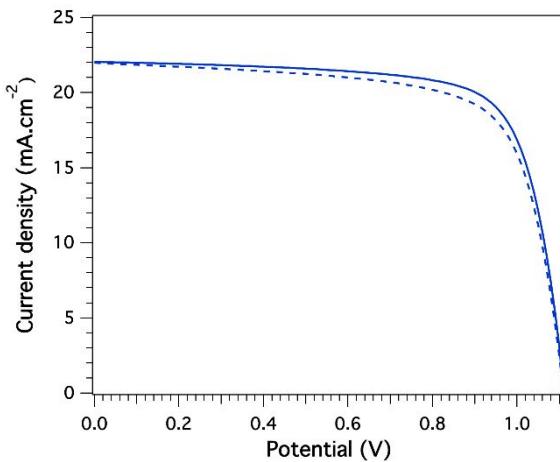


Figure S14. Hysteresis curve of a device with **TbT-3** on $(\text{FAPbI}_3)_{0.85}(\text{MAPbBr}_3)_{0.15}$ perovskite measured at $10 \text{ mV}\cdot\text{s}^{-1}$.

Table S3. Reverse and forward scan photovoltaic parameters measured for TbT-based HTMs

HTM	Scan	V _{oc} (V)	J _{sc} (mA/cm ²)	FF (%)	PCE (%)
TbT-1	Reverse	1.05	19.99	69.0	14.45
	Forward	1.04	19.88	59.6	12.36
TbT-2	Reverse	1.03	19.50	68.4	13.79
	Forward	1.05	19.28	65.0	13.22
TbT-3	Reverse	1.11	22.05	71.9	18.15
	Forward	1.10	21.99	71.8	17.36

3.3. Device Statistics

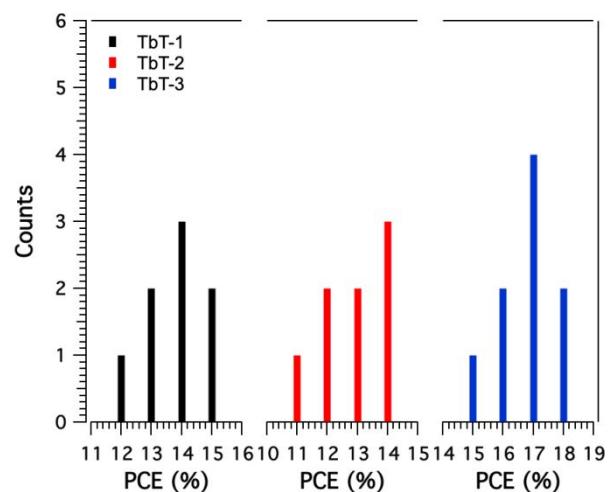


Figure S15. Devices efficiency statistics for TbT-based HTMs.

4. UV-vis spectra of oxidized TbT-based HTMs

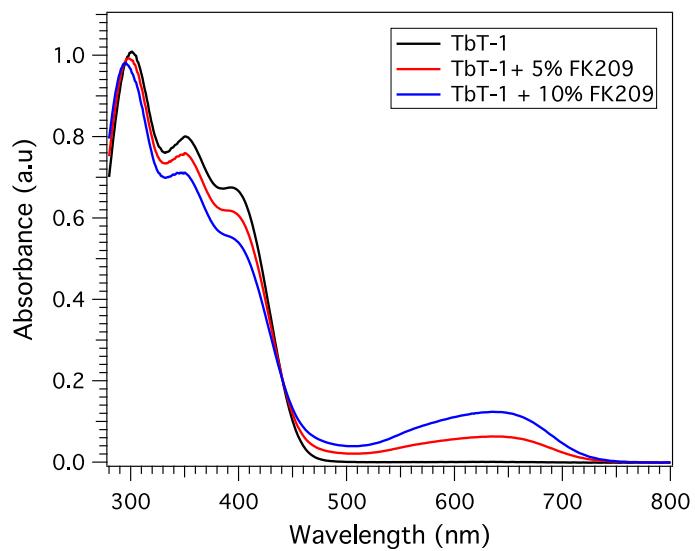


Figure S16. UV-vis absorption of **TbT-1** upon stepwise addition of FK-209.

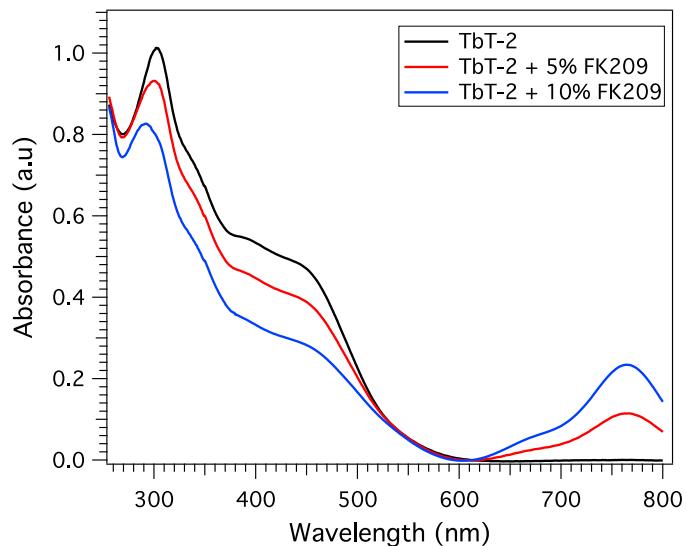


Figure S17. UV-vis absorption of **TbT-2** upon stepwise addition of FK-209.

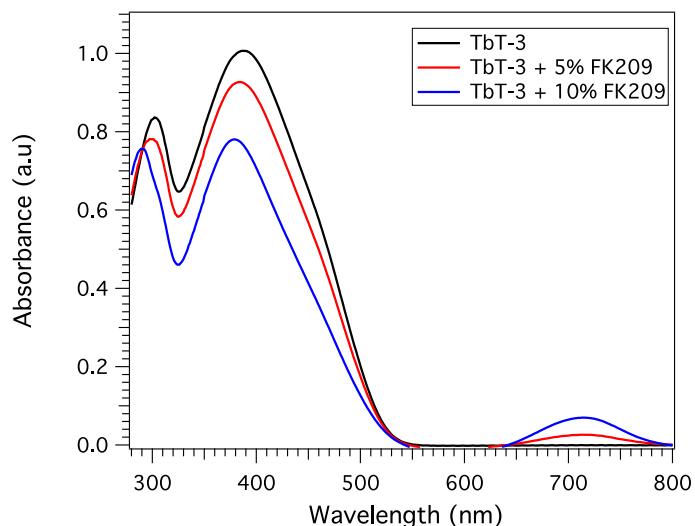


Figure S18. UV-vis absorption of **TbT-3** upon stepwise addition of FK-209.

5. Supplementary figures

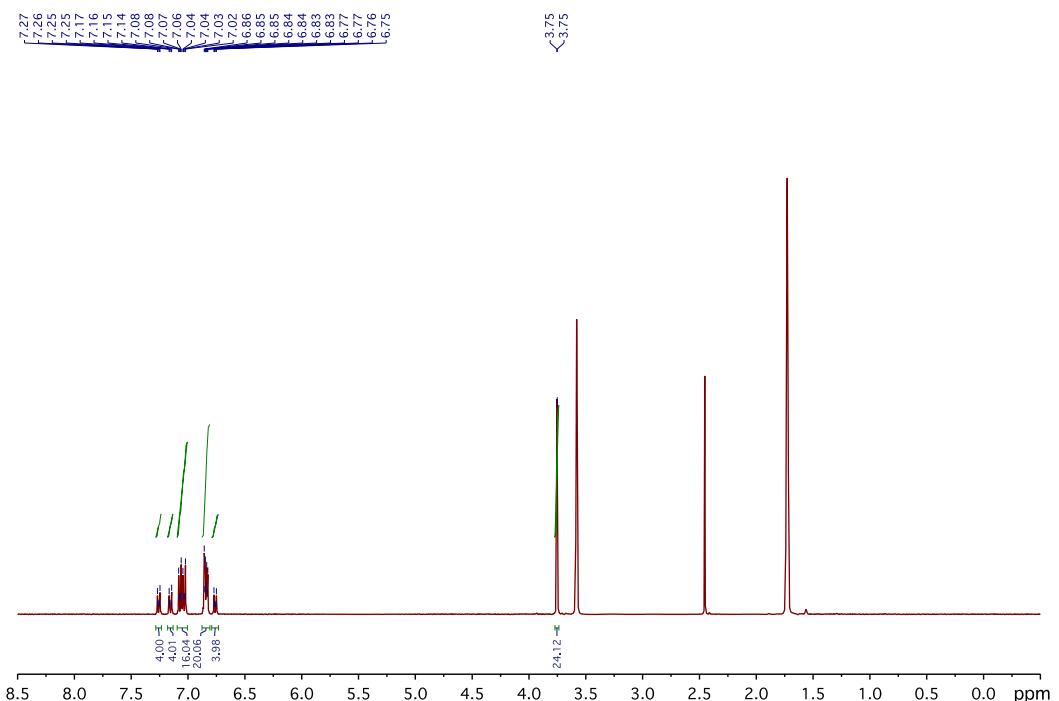


Figure S19. ¹H NMR (400 MHz, THF-*d*₈, 298 K) of **TbT-1**.

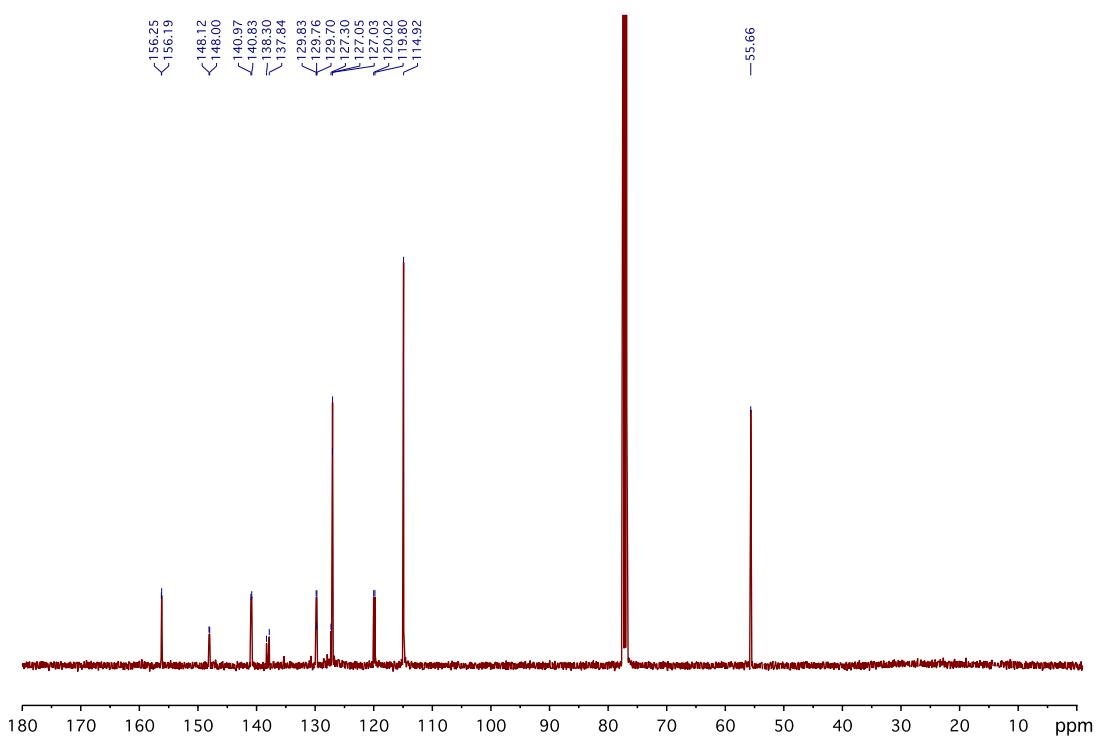


Figure S20. ¹³C NMR (100 MHz, CDCl₃, 298 K) of **TbT-1**.

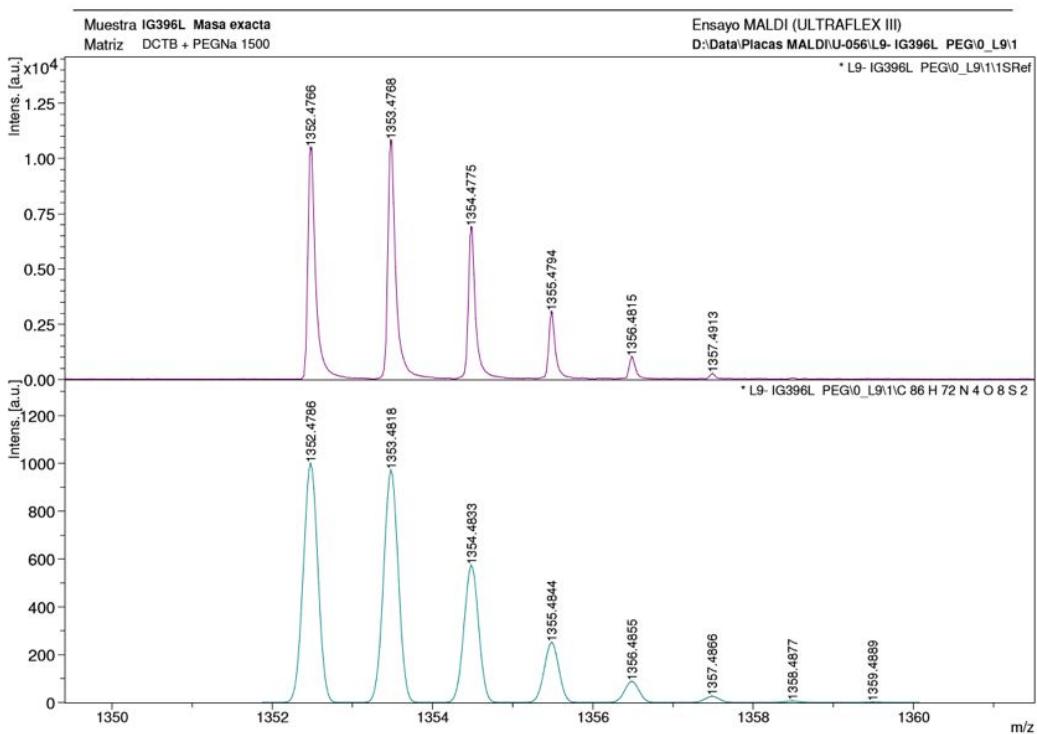
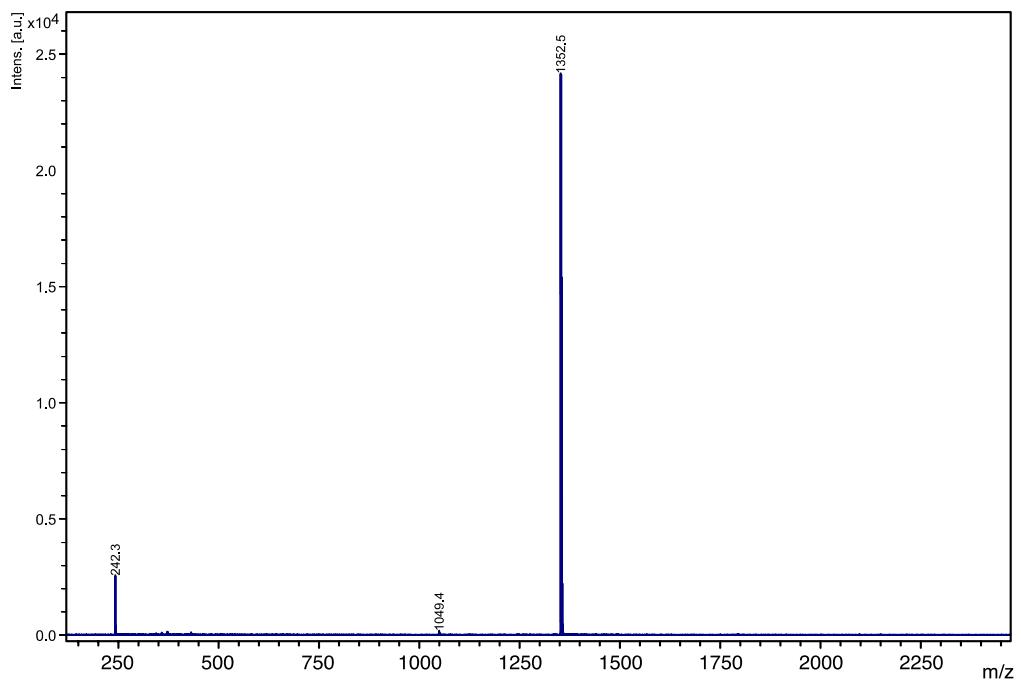


Figure S21. HR-MALDI-TOF mass spectrum of TbT-1.

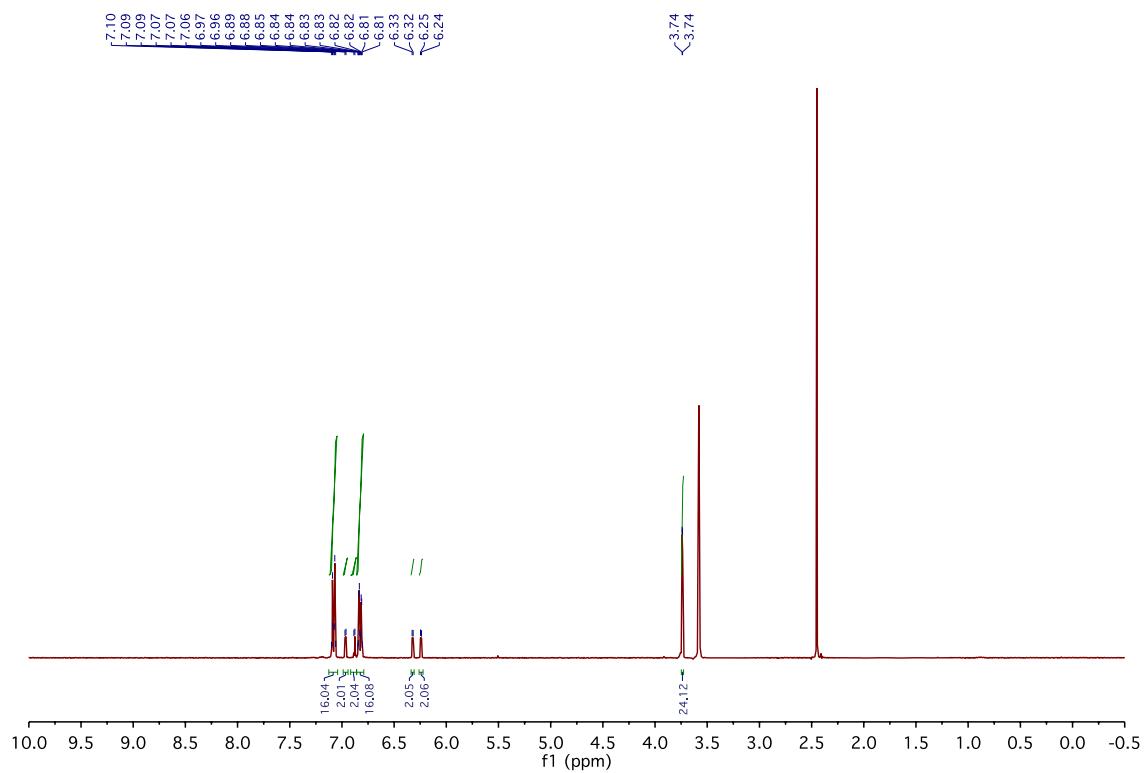


Figure S22. ^1H NMR (400 MHz, THF- d_8 , 298 K) of TbT-2.

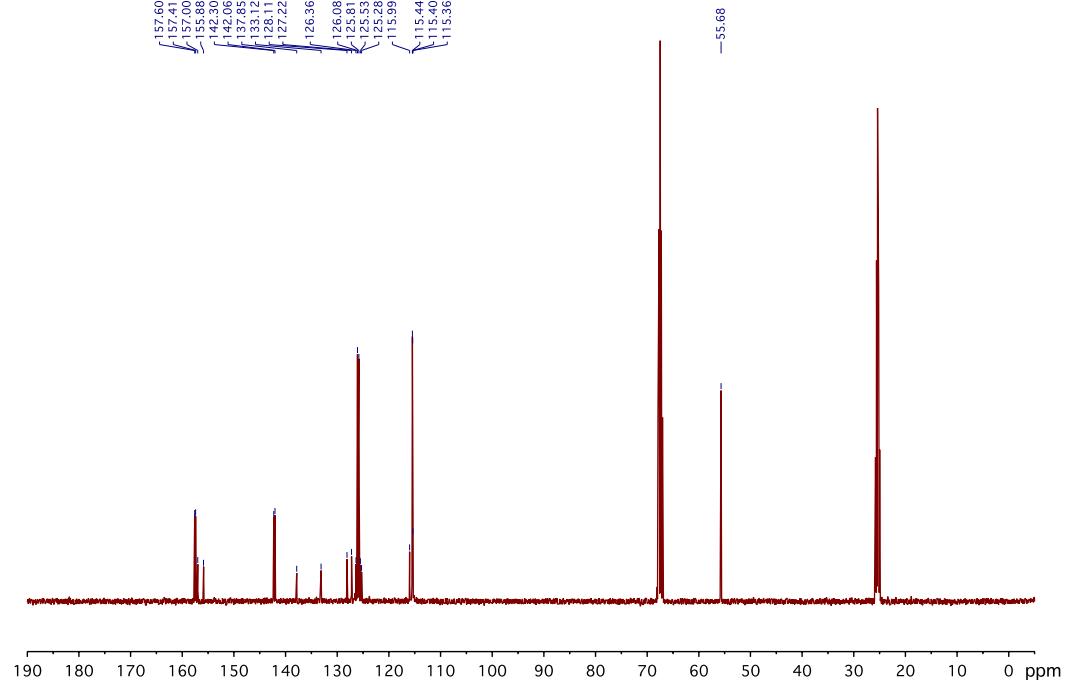


Figure S23. ^{13}C NMR (100 MHz, THF- d_8 , 298 K) of TbT-2.

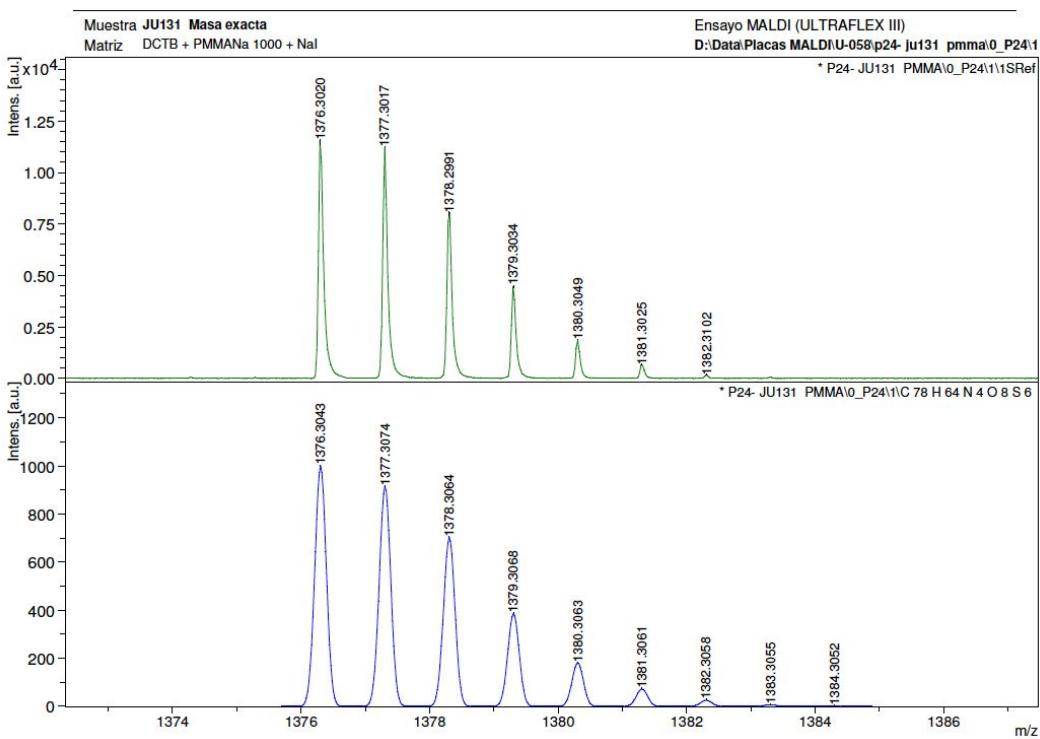
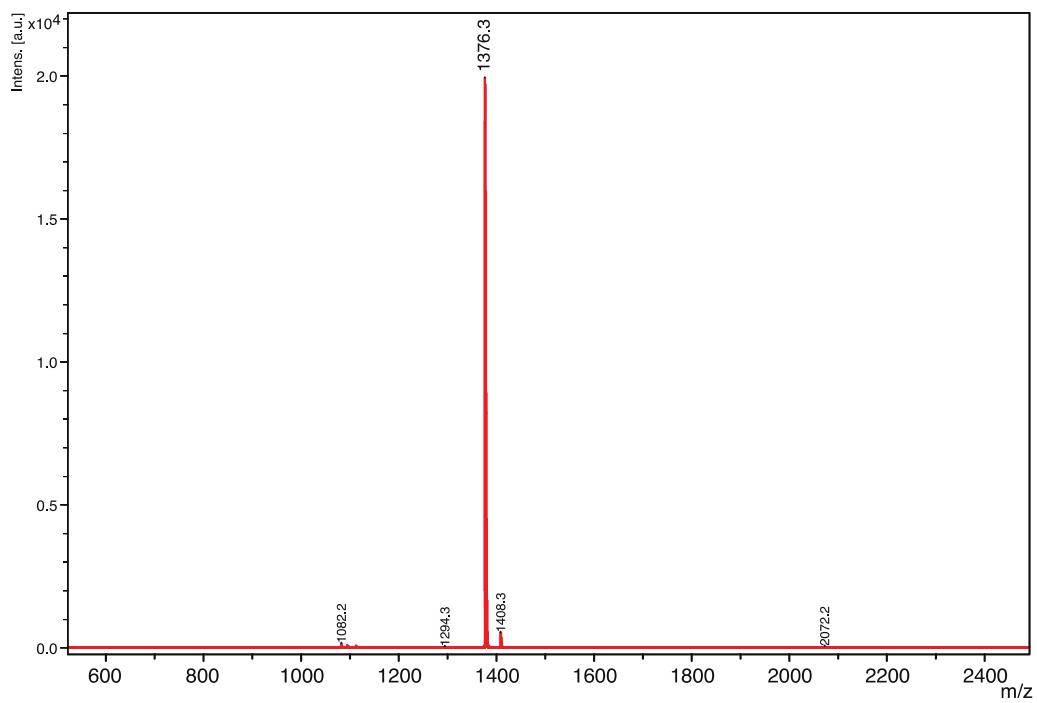


Figure S24. HR-MALDI-TOF mass spectrum of **TbT-2**.

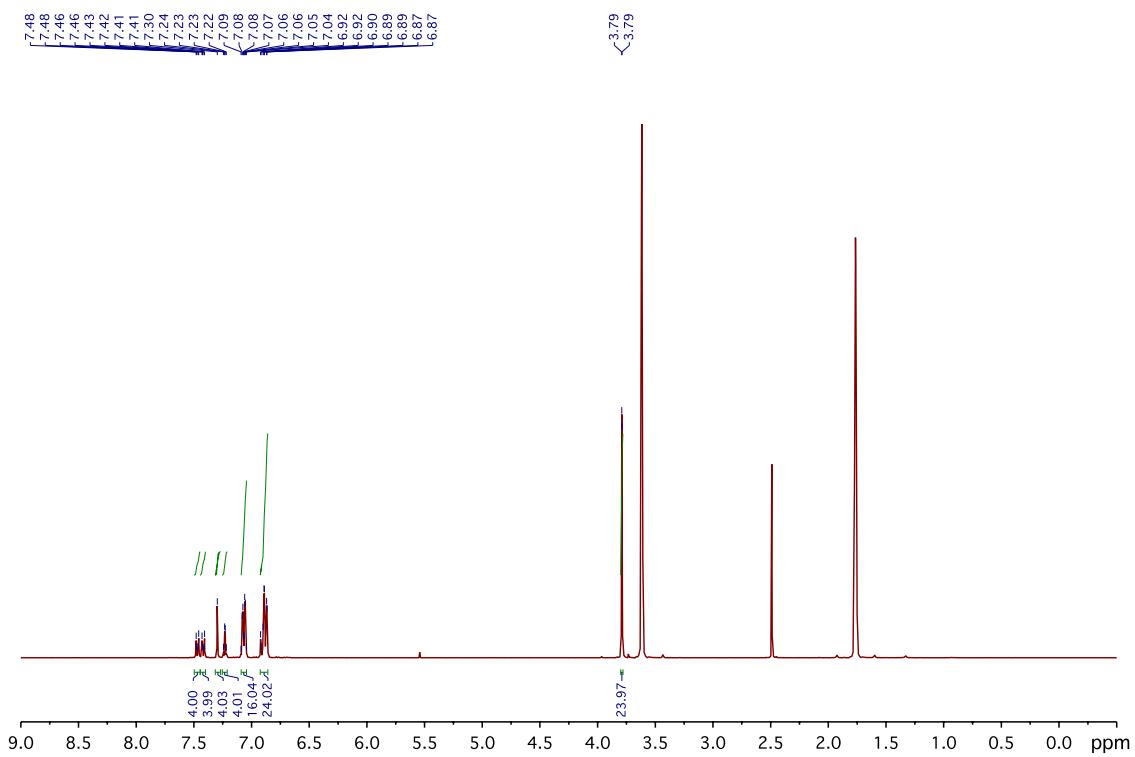


Figure S25. ^1H NMR (400 MHz, THF- d_8 , 298 K) of TbT-3.

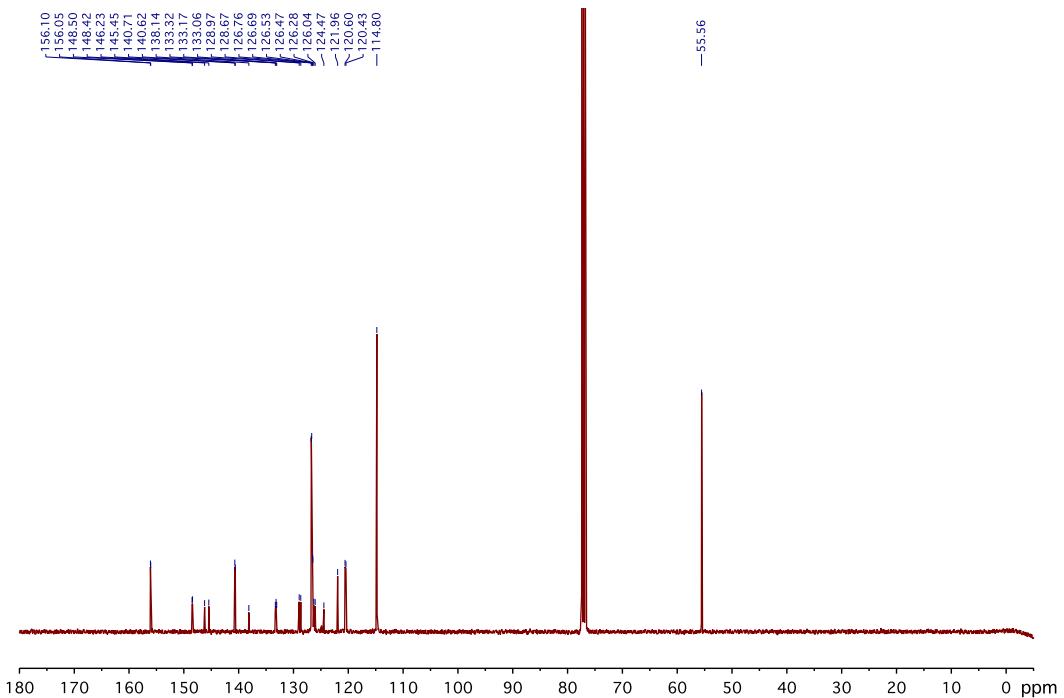


Figure S26. ^{13}C NMR (100 MHz, CDCl_3 , 298 K) of TbT-3.

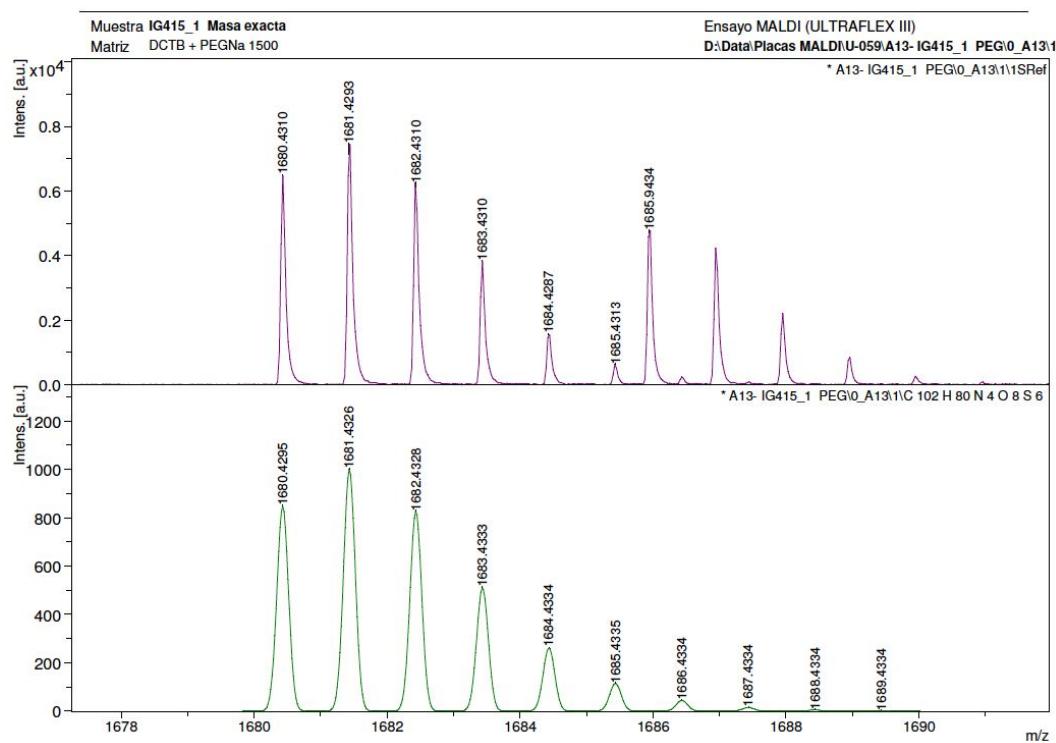
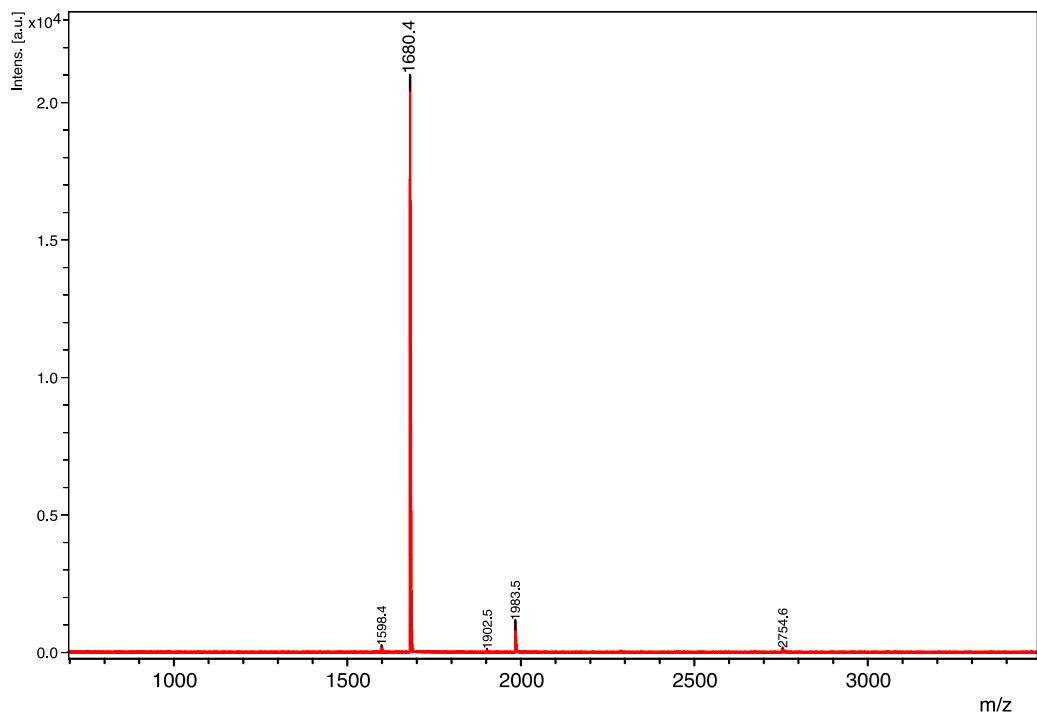


Figure S27. HR-MALDI-TOF mass spectrum of TbT-3.

6. References

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7. Energies and coordinates of the optimized structures in gas phase.

TbT (Neutral)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.868645	2.125024	0.000000
16	0.868645	1.905447	0.000000
6	0.674352	0.170235	0.000000
6	-0.674352	-0.170235	0.000000
6	-1.560464	0.946713	0.000000
6	1.560464	-0.946713	0.000000
6	0.868645	-2.125024	0.000000
16	-0.868645	-1.905447	0.000000
1	2.641796	-0.885382	0.000000
1	1.272247	-3.127954	0.000000
1	-2.641796	0.885382	0.000000
1	-1.272247	3.127954	0.000000

E = -1027.4088686 au; all frequencies positive

6	-0.898474	4.586919	0.669282
6	-0.767848	5.965624	0.341951
6	0.166051	6.191003	-0.632728
16	0.898474	4.719177	-1.176529
16	3.121958	2.934756	1.279312
6	4.752486	2.750413	0.724667
6	4.832217	1.896109	-0.340605
6	3.562007	1.377702	-0.725621
1	1.574131	-4.204745	1.426022
1	1.335639	-6.755446	0.819777
1	-0.477577	-7.135944	-1.055969
1	-5.552850	-3.286785	1.215213
1	-5.761700	-1.647209	-0.839338
1	-3.413387	-0.694895	-1.554461
1	-1.574131	4.204745	1.426022
1	-1.335639	6.755446	0.819777
1	0.477577	7.135944	-1.055969
1	5.552850	3.286785	1.215213
1	5.761700	1.647209	-0.839338
1	3.413387	0.694895	-1.554461

E = -3234.6677339 au; all frequencies positive

TbT (Radical cation)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.856015	2.101003	0.000000
16	0.856015	1.942576	0.000000
6	0.687925	0.188660	0.000000
6	-0.687925	-0.188660	0.000000
6	-1.566602	0.882743	0.000000
6	1.566602	-0.882743	0.000000
6	0.856015	-2.101003	0.000000
16	-0.856015	-1.942576	0.000000
1	2.648566	-0.831226	0.000000
1	1.297570	-3.091232	0.000000
1	-2.648566	0.831226	0.000000
1	-1.297570	3.091232	0.000000

E = -1027.1272439 au; all frequencies positive

exTbT (Radical cation)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.936841	2.110996	-0.130307
16	-1.987001	0.676524	-0.127710
6	-0.596723	-0.372165	-0.096013
6	0.596723	0.372165	-0.096013
6	0.444359	1.764850	-0.146925
6	-0.444359	-1.764850	-0.146925
6	0.936841	-2.110996	-0.130307
16	1.987001	-0.676524	-0.127710
6	1.561703	-3.388564	-0.045288
6	-1.561703	3.388564	-0.045288
6	1.561703	2.706728	-0.240236
6	-1.561703	-2.706728	-0.240236
6	2.934318	-3.642693	-0.165687
6	3.284662	-4.983575	0.056280
6	2.188721	-5.767382	0.356894
16	0.711971	-4.885744	0.352405
16	-2.853851	-2.705121	0.947622
6	-3.703120	-3.942819	0.090037
6	-3.039146	-4.332006	-1.043084
6	-1.819662	-3.627040	-1.233739
6	-2.934318	3.642693	-0.165687
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
16	-0.711971	4.885744	0.352405
16	2.853851	2.705121	0.947622
6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
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6	1.819662	3.627040	-1.233739
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6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
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6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
16	-0.711971	4.885744	0.352405
16	2.853851	2.705121	0.947622
6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
16	-0.711971	4.885744	0.352405
16	2.853851	2.705121	0.947622
6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
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16	2.853851	2.705121	0.947622
6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
16	-0.711971	4.885744	0.352405
16	2.853851	2.705121	0.947622
6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
16	-0.711971	4.885744	0.352405
16	2.853851	2.705121	0.947622
6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
16	-0.711971	4.885744	0.352405
16	2.853851	2.705121	0.947622
6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
16	-0.711971	4.885744	0.352405
16	2.853851	2.705121	0.947622
6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	0.356894
16	-0.711971	4.885744	0.352405
16	2.853851	2.705121	0.947622
6	3.703120	3.942819	0.090037
6	3.039146	4.332006	-1.043084
6	1.819662	3.627040	-1.233739
6	-3.284662	4.983575	0.056280
6	-2.188721	5.767382	

E = -3234.4406999 au; all frequencies positive

TbT-1 (Neutral)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.621433	0.306067	-0.175311
6	0.621433	-0.306067	-0.175311
16	1.884526	0.894402	-0.116049
6	0.696545	2.210741	-0.084571
6	-0.607374	1.737285	-0.109003
6	1.206147	3.588576	-0.124461
6	0.604890	4.574764	-0.929768
6	1.124669	5.859776	-1.012400
6	2.275315	6.221470	-0.286699
6	2.877297	5.245577	0.527451
6	2.354131	3.960744	0.599588
1	-0.265569	4.317484	-1.523186
1	0.651549	6.589119	-1.660677
1	3.755763	5.502428	1.108929
1	2.831537	3.234523	1.251244
6	0.607374	-1.737285	-0.109003
16	-1.884526	-0.894402	-0.116049
6	-0.696545	-2.210741	-0.084571
6	-1.844111	2.545945	-0.008642
6	-2.001424	3.536731	0.975087
6	-3.189686	4.244500	1.108487
6	-4.275381	3.997439	0.247606
6	-4.120118	3.019042	-0.749726
6	-2.932549	2.304076	-0.863605
1	-1.186615	3.733586	1.664290
1	-3.288975	4.984514	1.894950
1	-4.935941	2.819909	-1.435672
1	-2.839976	1.559300	-1.648671
6	1.844111	-2.545945	-0.008642
6	2.932549	-2.304076	-0.863605
6	4.120118	-3.019042	-0.749726
6	4.275381	-3.997439	0.247606
6	3.189686	-4.244500	1.108487
6	2.001424	-3.536731	0.975087
1	2.839976	-1.559300	-1.648671
1	4.935941	-2.819909	-1.435672
1	3.288975	-4.984514	1.894950
1	1.186615	-3.733586	1.664290
6	-1.206147	-3.588576	-0.124461
6	-2.354131	-3.960744	0.599588
6	-2.877297	-5.245577	0.527451
6	-2.275315	-6.221470	-0.286699
6	-1.124669	-5.859776	-1.012400
6	-0.604890	-4.574764	-0.929768
1	-2.831537	-3.234523	1.251244
1	-3.755763	-5.502428	1.108929
1	-0.651549	-6.589119	-1.660677
1	0.265569	-4.317484	-1.523186
7	-2.819797	-7.521337	-0.378824
6	-1.981760	-8.655824	-0.575158
6	-4.230226	-7.718964	-0.305033
6	-2.321680	-9.637607	-1.522624
6	-1.527179	-10.761073	-1.697471
6	-0.356515	-10.927245	-0.943805
6	0.000039	-9.951010	-0.007243
6	-0.816924	-8.833690	0.179516
6	-4.767238	-8.719535	0.523208
6	-6.137054	-8.931515	0.582624
6	-7.012400	-8.134467	-0.169495
6	-6.490254	-7.128632	-0.990349
6	-5.108954	-6.936838	-1.062064
6	1.536305	-12.298190	-0.449934
6	-9.270712	-7.647478	-0.776078
8	0.356515	-12.067090	-1.197896
8	-8.342501	-8.417611	-0.030726
1	-3.220899	-9.514005	-2.116741
1	-1.788106	-11.522720	-2.424801

1	0.894520	-10.053413	0.595732
1	-4.098530	-9.333899	1.117098
1	-6.556509	-9.703922	1.218760
1	-7.140267	-6.501001	-1.588244
1	-4.709451	-6.164109	-1.710659
1	1.934298	-13.252371	-0.798792
1	2.285879	-11.513303	-0.620203
1	1.329195	-12.366334	0.626347
1	-10.258394	-8.033466	-0.519597
1	-9.220211	-6.583104	-0.511783
1	-9.112102	-7.754290	-1.857071
1	-0.542788	-8.089294	0.919694
7	5.492068	-4.702896	0.385657
6	6.733954	-4.066846	0.091518
6	5.508622	-6.049549	0.848062
6	7.700037	-4.720657	-0.692629
6	8.919384	-4.117662	-0.965849
6	9.200361	-2.832353	-0.480222
6	8.242934	-2.167542	0.293870
6	7.027683	-2.790912	0.584330
6	6.426125	-6.453135	1.834182
6	6.467742	-7.769315	2.270013
6	5.578086	-8.718710	1.747684
6	4.652019	-8.327572	0.774792
6	4.631628	-7.005808	0.324156
6	10.758353	-1.026484	-0.350653
6	4.832643	-10.987943	1.750284
8	10.423880	-2.323176	-0.816405
8	5.697586	-9.985368	2.251658
1	7.486791	-5.710389	-1.082750
1	9.668670	-4.619257	-1.569345
1	8.432759	-1.176661	0.688743
1	7.111894	-5.723855	2.252255
1	7.176373	-8.084765	3.028680
1	3.955519	-9.038294	0.345799
1	3.920700	-6.714367	-0.441886
1	11.759428	-0.817879	-0.731066
1	10.063053	-0.266509	-0.730535
1	10.773270	-0.979432	0.746071
1	5.096256	-11.906683	2.276622
1	3.778229	-10.751260	1.947646
1	4.968356	-11.140299	0.671118
1	6.295179	-2.274172	1.195620
7	2.819797	7.521337	-0.378824
6	4.230226	7.718964	-0.305033
6	1.981760	8.655824	-0.575158
6	4.767238	8.719535	0.523208
6	6.137054	8.931515	0.582624
6	7.012400	8.134467	-0.169495
6	6.490254	7.128632	-0.990349
6	5.108954	6.936838	-1.062064
6	2.321680	9.637607	-1.522624
6	1.527179	10.761073	-1.697471
6	0.356515	10.927245	-0.943805
6	-0.000039	9.951010	-0.007243
6	0.816924	8.833690	0.179516
6	9.270712	7.647478	-0.776078
6	-1.536305	12.298190	-0.449934
8	8.342501	8.417611	-0.030726
8	-0.356515	12.067090	-1.197896
1	4.098530	9.333899	1.117098
1	6.556509	9.703922	1.218760
1	7.140267	6.501001	-1.588244
1	3.220899	9.514005	-2.116741
1	1.788106	11.522720	-2.424801
1	-0.894520	10.053413	0.595732
1	0.542788	8.089294	0.919694
1	10.258394	8.033466	-0.519597
1	9.220211	6.583104	-0.511783
1	9.112102	7.754290	-1.857071
1	-1.934298	13.252371	-0.798792
1	-2.285879	11.513303	-0.620203
1	-1.329195	12.366334	0.626347
1	4.709451	6.164109	-1.710659
7	-5.492068	4.702896	0.385657
6	-5.508622	6.049549	0.848062

6	-6.733954	4.066846	0.091518	1	-5.872942	0.773364	1.947965
6	-6.426125	6.453135	1.834182	1	-3.579032	1.570255	1.642867
6	-6.467742	7.769315	2.270013	6	-1.918147	3.239943	-0.179372
6	-5.578086	8.718710	1.747684	6	-1.358341	4.414195	0.378326
6	-4.652019	8.327572	0.774792	6	-1.983039	5.641688	0.275285
6	-4.631628	7.005808	0.324156	6	-3.216474	5.770600	-0.406552
6	-7.700037	4.720657	-0.692629	6	-3.787241	4.601948	-0.965405
6	-8.919384	4.117662	-0.965849	6	-3.155887	3.378287	-0.853324
6	-9.200361	2.832353	-0.480222	1	-0.429331	4.348900	0.936983
6	-8.242934	2.167542	0.293870	1	-1.535897	6.512831	0.738686
6	-7.027683	2.790912	0.584330	1	-4.714721	4.676110	-1.520602
6	-4.832643	10.987943	1.750284	1	-3.598660	2.514335	-1.333764
6	-10.758353	1.026484	-0.350653	7	-3.839437	7.009133	-0.529195
8	-5.697586	9.985368	2.251658	6	-5.249945	7.117022	-0.737526
8	-10.423880	2.323176	-0.816405	6	-3.085271	8.223998	-0.469648
1	-7.111894	5.723855	2.252255	6	-5.748019	7.926557	-1.772436
1	-7.176373	8.084765	3.028680	6	-7.113335	8.065411	-1.961138
1	-3.955519	9.038294	0.345799	6	-8.018411	7.393475	-1.122795
1	-7.486791	5.710389	-1.082750	6	-7.529670	6.582465	-0.089947
1	-9.668670	4.619257	-1.569345	6	-6.153200	6.456226	0.101075
1	-8.432759	1.176661	0.688743	6	-3.486856	9.260530	0.389380
1	-6.295179	2.274172	1.195620	6	-2.780428	10.451678	0.430443
1	-5.096256	11.906683	2.276622	6	-1.648969	10.635683	-0.382318
1	-3.778229	10.751260	1.947646	6	-1.241658	9.605602	-1.240975
1	-4.968356	11.140299	0.671118	6	-1.965058	8.413545	-1.285232
1	-11.759428	0.817879	-0.731066	6	-10.305334	6.973298	-0.566783
1	-10.063053	0.266509	-0.730535	6	0.112005	12.098419	-1.072041
1	-10.773270	0.979432	0.746071	8	-9.334554	7.597392	-1.394954
1	-3.920700	6.714367	-0.441886	8	-1.028118	11.837783	-0.262877

E = -4937.7062815 au; all frequencies positive

TbT-1 (Radical cation)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.641307	0.271959	-0.206754
6	-0.641307	-0.271959	-0.206754
16	-0.561425	-2.014154	-0.143124
6	1.211133	-1.974242	-0.120470
6	1.710404	-0.658211	-0.134731
6	1.918147	-3.239943	-0.179372
6	3.155887	-3.378287	-0.853324
6	3.787241	-4.601948	-0.965405
6	3.216474	-5.770600	-0.406552
6	1.983039	-5.641688	0.275285
6	1.358341	-4.414195	0.378326
1	3.598660	-2.514335	-1.333764
1	4.714721	-4.676110	-1.520602
1	1.535897	-6.512831	0.738686
1	0.429331	-4.348900	0.936983
6	-1.710404	0.658211	-0.134731
16	0.561425	2.014154	-0.143124
6	-1.211133	1.974242	-0.120470
6	3.120120	-0.248841	-0.001232
6	3.964179	-0.800343	0.982273
6	5.262588	-0.349911	1.159109
6	5.791257	0.677213	0.345369
6	4.955254	1.222395	-0.652513
6	3.651481	0.774981	-0.808598
1	3.579032	-1.570255	1.642867
1	5.872942	-0.773364	1.947965
1	5.339580	1.993041	-1.310066
1	3.042692	1.203569	-1.599337
6	-3.120120	0.248841	-0.001232
6	-3.651481	-0.774981	-0.808598
6	-4.955254	-1.222395	-0.652513
6	-5.791257	-0.677213	0.345369
6	-5.262588	0.349911	1.159109
6	-3.964179	0.800343	0.982273
1	-3.042692	-1.203569	-1.599337
1	-5.339580	-1.993041	-1.310066

6	5.249945	-7.117022	-0.737526
6	3.486856	-9.260530	0.389380
6	2.780428	-10.451678	0.430443
6	1.648969	-10.635683	-0.382318
6	1.241658	-9.605602	-1.240975
6	1.965058	-8.413545	-1.285232
6	5.748019	-7.926557	-1.772436
6	7.113335	-8.065411	-1.961138
6	8.018411	-7.393475	-1.122795
6	7.529670	-6.582465	-0.089947
6	6.153200	-6.456226	0.101075
6	-0.112005	-12.098419	-1.072041
6	10.305334	-6.973298	-0.566783
8	1.028118	-11.837783	-0.262877
8	9.334554	-7.597392	-1.394954
1	4.357453	-9.123639	1.022162
1	3.079629	-11.258509	1.090596
1	0.380721	-9.725146	-1.887233
1	5.054407	-8.446971	-2.424216
1	7.508857	-8.686724	-2.757261
1	8.204705	-6.063654	0.579734
1	5.778657	-5.842813	0.914171
1	-0.436032	-13.107202	-0.815513
1	-0.924686	-11.392375	-0.861061
1	0.135109	-12.058099	-2.139887
1	11.275320	-7.279665	-0.959134
1	10.227859	-5.879286	-0.610069
1	10.216315	-7.302261	0.476009
1	1.657919	-7.624757	-1.964385
7	7.097280	1.143814	0.524314
6	8.099780	0.330682	1.138644
6	7.470487	2.466585	0.127729
6	8.859260	0.836331	2.207064
6	9.856146	0.069725	2.789735
6	10.113976	-1.230258	2.326686
6	9.359449	-1.744923	1.265104
6	8.367702	-0.960256	0.673206
6	8.610783	2.667607	-0.667562
6	9.001741	3.947274	-1.029906
6	8.254400	5.061884	-0.616495
6	7.113335	4.870834	0.173199
6	6.736218	3.580181	0.547469
6	11.438205	-3.208953	2.535793
6	8.018412	7.440180	-0.629326
8	11.109804	-1.899086	2.971493
8	8.719185	6.271727	-1.031558
1	8.663133	1.838671	2.572897
1	10.447872	0.452357	3.614330
1	9.544967	-2.740080	0.879124
1	9.190276	1.810584	-0.994643
1	9.881332	4.112164	-1.642833
1	6.524187	5.712785	0.515938
1	5.861125	3.438648	1.173620
1	12.252876	-3.544243	3.178446
1	10.588221	-3.895377	2.643987
1	11.776492	-3.214255	1.491762
1	8.560065	8.279756	-1.066000
1	6.987065	7.440976	-1.004306
1	8.005383	7.547192	0.462508
1	7.797339	-1.356055	-0.161011

E = -4937.5236915 au; all frequencies positive

TbT-2 (Neutral)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	2.079883	-1.032680	-0.642173
16	1.953069	0.741221	-0.666792
6	0.212216	0.658206	-0.648838
6	-0.212216	-0.658206	-0.648838
6	0.824364	-1.637340	-0.643050
6	-0.824364	1.637340	-0.643050
6	-2.079883	1.032680	-0.642173
16	-1.953069	-0.741221	-0.666792
6	-3.401797	1.615774	-0.623932
6	3.401797	-1.615774	-0.623932
6	0.568628	-3.088540	-0.645332
6	-0.568628	3.088540	-0.645332
6	-4.603968	0.956541	-0.453946
6	-5.750199	1.778880	-0.565755
6	-5.443914	3.100447	-0.806202
16	-3.695910	3.336938	-0.898143
16	-0.421881	3.998386	0.854966
6	0.002306	5.470233	-0.024855
6	0.009974	5.240267	-1.380833
6	-0.314146	3.899257	-1.723386
6	4.603968	-0.956541	-0.453946
6	5.750199	-1.778880	-0.565755
6	5.443914	-3.100447	-0.806202
16	3.695910	-3.336938	-0.898143
16	0.421881	-3.998386	0.854966
6	-0.002306	-5.470233	-0.024855
6	-0.009974	-5.240267	-1.380833
6	0.314146	-3.899257	-1.723386
1	-4.663078	-0.110127	-0.267843
1	-6.766177	1.420397	-0.458317
1	0.233140	6.017526	-2.101363
1	-0.340844	3.529341	-2.742159
1	4.663078	0.110127	-0.267843
1	6.766177	-1.420397	-0.458317
1	-0.233140	-6.017526	-2.101363
1	0.340844	-3.529341	-2.742159
7	6.324122	-4.179176	-0.858032
6	7.488708	-4.172734	-0.027461
6	6.068441	-5.305225	-1.691439
6	8.747175	-4.470623	-0.574656
6	9.880188	-4.484126	0.226507
6	9.786733	-4.180371	1.592620
6	8.537360	-3.872191	2.144215
6	7.399147	-3.880117	1.336353
6	6.302237	-6.607074	-1.214366
6	6.056378	-7.709942	-2.019509
6	5.543569	-7.545885	-3.314740
6	5.308486	-6.255256	-3.799298
6	5.584472	-5.147896	-2.994875
6	10.923749	-3.916193	3.677122
6	4.802642	-8.586462	-5.336605
8	10.960846	-4.210590	2.289796
8	5.308486	-8.699436	-4.014116
1	8.828516	-4.695906	-1.632958
1	10.855962	-4.714386	-0.188064
1	8.433303	-3.638867	3.197000
1	6.682676	-6.747300	-0.208507
1	6.247967	-8.715154	-1.658238
1	4.923451	-6.094175	-4.798887
1	5.414305	-4.150249	-3.384715
1	11.953109	-3.995058	4.029597
1	10.554935	-2.899851	3.866545
1	10.298861	-4.631480	4.227239
1	4.691694	-9.606967	-5.705307
1	3.825476	-8.087812	-5.354507
1	5.496888	-8.040915	-5.988092
1	6.431916	-3.648354	1.769673
7	-0.171580	-6.690314	0.629959
6	-0.978813	-6.782289	1.798923
6	0.481815	-7.850400	0.109394
6	-0.585987	-7.593845	2.877953
6	-1.372216	-7.683947	4.016945
6	-2.563104	-6.950307	4.120671
6	-2.958593	-6.133847	3.056343
6	-2.175133	-6.064865	1.902598
6	-3.656118	11.284021	-1.818893
6	4.462856	6.374794	5.448169
8	-2.283912	11.279754	-1.452260

8	3.256205	7.101719	5.290231	6	0.900727	-12.559257	1.593215
1	1.263989	9.108840	0.248614	6	-6.708920	-6.745404	-5.079853
1	0.121092	11.119707	-0.668904	8	0.458918	-12.295214	0.266151
1	-3.503070	8.843000	-1.096089	8	-6.521151	-7.231203	-3.753354
1	-0.340521	8.154274	2.815410	1	-1.226213	-9.490218	-2.798122
1	1.073675	8.308539	4.852410	1	-0.364888	-11.701279	-2.045253
1	3.875139	5.558119	3.103061	1	0.249360	-10.105397	1.901932
1	2.496773	5.441778	1.074829	1	-3.795251	-8.239853	-0.332269
1	-3.862421	12.287059	-2.195971	1	-6.012727	-8.190090	-1.467604
1	-3.877655	10.548668	-2.601904	1	-4.209562	-6.278236	-4.876091
1	-4.303237	11.086376	-0.953954	1	-2.020670	-6.342169	-3.753439
1	4.842475	6.630463	6.438641	1	1.216620	-13.602461	1.599965
1	4.294369	5.291229	5.395625	1	1.749830	-11.921711	1.867790
1	5.209096	6.656205	4.693538	1	0.091597	-12.420999	2.320450
1	-2.380229	6.875677	-0.161648	1	-7.768709	-6.876930	-5.298737

E = -6220.706918 au; all frequencies positive

TbT-2 (Radical Cation)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.150567	-2.309816	-0.489820
16	1.446905	-1.518235	-0.501499
6	0.697437	0.055878	-0.531563
6	-0.697437	-0.055878	-0.531563
6	-1.205833	-1.366973	-0.475005
6	1.205833	1.366973	-0.475005
6	0.150567	2.309816	-0.489820
16	-1.446905	1.518235	-0.501499
6	0.210825	3.724920	-0.582428
6	-0.210825	-3.724920	-0.582428
6	-2.634476	-1.682531	-0.382535
6	2.634476	1.682531	-0.382535
6	-0.843678	4.631705	-0.433353
6	-0.513917	5.964171	-0.685478
6	0.828508	6.128771	-1.043719
16	1.682869	4.590571	-1.057640
16	3.332542	2.359213	1.092747
6	4.961486	2.256023	0.421738
6	4.935435	1.720002	-0.852435
6	3.628163	1.394457	-1.290902
6	0.843678	-4.631705	-0.433353
6	0.513917	-5.964171	-0.685478
6	-0.828508	-6.128771	-1.043719
16	-1.682869	-4.590571	-1.057640
16	-3.332542	-2.359213	1.092747
6	-4.961486	-2.256023	0.421738
6	-4.935435	-1.720002	-0.852435
6	-3.628163	-1.394457	-1.290902
1	-1.841288	4.317446	-0.146619
1	-1.210505	6.788599	-0.618386
1	5.829783	1.576965	-1.444634
1	3.416654	0.958156	-2.261206
1	1.841288	-4.317446	-0.146619
1	1.210505	-6.788599	-0.618386
1	-5.829783	-1.576965	-1.444634
1	-3.416654	-0.958156	-2.261206
7	-1.491024	-7.295615	-1.305560
6	-0.966816	-8.558734	-0.869566
6	-2.767466	-7.276168	-1.964896
6	-0.900727	-9.630886	-1.772831
6	-0.423900	-10.863939	-1.358617
6	0.004947	-11.052404	-0.033394
6	-0.061568	-9.984195	0.871684
6	-0.553889	-8.748281	0.451682
6	-3.895242	-7.810258	-1.323432
6	-5.130776	-7.785120	-1.951585
6	-5.262875	-7.224140	-3.233180
6	-4.136627	-6.702975	-3.882794
6	-2.895157	-6.737815	-3.247355

1	-1.216620	13.602461	1.599965
1	-1.749830	11.921711	1.867790
1	-0.091597	12.420999	2.320450
1	2.020670	6.342169	-3.753439
7	6.051484	2.751644	1.114015
6	7.155679	3.318245	0.397253
6	6.081395	2.748315	2.543545
6	8.466523	2.917201	0.698596
6	9.544775	3.486953	0.037898
6	9.337131	4.460720	-0.951486
6	8.031320	4.859531	-1.265354
6	6.952743	4.293601	-0.582890
6	6.438219	3.912727	3.244024
6	6.483587	3.913614	4.629266
6	6.159144	2.754320	5.352396
6	5.800391	1.590522	4.661668
6	5.776291	1.591110	3.265978
6	10.319980	5.956218	-2.534788
6	5.928642	1.721250	7.495206
8	10.462765	4.952272	-1.541274
8	6.226223	2.865670	6.707754
1	8.632858	2.162056	1.459763
1	10.562333	3.187630	0.265022
1	7.839462	5.614402	-2.018919
1	6.684243	4.813598	2.691947
1	6.759498	4.806490	5.179965
1	5.556318	0.678548	5.192600
1	5.519611	0.680453	2.734748
1	11.331715	6.209489	-2.853479
1	9.749984	5.590139	-3.398547
1	9.829170	6.853293	-2.137590
1	6.046075	2.032832	8.533572
1	4.898820	1.377721	7.335232
1	6.620588	0.896038	7.285440
1	5.943843	4.617141	-0.817046

E = -6220.5308216 au; all frequencies positive

TbT-3 (Neutral)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.203580	1.977428	-0.250610
16	-2.046297	0.418796	-0.285704
6	-0.533001	-0.442610	-0.336703
6	0.533001	0.442610	-0.336703
6	0.179175	1.827691	-0.270170
6	-0.179175	-1.827691	-0.270170
6	1.203580	-1.977428	-0.250610
16	2.046297	-0.418796	-0.285704
6	2.021223	-3.176726	-0.285964
6	-2.021223	3.176726	-0.285964
6	1.184084	2.889912	-0.177813
6	-1.184084	-2.889912	-0.177813
6	3.202343	-3.412617	0.387896
6	3.801745	-4.656966	0.073317
6	3.096737	-5.396776	-0.854230
16	1.669282	-4.517354	-1.364956
16	-1.120785	-4.129695	1.059151
6	-2.628646	-4.844598	0.522693
6	-3.141052	-4.125207	-0.536029
6	-2.334346	-3.023665	-0.923572
6	-3.202343	3.412617	0.387896
6	-3.801745	4.656966	0.073317
6	-3.096737	5.396776	-0.854230
16	-1.669282	4.517354	-1.364956
16	1.120785	4.129695	1.059151
6	2.628646	4.844598	0.522693
6	3.141052	4.125207	-0.536029
6	2.334346	3.023665	-0.923572
1	3.604416	-2.716086	1.115204
1	4.704421	-5.020417	0.550346
1	-4.055221	-4.403394	-1.047429
1	-2.572563	-2.364544	-1.750935
1	-3.604416	2.716086	1.115204
1	-4.704421	5.020417	0.550346
1	4.055221	4.403394	-1.047429
1	2.572563	2.364544	-1.750935
6	-3.409765	6.721050	-1.391694
6	-2.416038	7.575387	-1.904504
6	-2.724154	8.833909	-2.402969
6	-4.052571	9.297733	-2.417576
6	-5.054632	8.447644	-1.911832
6	-4.736508	7.192732	-1.412579
7	-4.372155	10.573930	-2.926609
6	-5.441002	11.332188	-2.365886
6	-3.630535	11.130376	-4.009502
6	-6.382093	11.962876	-3.197979
6	-7.412043	12.719396	-2.657860
6	-7.543690	12.851025	-1.267677
6	-6.617985	12.220460	-0.428866
6	-5.570685	11.480015	-0.980680
6	-3.180515	12.460925	-3.957400
6	-2.476236	13.013421	-5.017447
6	-2.182954	12.244761	-6.153362
6	-2.618326	10.916192	-6.212976
6	-3.346704	10.374521	-5.152106
6	-8.773360	13.778093	0.558327
6	-1.155306	12.148179	-8.307504
8	-8.598082	13.607514	-0.838514
8	-1.474621	12.879369	-7.135087
1	-1.931158	9.473603	-2.773796
1	-6.088832	8.773091	-1.929145
1	-5.537527	6.548356	-1.063497
1	-6.295102	11.857987	-4.274360
1	-8.139647	13.209657	-3.296167
1	-6.688484	12.309338	0.648612
1	-4.847789	11.006347	-0.324602
1	-3.392567	13.060242	-3.078192
1	-2.128364	14.040537	-4.982553
1	-2.413475	10.298839	-7.079396
1	-3.693199	9.347988	-5.211416
1	-9.659303	14.403525	0.677331
1	-8.938466	12.819420	1.067124
1	-7.912781	14.281953	1.017248
1	-0.595103	12.832157	-8.946715
1	-0.531951	11.272833	-8.083196
1	-2.057449	11.817134	-8.838185
1	-1.376030	7.262488	-1.881002
6	3.186823	6.030048	1.175817
6	4.571709	6.281849	1.145385
6	5.120682	7.402760	1.752156
6	4.303456	8.332215	2.423052
6	2.918461	8.087724	2.460433
6	2.378834	6.961705	1.853081
7	4.858105	9.472441	3.042637
6	4.288052	9.997969	4.238668
6	5.999144	10.118377	2.484051
6	4.062779	11.378651	4.375652
6	3.526857	11.897304	5.545611
6	3.180515	11.047715	6.606412
6	3.392048	9.670418	6.478366
6	3.953561	9.158649	5.306956
6	7.080699	10.490295	3.301272
6	8.184946	11.137299	2.765631
6	8.249751	11.413591	1.392090
6	7.183060	11.040279	0.566941
6	6.065054	10.410371	1.117317
6	2.285075	10.843500	8.811369
6	9.498751	12.351393	-0.415134
8	2.649122	11.657277	7.708559
8	9.385113	12.043364	0.964339
1	6.193567	7.557829	1.725168
1	2.264771	8.794624	2.959069
1	1.302013	6.820131	1.876019
1	4.316642	12.042978	3.556273
1	3.352902	12.962512	5.656486
1	3.141297	8.988904	7.282397
1	4.127563	8.091152	5.220431
1	7.044935	10.270878	4.363224
1	9.021236	11.427853	3.392860
1	7.200119	11.246340	-0.496588
1	5.235205	10.137094	0.473857
1	1.886236	11.520896	9.567897
1	1.512579	10.112478	8.539345
1	3.150419	10.310300	9.226087
1	10.466273	12.840669	-0.536646
1	9.472057	11.447028	-1.036928
1	8.705774	13.034886	-0.745521
1	5.233531	5.565976	0.667632
6	3.409765	-6.721050	-1.391694
6	4.736508	-7.192732	-1.412579
6	5.054632	-8.447644	-1.911832
6	4.052571	-9.297733	-2.417576
6	2.724154	-8.833909	-2.402969
6	2.416038	-7.575387	-1.904504
7	4.372155	-10.573930	-2.926609
6	3.630535	-11.130376	-4.009502
6	5.441002	-11.332188	-2.365886
6	3.180515	-12.460925	-3.957400
6	2.476236	-13.013421	-5.017447
6	2.182954	-12.244761	-6.153362
6	2.618326	-10.916192	-6.212976
6	3.346704	-10.374521	-5.152106
6	6.382093	-11.962876	-3.197979
6	7.412043	-12.719396	-2.657860
6	7.543690	-12.851025	-1.267677
6	6.617985	-12.220460	-0.428866
6	5.570685	-11.480015	-0.980680
6	1.155306	-12.148179	-8.307504
6	8.773360	-13.778093	0.558327
8	1.474621	-12.879369	-7.135087
8	8.598082	-13.607514	-0.838514
1	6.088832	-8.773091	-1.929145
1	1.931158	-9.473603	-2.773796
1	1.376030	-7.262488	-1.881002
1	3.392567	-13.060242	-3.078192

1	2.128364	-14.040537	-4.982553	6	2.582128	1.740340	-0.457822
1	2.413475	-10.298839	-7.079396	6	-0.963314	4.591296	-0.203515
1	3.693199	-9.347988	-5.211416	6	-0.735946	5.947788	-0.482487
1	6.295102	-11.857987	-4.274360	6	0.467814	6.194494	-1.133367
1	8.139647	-13.209657	-3.296167	16	1.321752	4.688220	-1.408574
1	6.688484	-12.309338	0.648612	16	3.230523	2.677625	0.875303
1	4.847789	-11.006347	-0.324602	6	4.877350	2.477261	0.307710
1	0.595103	-12.832157	-8.946715	6	4.892341	1.696733	-0.833088
1	0.531951	-11.272833	-8.083196	6	3.608173	1.274467	-1.254041
1	2.057449	-11.817134	-8.838185	6	0.963314	-4.591296	-0.203515
1	9.659303	-14.403525	0.677331	6	0.735946	-5.947788	-0.482487
1	8.938466	-12.819420	1.067124	6	-0.467814	-6.194494	-1.133367
1	7.912781	-14.281953	1.017248	16	-1.321752	-4.688220	-1.408574
1	5.537527	-6.548356	-1.063497	16	-3.230523	-2.677625	0.875303
6	-3.186823	-6.030048	1.175817	6	-4.877350	-2.477261	0.307710
6	-2.378834	-6.961705	1.853081	6	-4.892341	-1.696733	-0.833088
6	-2.918461	-8.087724	2.460433	6	-3.608173	-1.274467	-1.254041
6	-4.303456	-8.332215	2.423052	1	-1.838307	4.226711	0.322880
6	-5.120682	-7.402760	1.752156	1	-1.415471	6.735749	-0.182054
6	-4.571709	-6.281849	1.145385	1	5.801846	1.465638	-1.374497
7	-4.858105	-9.472441	3.042637	1	3.431755	0.675473	-2.140565
6	-5.999144	-10.118377	2.484051	1	1.838307	-4.226711	0.322880
6	-4.288052	-9.997969	4.238668	1	1.415471	-6.735749	-0.182054
6	-7.080699	-10.490295	3.301272	1	-5.801846	-1.465638	-1.374497
6	-8.184946	-11.137299	2.765631	1	-3.431755	-0.675473	-2.140565
6	-8.249751	-11.413591	1.392090	6	-1.017988	-7.467836	-1.557393
6	-7.183060	-11.040279	0.566941	6	-2.379078	-7.622624	-1.901056
6	-6.065054	-10.410371	1.117317	6	-2.894390	-8.839634	-2.307655
6	-4.062779	-11.378651	4.375652	6	-2.068107	-9.983313	-2.393050
6	-3.526857	-11.897304	5.545611	6	-0.703645	-9.839085	-2.051165
6	-3.180515	-11.047715	6.606412	6	-0.199462	-8.616650	-1.648791
6	-3.392048	-9.670418	6.478366	7	-2.582128	-11.215094	-2.802028
6	-3.953561	-9.158649	5.306956	6	-1.984716	-12.441183	-2.374969
6	-9.498751	-12.351393	-0.415134	6	-3.719655	-11.288626	-3.663671
6	-2.285075	-10.843500	8.811369	6	-1.685459	-13.445444	-3.311223
8	-9.385113	-12.043364	0.964339	6	-1.128904	-14.646360	-2.900912
8	-2.649122	-11.657277	7.708559	6	-0.846549	-14.872489	-1.543483
1	-2.264771	-8.794624	2.959069	6	-1.140184	-13.875588	-0.603684
1	-6.193567	-7.557829	1.725168	6	-1.714325	-12.675062	-1.022519
1	-5.233531	-5.565976	0.667632	6	-4.792746	-12.138807	-3.346981
1	-7.044935	-10.270878	4.363224	6	-5.886857	-12.235287	-4.192042
1	-9.021236	-11.427853	3.392860	6	-5.942515	-11.476464	-5.372875
1	-7.200119	-11.246340	-0.496588	6	-4.877805	-10.624608	-5.694960
1	-5.235205	-10.137094	0.473857	6	-3.773244	-10.543784	-4.846659
1	-4.316642	-12.042978	3.556273	6	0.005229	-16.375950	0.108674
1	-3.352902	-12.962512	5.656486	6	-7.170267	-10.916879	-7.346274
1	-3.141297	-8.988904	7.282397	8	-0.295886	-16.080104	-1.248887
1	-4.127563	-8.091152	5.220431	8	-7.061838	-11.640731	-6.127626
1	-10.466273	-12.840669	-0.536646	1	-3.948770	-8.924654	-2.542059
1	-9.472057	-11.447028	-1.036928	1	-0.041297	-10.692955	-2.129579
1	-8.705774	-13.034886	-0.745521	1	0.861214	-8.538631	-1.434141
1	-1.886236	-11.520896	9.567897	1	-1.894250	-13.275256	-4.362113
1	-1.512579	-10.112478	8.539345	1	-0.892519	-15.427246	-3.615569
1	-3.150419	-10.310300	9.226087	1	-0.944110	-14.027079	0.450693
1	-1.302013	-6.820131	1.876019	1	-1.956664	-11.912980	-0.288953

E = -7144.9795149 au; all frequencies positive

TbT-3 (Radical cation)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.079515	-2.313643	-0.555851
16	1.485742	-1.473409	-0.582232
6	0.691150	0.076797	-0.627311
6	-0.691150	-0.076797	-0.627311
6	-1.159283	-1.415513	-0.563531
6	1.159283	1.415513	-0.563531
6	0.079515	2.313643	-0.555851
16	-1.485742	1.473409	-0.582232
6	0.060814	3.747484	-0.622687
6	-0.060814	-3.747484	-0.622687
6	-2.582128	-1.740340	-0.457822

6	2.582128	1.740340	-0.457822
6	-0.963314	4.591296	-0.203515
6	-0.735946	5.947788	-0.482487
6	0.467814	6.194494	-1.133367
16	1.321752	4.688220	-1.408574
16	3.230523	2.677625	0.875303
6	4.877350	2.477261	0.307710
6	4.892341	1.696733	-0.833088
6	3.608173	1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487
6	-0.467814	-6.194494	-1.133367
16	-1.321752	-4.688220	-1.408574
16	-3.230523	-2.677625	0.875303
6	-4.877350	-2.477261	0.307710
6	-4.892341	-1.696733	-0.833088
6	-3.608173	-1.274467	-1.254041
6	0.963314	-4.591296	-0.203515
6	0.735946	-5.947788	-0.482487

6	-9.584906	-7.390207	5.705423	1	2.942714	9.896725	-5.109487
6	-8.840261	-6.813575	6.746760	1	1.894250	13.275256	-4.362113
6	-8.250291	-5.557604	6.556535	1	0.892519	15.427246	-3.615569
6	-8.414821	-4.890065	5.342158	1	0.944110	14.027079	0.450693
6	-11.704051	-4.258267	3.346407	1	1.956664	11.912980	-0.288953
6	-12.993885	-4.178947	2.844649	1	8.129317	11.202081	-7.779487
6	-13.256155	-4.501479	1.503520	1	7.159091	9.833391	-7.173993
6	-12.203403	-4.914393	0.677149	1	6.365866	11.180146	-8.044070
6	-10.910789	-5.009143	1.194669	1	-0.431822	17.379296	0.108686
6	-8.029551	-7.010048	8.986584	1	-0.737898	15.671464	0.521560
6	-14.884932	-4.703043	-0.234077	1	0.897008	16.366683	0.732575
8	-8.753670	-7.549025	7.889682	1	-0.861214	8.538631	-1.434141
8	-14.554084	-4.381750	1.109416	6	6.004157	3.074515	1.016860
1	-9.365307	-2.638138	1.444826	6	5.853804	4.198225	1.853078
1	-6.781549	-5.635988	3.139292	6	6.931220	4.759500	2.519821
1	-4.877346	-4.662960	1.957019	6	8.226700	4.217579	2.383896
1	-10.300359	-7.183702	3.693553	6	8.385859	3.089878	1.549988
1	-10.033464	-8.364437	5.867684	6	7.301417	2.537273	0.888863
1	-7.679216	-5.083498	7.345466	7	9.320159	4.778938	3.057316
1	-7.970123	-3.909589	5.206299	6	10.641787	4.675522	2.526327
1	-11.508409	-3.999504	4.381676	6	9.144625	5.466071	4.296805
1	-13.819363	-3.857679	3.470734	6	11.704051	4.258267	3.346407
1	-12.377579	-5.179418	-0.358606	6	12.993885	4.178947	2.844649
1	-10.101675	-5.345796	0.554650	6	13.256155	4.501479	1.503520
1	-8.093276	-7.752962	9.782294	6	12.203403	4.914393	0.677149
1	-6.975288	-6.843148	8.731904	6	10.910789	5.009143	1.194669
1	-8.469065	-6.067629	9.336501	6	9.728977	6.728545	4.495704
1	-15.958721	-4.537168	-0.326578	6	9.584906	7.390207	5.705423
1	-14.356936	-4.055931	-0.945866	6	8.840261	6.813575	6.746760
1	-14.660418	-5.751827	-0.465575	6	8.250291	5.557604	6.556535
1	-7.454469	-1.646094	0.288371	6	8.414821	4.890065	5.342158
6	1.017988	7.467836	-1.557393	6	14.884932	4.703043	-0.234077
6	0.199462	8.616650	-1.648791	6	8.029551	7.010048	8.986584
6	0.703645	9.839085	-2.051165	8	14.554084	4.381750	1.109416
6	2.068107	9.983313	-2.393050	8	8.753670	7.549025	7.889682
6	2.894390	8.839634	-2.307655	1	6.781549	5.635988	3.139292
6	2.379078	7.622624	-1.901056	1	9.365307	2.638138	1.444826
7	2.582128	11.215094	-2.802028	1	7.454469	1.646094	0.288371
6	3.719655	11.288626	-3.663671	1	11.508409	3.999504	4.381676
6	1.984716	12.441183	-2.374969	1	13.819363	3.857679	3.470734
6	4.792746	12.138807	-3.346981	1	12.377579	5.179418	-0.358606
6	5.886857	12.235287	-4.192042	1	10.101675	5.345796	0.554650
6	5.942515	11.476464	-5.372875	1	10.300359	7.183702	3.693553
6	4.877805	10.624608	-5.694960	1	10.033464	8.364437	5.867684
6	3.773244	10.543784	-4.846659	1	7.679216	5.083498	7.345466
6	1.685459	13.445444	-3.311223	1	7.970123	3.909589	5.206299
6	1.128904	14.646360	-2.900912	1	15.958721	4.537168	-0.326578
6	0.846549	14.872489	-1.543483	1	14.356936	4.055931	-0.945866
6	1.140184	13.875588	-0.603684	1	14.660418	5.751827	-0.465575
6	1.714325	12.675062	-1.022519	1	8.093276	7.752962	9.782294
6	7.170267	10.916879	-7.346274	1	6.975288	6.843148	8.731904
6	-0.005229	16.375950	0.108674	1	8.469065	6.067629	9.336501
8	7.061838	11.640731	-6.127626	1	4.877346	4.662960	1.957019
8	0.295886	16.080104	-1.248887				
1	0.041297	10.692955	-2.129579				
1	3.948770	8.924654	-2.542059				
1	3.054706	6.776563	-1.814615				
1	4.759031	12.723644	-2.433870				
1	6.720520	12.887980	-3.956588				
1	4.888209	10.036878	-6.604667				

E = -7144.7978336 au; all frequencies positive

8. Energies and coordinates of the optimized structures in solution (CH_2Cl_2).

TbT (Neutral)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.869500	2.127172	0.000000
16	0.869500	1.905656	0.000000
6	0.674716	0.168970	0.000000
6	-0.674716	-0.168970	0.000000
6	-1.561470	0.948742	0.000000
6	1.561470	-0.948742	0.000000
6	0.869500	-2.127172	0.000000
16	-0.869500	-1.905656	0.000000
1	2.642763	-0.887429	0.000000
1	1.271063	-3.131032	0.000000
1	-2.642763	0.887429	0.000000
1	-1.271063	3.131032	0.000000

E = -1027.4123997 au; all frequencies positive

exTbT (Neutral)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.005615	2.313793	0.025650
16	1.526697	1.425572	0.060441
6	0.685648	-0.099186	0.107603
6	-0.685648	0.099186	0.107603
6	-1.105442	1.466068	0.044397
6	1.105442	-1.466068	0.044397
6	0.005615	-2.313793	0.025650
16	-1.526697	-1.425572	0.060441
6	-0.060902	-3.767373	0.059385
6	0.060902	3.767373	0.059385
6	-2.518326	1.854300	-0.042412
6	2.518326	-1.854300	-0.042412
6	-0.918040	-4.589401	-0.641240
6	-0.781716	-5.968165	-0.312162
6	0.171863	-6.193163	0.643463
16	0.918040	-4.719147	1.167509
16	3.115510	-2.912489	-1.307935
6	4.748847	-2.747678	-0.750075
6	4.831156	-1.918223	0.334534
6	3.562243	-1.403369	0.733119
6	0.918040	4.589401	-0.641240
6	0.781716	5.968165	-0.312162
6	-0.171863	6.193163	0.643463
16	-0.918040	4.719147	1.167509
16	-3.115510	2.912489	-1.307935
6	-4.748847	2.747678	-0.750075
6	-4.831156	1.918223	0.334534
6	-3.562243	1.403369	0.733119
1	-1.610962	-4.211511	-1.384490
1	-1.360792	-6.758296	-0.775526
1	0.491962	-7.136179	1.064803
1	5.545694	-3.275996	-1.255045
1	5.761713	-1.684186	0.838319
1	3.419238	-0.739357	1.578123
1	1.610962	4.211511	-1.384490
1	1.360792	6.758296	-0.775526
1	-0.491962	7.136179	1.064803
1	-5.545694	3.275996	-1.255045
1	-5.761713	1.684186	0.838319
1	-3.419238	0.739357	1.578123

E = -3234.6755146 au; all frequencies positive

TbT-1 (Neutral)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.620494	-0.307744	-0.206690
6	-0.620494	0.307744	-0.206690
16	-1.885632	-0.891937	-0.143670
6	-0.698405	-2.212446	-0.107534
6	0.606333	-1.739446	-0.132641
6	-1.212172	-3.588265	-0.146163
6	-0.604243	-4.583207	-0.937141
6	-1.124955	-5.868028	-1.013964
6	-2.286422	-6.222972	-0.299192
6	-2.898347	-5.235646	0.495850
6	-2.371699	-3.952023	0.564864
1	0.273710	-4.335474	-1.523844
1	-0.642680	-6.602825	-1.649047
1	-3.785713	-5.481764	1.068090
1	-2.858000	-3.221608	1.205381
6	-0.606333	1.739446	-0.132641
16	1.885632	0.891937	-0.143670
6	0.698405	2.212446	-0.107534
6	1.842833	-2.547857	-0.024368
6	1.990862	-3.545629	0.954740
6	3.176027	-4.257706	1.093131
6	4.272467	-4.006953	0.244548
6	4.127156	-3.017999	-0.745781
6	2.940919	-2.301503	-0.866456
1	1.171106	-3.747551	1.636807
1	3.263549	-5.004612	1.874288
1	4.947791	-2.812866	-1.424054
1	2.858383	-1.554625	-1.650718
6	-1.842833	2.547857	-0.024368
6	-2.940919	2.301503	-0.866456
6	-4.127156	3.017999	-0.745781
6	-4.272467	4.006953	0.244548
6	-3.176027	4.257706	1.093131
6	-1.990862	3.545629	0.954740
1	-2.858383	1.554625	-1.650718
1	-4.947791	2.812866	-1.424054
1	-3.263549	5.004612	1.874288
1	-1.171106	3.747551	1.636807
6	1.212172	3.588265	-0.146163
6	2.371699	3.952023	0.564864
6	2.898347	5.235646	0.495850
6	2.286422	6.222972	-0.299192
6	1.124955	5.868028	-1.013964
6	0.604243	4.583207	-0.937141
1	2.858000	3.221608	1.205381
1	3.785713	5.481764	1.068090
1	0.642680	6.602825	-1.649047
1	-0.273710	4.335474	-1.523844
7	2.825851	7.521771	-0.381629
6	1.985521	8.655363	-0.587788
6	4.234897	7.729077	-0.281165
6	2.318922	9.622111	-1.551940
6	1.522724	10.744156	-1.735779
6	0.357573	10.921950	-0.974274
6	0.008364	9.958867	-0.019663
6	0.827833	8.844831	0.175497
6	4.750773	8.705944	0.587566
6	6.118593	8.928672	0.670915
6	7.011468	8.165685	-0.098113
6	6.508715	7.183597	-0.961261
6	5.130145	6.981853	-1.055175
6	-1.540695	12.295373	-0.483003
6	9.283662	7.711091	-0.695910
8	-0.357573	12.055928	-1.237707
8	8.336239	8.454674	0.065321
1	3.212146	9.490317	-2.153534
1	1.780802	11.493518	-2.476997
1	-0.881219	10.069839	0.588471
1	4.070590	9.293869	1.195635
1	6.519118	9.684228	1.339468
1	7.171316	6.583703	-1.573770
1	4.747559	6.229703	-1.737959
1	-1.942537	13.241915	-0.845493
1	-2.283437	11.504027	-0.639579
1	10.263900	8.098154	-0.416060
1	9.236008	6.640969	-0.461502
1	9.132906	7.851376	-1.772879
1	0.560137	8.113400	0.930810
7	-5.481334	4.718598	0.386529
6	-6.729846	4.104743	0.066137
6	-5.490606	6.058908	0.874985
6	-7.665863	4.777084	-0.738159
6	-8.892781	4.198173	-1.034057
6	-9.210390	2.919515	-0.550278
6	-8.281919	2.236816	0.245402
6	-7.059748	2.836449	0.557285
6	-6.380240	6.438335	1.894965
6	-6.416648	7.747839	2.354273
6	-5.549179	8.713128	1.820604
6	-4.651358	8.344584	0.811017
6	-4.637000	7.029970	0.339059
6	-10.807045	1.139319	-0.443159
6	-4.808466	10.990823	1.841373
8	-10.436071	2.433936	-0.908146
8	-5.659093	9.968471	2.349334
1	-7.425783	5.761198	-1.127431
1	-9.617646	4.716605	-1.653587
1	-8.500903	1.252072	0.640064
1	-7.048173	5.698185	2.323098
1	-7.104787	8.042480	3.140108
1	-3.974978	9.068019	0.371922
1	-3.950257	6.758201	-0.456092
1	-11.803961	0.950941	-0.843070
1	-10.118351	0.368625	-0.809078
1	-10.843052	1.100057	0.651976
1	-5.066063	11.897026	2.390302
1	-3.751179	10.755244	2.010495
1	-4.974349	11.157144	0.770723
1	-6.352531	2.306685	1.187329
7	-2.825851	-7.521771	-0.381629
6	-4.234897	-7.729077	-0.281165
6	-1.985521	-8.655363	-0.587788
6	-4.750773	-8.705944	0.587566
6	-6.118593	-8.928672	0.670915
6	-7.011468	-8.165685	-0.098113
6	-6.508715	-7.183597	-0.961261
6	-5.130145	-6.981853	-1.055175
6	-2.318922	-9.622111	-1.551940
6	-1.522724	-10.744156	-1.735779
6	-0.357573	-10.921950	-0.974274
6	-0.008364	-9.958867	-0.019663
6	-0.827833	-8.844831	0.175497
6	-9.283662	-7.711091	-0.695910
6	1.540695	-12.295373	-0.483003
8	-8.336239	-8.454674	0.065321
8	0.357573	-12.055928	-1.237707
1	-4.070590	-9.293869	1.195635
1	-6.519118	-9.684228	1.339468
1	-7.171316	-6.583703	-1.573770
1	-3.212146	-9.490317	-2.153534
1	-1.780802	-11.493518	-2.476997
1	0.881219	-10.069839	0.588471
1	-0.560137	-8.113400	0.930810
1	-10.263900	-8.098154	-0.416060
1	-9.236008	-6.640969	-0.461502
1	-9.132906	-7.851376	-1.772879
1	1.942537	-13.241915	-0.845493
1	2.283437	-11.504027	-0.639579
1	1.324430	-12.380422	0.588366
1	-4.747559	-6.229703	-1.737959
7	5.481334	-4.718598	0.386529
6	5.490606	-6.058908	0.874985
6	6.729846	-4.104743	0.066137
6	6.380240	-6.438335	1.894965

6	6.416648	-7.747839	2.354273
6	5.549179	-8.713128	1.820604
6	4.651358	-8.344584	0.811017
6	4.637000	-7.029970	0.339059
6	7.665863	-4.777084	-0.738159
6	8.892781	-4.198173	-1.034057
6	9.210390	-2.919515	-0.550278
6	8.281919	-2.236816	0.245402
6	7.059748	-2.836449	0.557285
6	4.808466	-10.990823	1.841373
6	10.807045	-1.139319	-0.443159
8	5.659093	-9.968471	2.349334
8	10.436071	-2.433936	-0.908146
1	7.048173	-5.698185	2.323098
1	7.104787	-8.042480	3.140108
1	3.974978	-9.068019	0.371922
1	7.425783	-5.761198	-1.127431
1	9.617646	-4.716605	-1.653587
1	8.500903	-1.252072	0.640064
1	6.352531	-2.306685	1.187329
1	5.066063	-11.897026	2.390302
1	3.751179	-10.755244	2.010495
1	4.974349	-11.157144	0.770723
1	11.803961	-0.950941	-0.843070
1	10.118351	-0.368625	-0.809078
1	10.843052	-1.100057	0.651976
1	3.950257	-6.758201	-0.456092

E = -4937.7345803 au; all frequencies positive

TbT-1 (Radical Cation)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.624220	-0.309968	-0.276772
6	-0.624179	0.310107	-0.276787
16	-1.896189	-0.883728	-0.214236
6	-0.711554	-2.203904	-0.192983
6	0.612308	-1.726239	-0.202889
6	-1.205388	-3.566212	-0.249043
6	-0.500300	-4.589045	-0.930095
6	-0.997630	-5.873950	-1.021153
6	-2.237956	-6.218140	-0.431134
6	-2.953144	-5.201882	0.246858
6	-2.449632	-3.918083	0.327328
1	0.430201	-4.351661	-1.430987
1	-0.446687	-6.620601	-1.580241
1	-3.893390	-5.439114	0.729422
1	-3.010489	-3.174726	0.885827
6	-0.612273	1.726381	-0.202928
16	1.896228	0.883874	-0.214209
6	0.711590	2.204045	-0.193017
6	1.834793	-2.536409	-0.050356
6	1.934552	-3.539046	0.933974
6	3.105698	-4.255590	1.121112
6	4.241636	-4.009896	0.318887
6	4.147475	-3.008475	-0.669763
6	2.973466	-2.286543	-0.839132
1	1.088137	-3.734910	1.583829
1	3.156194	-5.000960	1.906034
1	4.995726	-2.808512	-1.313776
1	2.928117	-1.540977	-1.627443
6	-1.834785	2.536519	-0.050387
6	-2.973437	2.286651	-0.839195
6	-4.147478	3.008526	-0.669797
6	-4.241693	4.009882	0.318911
6	-3.105767	4.255600	1.121142
6	-1.934589	3.539111	0.933981
1	-2.928036	1.541154	-1.627567
1	-4.995708	2.808583	-1.313844
1	-3.156289	5.000952	1.906081
1	-1.088176	3.735004	1.583828
6	1.205409	3.566356	-0.249055

6	2.449651	3.918218	0.327316
6	2.953155	5.202021	0.246874
6	2.237958	6.218288	-0.431089
6	0.997645	5.874103	-1.021139
6	0.500323	4.589192	-0.930110
1	3.010528	3.174840	0.885768
1	3.893414	5.439246	0.729418
1	0.446721	6.620759	-1.580240
1	-0.430153	4.351799	-1.431043
7	2.743085	7.511966	-0.520384
6	1.879528	8.635656	-0.707928
6	4.149037	7.760773	-0.436086
6	2.166364	9.584472	-1.703888
6	1.352950	10.694265	-1.871241
6	0.226434	10.880795	-1.052058
6	-0.068584	9.936362	-0.059136
6	0.762080	8.828563	0.112056
6	4.639932	8.742912	0.440244
6	5.999458	9.005649	0.508471
6	6.903867	8.287676	-0.292768
6	6.420730	7.306402	-1.169406
6	5.050473	7.056088	-1.241352
6	-1.648988	12.259235	-0.489234
6	9.181351	7.929544	-0.938963
8	-0.503907	12.001473	-1.298972
8	8.214908	8.618125	-0.146627
1	3.030274	9.444636	-2.344799
1	1.566476	11.430494	-2.638821
1	-0.923937	10.059291	0.593950
1	3.948876	9.295559	1.067816
1	6.387630	9.759786	1.184794
1	7.092940	6.746480	-1.807397
1	4.677975	6.308469	-1.934823
1	-2.064339	13.200199	-0.850019
1	-2.399701	11.467522	-0.595071
1	-1.376753	12.363297	0.567241
1	10.148556	8.346792	-0.658827
1	9.175689	6.853580	-0.730754
1	9.011232	8.093806	-2.009053
1	0.541087	8.111761	0.895929
7	-5.424262	4.738442	0.502489
6	-6.695716	4.178498	0.169173
6	-5.392727	6.060044	1.045132
6	-7.609162	4.909913	-0.608158
6	-8.857231	4.384895	-0.911865
6	-9.220107	3.106296	-0.458739
6	-8.313798	2.367247	0.312467
6	-7.067851	2.910738	0.629554
6	-6.223089	6.403738	2.124757
6	-6.209886	7.690696	2.643433
6	-5.354146	8.665192	2.105165
6	-4.520891	8.331249	1.029746
6	-4.554136	7.039312	0.502202
6	-10.888990	1.391984	-0.376380
6	-4.574649	10.926791	2.176843
8	-10.463905	2.678775	-0.818100
8	-5.408619	9.894010	2.693711
1	-7.334414	5.895056	-0.970522
1	-9.566297	4.946405	-1.511232
1	-8.568978	1.382441	0.683789
1	-6.879928	5.654293	2.553894
1	-6.848724	7.961258	3.477677
1	-3.858330	9.064327	0.585969
1	-3.917397	6.791011	-0.340709
1	-11.895675	1.256784	-0.772466
1	-10.237860	0.599407	-0.763382
1	-10.919303	1.332954	0.717874
1	-4.776466	11.808508	2.785457
1	-3.512716	10.665200	2.259392
1	-4.812423	11.147037	1.129458
1	-6.377917	2.339714	1.242253
7	-2.743055	-7.511825	-0.520450
6	-4.148998	-7.760692	-0.436126
6	-1.879465	-8.635478	-0.708048
6	-4.639830	-8.742846	0.440222
6	-5.999340	-9.005662	0.508457

6	-6.903795	-8.287758	-0.292792	6	-2.940287	-5.219455	0.293543
6	-6.420720	-7.306476	-1.169457	6	-2.431242	-3.941021	0.411915
6	-5.050477	-7.056082	-1.241409	1	0.382907	-4.298933	-1.469618
6	-2.166260	-9.584250	-1.704061	1	-0.506845	-6.559751	-1.688961
6	-1.352785	-10.693987	-1.871491	1	-3.861306	-5.479427	0.800856
6	-0.226249	-10.880501	-1.052332	1	-2.967297	-3.220782	1.022184
6	0.068719	-9.936120	-0.059345	6	-0.608274	1.731337	-0.119934
6	-0.762006	-8.828379	0.111923	16	1.894549	0.887485	-0.128997
6	-9.181310	-7.929774	-0.938973	6	0.712227	2.206359	-0.107769
6	1.649283	-12.258835	-0.489630	6	1.822138	-2.542632	0.035296
8	-8.214815	-8.618291	-0.146646	6	1.891119	-3.595784	0.974035
8	0.504167	-12.001111	-1.299332	6	3.056945	-4.313159	1.168610
1	-3.948736	-9.295448	1.067792	6	4.218617	-4.013819	0.420479
1	-6.387465	-9.759815	1.184789	6	4.157461	-2.967421	-0.526324
1	-7.092962	-6.746614	-1.807467	6	2.987994	-2.247298	-0.702837
1	-3.030182	-9.444418	-2.344959	1	1.025924	-3.819389	1.588043
1	-1.566276	-11.430178	-2.639117	1	3.092606	-5.086751	1.926394
1	0.924081	-10.059044	0.593731	1	5.024498	-2.743196	-1.136000
1	-0.541045	-8.111610	0.895835	1	2.962066	-1.472028	-1.461757
1	-10.148487	-8.347075	-0.658819	6	-1.822228	2.542737	0.035260
1	-9.175707	-6.853807	-0.730773	6	-2.988007	2.247501	-0.703010
1	-9.011201	-8.094032	-2.009064	6	-4.157457	2.967664	-0.526577
1	2.064739	-13.199709	-0.850526	6	-4.218690	4.013998	0.420287
1	2.399904	-11.467021	-0.595377	6	-3.057094	4.313243	1.168549
1	1.377062	-12.363052	0.566833	6	-1.891277	3.595832	0.974048
1	-4.679842	-6.308465	-1.934906	1	-2.962021	1.472284	-1.461975
7	5.424164	-4.738518	0.502445	1	-5.024426	2.743518	-1.136364
6	5.392581	-6.060098	1.045145	1	-3.092808	5.086786	1.926375
6	6.695640	-4.178684	0.169013	1	-1.026144	3.819366	1.588155
6	6.222957	-6.403775	2.124763	6	1.207089	3.569067	-0.193318
6	6.209712	-7.690705	2.643508	6	2.431218	3.941047	0.411863
6	5.353910	-8.665191	2.105318	6	2.940295	5.219464	0.293463
6	4.520646	-8.331266	1.029899	6	2.252037	6.203304	-0.456468
6	4.553933	-7.039357	0.502286	6	1.030478	5.838927	-1.072878
6	7.608939	-4.910163	-0.608431	6	0.526916	4.560235	-0.942460
6	8.857025	-4.385251	-0.912250	1	2.967294	3.220787	1.022090
6	9.220065	-3.106698	-0.459124	1	3.861362	5.479401	0.800711
6	8.313902	-2.367586	0.312192	1	0.506755	6.559858	-1.688862
6	7.067936	-2.910971	0.629388	1	-0.383044	4.299068	-1.469489
6	4.574305	-10.926761	2.177188	7	2.769717	7.488408	-0.592754
6	10.889115	-1.392541	-0.376894	6	1.916658	8.604350	-0.842981
8	5.408337	-9.893974	2.693946	6	4.175315	7.726034	-0.513256
8	10.463868	-2.679286	-0.818595	6	2.236076	9.519185	-1.862225
1	6.879839	-5.654336	2.553846	6	1.421225	10.613076	-2.100280
1	6.848558	-7.961251	3.477750	6	0.264354	10.820704	-1.327832
1	3.858045	-9.064339	0.586174	6	-0.056488	9.915269	-0.305395
1	7.334062	-5.895270	-0.970793	6	0.771236	8.819843	-0.066437
1	9.565980	-4.946807	-1.511706	6	4.667424	8.774190	0.284357
1	8.569205	-1.382811	0.683512	6	6.028336	9.022556	0.350212
1	6.378113	-2.339899	1.242168	6	6.933150	8.228527	-0.377505
1	4.776109	-11.808443	2.785857	6	6.447662	7.184026	-1.178130
1	3.512386	-10.665123	2.259759	6	5.076819	6.943978	-1.246077
1	4.812029	-11.147092	1.129810	6	-1.655058	12.187906	-0.903872
1	11.895757	-1.257408	-0.773114	6	9.214521	7.784952	-0.954223
1	10.237996	-0.599901	-0.763781	8	-0.467396	11.917716	-1.647629
1	10.919584	-1.333551	0.717357	8	8.243585	8.552308	-0.241269
1	3.917179	-6.791067	-0.340617	1	3.120746	9.359878	-2.468948

E = -4937.5722034 au; all frequencies positive

TbT-1 (Dication (Triplet))

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.622981	-0.306293	-0.200365
6	-0.623084	0.306378	-0.200374
16	-1.894649	-0.887410	-0.129050
6	-0.712323	-2.206280	-0.107803
6	0.608175	-1.731252	-0.119945
6	-1.207167	-3.568998	-0.193342
6	-0.527013	-4.560135	-0.942537
6	-1.030548	-5.838840	-1.072938
6	-2.252051	-6.203264	-0.456445
6	10.181811	8.213753	-0.693403
1	9.189436	6.731939	-0.652509
1	9.063764	7.858778	-2.036829
1	0.530677	8.132883	0.737908
7	-5.403920	4.729693	0.617387
6	-6.669705	4.110924	0.410434
6	-5.377664	6.087440	1.042877
6	-7.675392	4.785567	-0.306829
6	-8.911576	4.194074	-0.499791
6	-9.177193	2.912396	0.017347

Atomic Number	Coordinates (Angstroms)			
	X	Y	Z	
6	-8.180153	2.236551	0.738003	1
6	-6.940065	2.838591	0.933534	1
6	-6.241512	6.522081	2.066014	1
6	-6.234145	7.844944	2.471754	1
6	-5.363554	8.770947	1.867782	1
6	-4.501321	8.344929	0.845441	1
6	-4.516264	7.013566	0.437745	1
6	-10.753765	1.126507	0.264403	1
6	-4.589706	11.035186	1.763848	1
8	-10.416137	2.423347	-0.231292	1
8	-5.435636	10.039194	2.339868	1
1	-7.473898	5.767893	-0.719652	1
1	-9.689921	4.700515	-1.060093	1
1	-8.363428	1.257358	1.162141	1
1	-6.907271	5.812326	2.544336	1
1	-6.888741	8.187588	3.265681	1
1	-3.833755	9.040058	0.351776	1
1	-3.864419	6.694635	-0.368333	1
1	-11.778153	0.943147	-0.058491	1
1	-10.095763	0.357350	-0.154601	1
1	-10.705182	1.094754	1.358187	1
1	-4.815870	11.959709	2.294309	1
1	-3.531466	10.785867	1.901157	1
1	-4.800576	11.166267	0.696736	1
1	-6.180220	2.321734	1.509622	7
7	-2.769672	-7.488396	-0.592693	6
6	-4.175239	-7.726152	-0.513047	6
6	-1.916565	-8.604276	-0.843040	6
6	-4.667145	-8.774342	0.284634	6
6	-6.028014	-9.022885	0.350616	6
6	-6.932997	-8.229008	-0.377049	6
6	-6.447718	-7.184470	-1.177733	6
6	-5.076913	-6.944236	-1.245800	6
6	-2.235955	-9.519019	-1.862378	6
6	-1.421084	-10.612876	-2.100533	6
6	-0.264226	-10.820569	-1.328082	6
6	0.056593	-9.915220	-0.305559	6
6	-0.771143	-8.819819	-0.066512	6
6	-9.214474	-7.785820	-0.953646	6
6	1.655262	-12.187735	-0.904312	8
8	-8.243375	-8.552975	-0.240710	8
8	0.467521	-11.917566	-1.647953	1
1	-3.975963	-9.384581	0.855750	1
1	-6.418549	-9.823992	0.968759	1
1	-7.120693	-6.568424	-1.760563	1
1	-3.120620	-9.359664	-2.469096	1
1	-1.653528	-11.319409	-2.889928	1
1	0.930334	-10.062096	0.317271	1
1	-0.530607	-8.132931	0.737903	1
1	-10.181683	-8.214734	-0.692728	1
1	-9.189514	-6.732792	-0.652018	1
1	-9.063789	-7.859710	-2.036246	1
1	2.079780	-13.092071	-1.339629	1
1	2.376309	-11.366982	-0.993924	1
1	1.431753	-12.363409	0.153842	1
1	-4.704854	-6.148926	-1.882792	7
7	5.403839	-4.729509	0.617647	6
6	5.377548	-6.087266	1.043081	6
6	6.669648	-4.110751	0.410785	6
6	6.241323	-6.521960	2.066265	6
6	6.233918	-7.844840	2.471950	6
6	5.363367	-8.770816	1.867869	6
6	4.501207	-8.344745	0.845485	6
6	4.516177	-7.013364	0.437854	6
6	7.675347	-4.785399	-0.306458	6
6	8.911576	-4.193967	-0.499282	6
6	9.177233	-2.912351	0.017985	6
6	8.180170	-2.236489	0.738596	6
6	6.940027	-2.838463	0.933978	6
6	4.589481	-11.035037	1.763776	6
6	10.753954	-1.126633	0.265369	8
8	5.435417	-10.039090	2.339884	8
8	10.416238	-2.423382	-0.230492	1
1	6.907048	-5.812227	2.544670	1
1	6.888453	-8.187520	3.265915	1
1	3.833683	-9.039853	0.351732	6

E = -4937.3946665 au; all frequencies positive

TbT-1 (Trication (Quadruplet))

$E = -4937.2059575$ au; all frequencies positive

TbT-1 (Tetracation (Quintuplet))

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.623045	-0.306535	-0.163186
6	-0.623082	0.306471	-0.163167
16	-1.891255	-0.884411	-0.094340
6	-0.710522	-2.199528	-0.076203
6	0.599379	-1.734749	-0.108677
6	-1.218109	-3.575083	-0.123597
6	-0.644499	-4.533668	-0.985830
6	-1.169984	-5.812239	-1.084342
6	-2.293021	-6.174911	-0.315326
6	-2.865322	-5.233709	0.561078
6	-2.335378	-3.956422	0.647972
1	0.189902	-4.254802	-1.618602
1	-0.747299	-6.517938	-1.789870
1	-3.702768	-5.516883	1.187443
1	-2.773254	-3.251328	1.346447
6	-0.599408	1.734687	-0.108640
16	1.891225	0.884337	-0.094389
6	0.710500	2.199457	-0.076187
6	1.827164	-2.553087	-0.010403
6	1.975649	-3.527861	0.994542
6	3.163973	-4.228266	1.140938
6	4.240864	-3.973798	0.271248
6	4.097576	-3.020220	-0.752712
6	2.907573	-2.317965	-0.881715
1	1.167485	-3.703028	1.695608

1	3.279976	-4.936894	1.952783	1	-3.852178	8.941751	0.247045
1	4.908348	-2.848619	-1.450776	1	-3.821903	6.586450	-0.430733
1	2.804840	-1.596571	-1.685749	1	-11.571993	0.505961	-0.332844
6	-1.827183	2.553036	-0.010368	1	-9.856361	0.050016	-0.523539
6	-2.907590	2.317900	-0.881677	1	-10.470001	0.603265	1.067360
6	-4.097581	3.020184	-0.752713	1	-5.006146	11.881909	2.084912
6	-4.240858	3.973801	0.271209	1	-3.700650	10.705502	1.772261
6	-3.163975	4.228274	1.140909	1	-4.880300	11.107634	0.481993
6	-1.975662	3.527844	0.994547	1	-6.029347	2.143493	1.168403
1	-2.804865	1.596475	-1.685683	7	-2.854937	-7.467018	-0.431618
1	-4.908354	2.848557	-1.450768	6	-4.254046	-7.635212	-0.365238
1	-3.279983	4.936926	1.952733	6	-2.031611	-8.593461	-0.632495
1	-1.167509	3.703007	1.695627	6	-4.802682	-8.740643	0.325224
6	1.218108	3.575005	-0.123590	6	-6.169160	-8.908240	0.386905
6	2.335427	3.956315	0.647924	6	-7.031950	-7.986186	-0.245907
6	2.865392	5.233591	0.561016	6	-6.490391	-6.885324	-0.939415
6	2.293057	6.174822	-0.315340	6	-5.116477	-6.714078	-0.992478
6	1.169964	5.812178	-1.084299	6	-2.448777	-9.622097	-1.508941
6	0.644469	4.533615	-0.985781	6	-1.654415	-10.730705	-1.703273
1	2.773323	3.251206	1.346373	6	-0.422281	-10.854041	-1.025422
1	3.702863	5.516742	1.187359	6	0.000832	-9.832065	-0.152235
1	0.747261	6.517890	-1.789803	6	-0.797941	-8.714572	0.037590
1	-0.189972	4.254774	-1.618511	6	-9.294886	-7.352959	-0.725912
7	2.854971	7.466919	-0.431632	6	1.532211	-12.187194	-0.641788
6	2.031643	8.593371	-0.632481	8	-8.343398	-8.244823	-0.127895
6	4.254083	7.635130	-0.365283	8	0.267549	-11.976858	-1.281718
6	2.448761	9.621991	-1.508969	1	-4.147267	-9.438298	0.833360
6	1.654387	10.730594	-1.703280	1	-6.606044	-9.736987	0.932132
6	0.422291	10.853941	-1.025358	1	-7.131932	-6.178924	-1.450037
6	-0.000765	9.831989	-0.152120	1	-3.381451	-9.522509	-2.051419
6	0.798020	8.714499	0.037680	1	-1.950825	-11.517626	-2.387276
6	4.802711	8.740552	0.325204	1	0.934239	-9.915257	0.390813
6	6.169185	8.908190	0.386842	1	-0.486128	-7.944880	0.734359
6	7.031980	7.986188	-0.246043	1	-10.272668	-7.771827	-0.493748
6	6.490427	6.885333	-0.939568	1	-9.212038	-6.349681	-0.296817
6	5.116517	6.714048	-0.992588	1	-9.161357	-7.309257	-1.810882
6	-1.532205	12.187063	-0.641665	1	1.893211	-13.144328	-1.014826
6	9.294916	7.353053	-0.726174	1	2.240165	-11.396654	-0.909117
8	-0.267564	11.976743	-1.281644	1	1.417103	-12.234757	0.445423
8	8.343421	8.244864	-0.128079	1	-4.701834	-5.882813	-1.550650
1	3.381409	9.522392	-2.051490	7	5.470139	-4.658462	0.436773
1	1.950750	11.517499	-2.387322	6	5.484881	-6.012302	0.827238
1	-0.934136	9.915198	0.390988	6	6.687510	-3.979750	0.232703
1	4.147285	9.438158	0.833393	6	6.451285	-6.468325	1.753857
1	6.606065	9.736928	0.932085	6	6.468213	-7.790277	2.140986
1	7.131973	6.178973	-1.450239	6	5.530150	-8.702464	1.610521
1	4.701874	5.882783	-1.550762	6	4.567737	-8.255548	0.682696
1	-1.893231	13.144194	-1.014686	6	4.546011	-6.922610	0.302607
1	-2.240159	11.396515	-0.908975	6	7.771018	-4.638578	-0.394651
1	-1.417057	12.234618	0.445541	6	8.962924	-3.975839	-0.591896
1	10.272691	7.771969	-0.494070	6	9.117185	-2.638821	-0.162593
1	9.212144	6.349770	-0.297078	6	8.042704	-1.979281	0.467207
1	9.161309	7.309357	-1.811134	6	6.842974	-2.644402	0.657385
1	0.486249	7.944810	0.734473	6	4.742113	-10.966278	1.558201
7	-5.470122	4.658502	0.436706	6	10.553192	-0.724065	-0.016687
6	-6.687515	3.979838	0.232597	8	5.637057	-9.963871	2.056484
6	-5.484844	6.012330	0.827201	8	10.316398	-2.086539	-0.400271
6	-7.770996	4.638734	-0.394731	1	7.157599	-5.768371	2.184485
6	-8.962935	3.976057	-0.591992	1	7.187139	-8.150260	2.868024
6	-9.117250	2.639035	-0.162726	1	3.852217	-8.941699	0.246988
6	-8.042791	1.979419	0.467025	1	7.650630	-5.655081	-0.750612
6	-6.843030	2.644482	0.657228	1	9.793968	-4.459021	-1.092720
6	-6.451253	6.468327	1.753831	1	8.145816	-0.963105	0.824196
6	-6.468188	7.790268	2.140992	1	6.029272	-2.143476	1.168593
6	-5.530136	8.702474	1.610543	1	5.006136	-11.881908	2.084801
6	-4.567704	8.255583	0.682721	1	3.700639	-10.705499	1.772164
6	-4.545970	6.922652	0.302601	1	4.880315	-11.107578	0.481903
6	-10.553333	0.724330	-0.016896	1	11.571831	-0.505639	-0.332660
6	-4.742118	10.966293	1.558288	1	9.856170	-0.049746	-0.523254
8	-10.316502	2.086820	-0.400384	1	10.469895	-0.603092	1.067581
8	-5.637075	9.963874	2.056515	1	3.821961	-6.586392	-0.430735
1	-7.650561	5.655239	-0.750670				
1	-9.793958	4.459294	-1.092796				
1	-8.145938	0.963229	0.823965				
1	-7.157554	5.768351	2.184445				
1	-7.187112	8.150232	2.868042				

E = -4937.0123046 au; all frequencies positive

TbT-2 (Neutral)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.241405	-1.965322	0.517170
16	-2.054853	-0.381452	0.555645
6	-0.522213	0.452943	0.568641
6	0.522213	-0.452943	0.568641
6	0.146714	-1.829538	0.523916
6	-0.146714	1.829538	0.523916
6	1.241405	1.965322	0.517170
16	2.054853	0.381452	0.555645
6	2.067108	3.148826	0.538664
6	-2.067108	-3.148826	0.538664
6	1.128721	-2.925029	0.486756
6	-1.128721	2.925029	0.486756
6	3.422751	3.241359	0.289521
6	3.982248	4.523720	0.505665
6	3.048531	5.456259	0.913894
16	1.445779	4.728200	1.044085
16	-1.425086	3.852249	-0.985769
6	-2.756104	4.731477	-0.224133
6	-2.934589	4.310799	1.074438
6	-2.016338	3.297276	1.466061
6	-3.422751	-3.241359	0.289521
6	-3.982248	-4.523720	0.505665
6	-3.048531	-5.456259	0.913894
16	-1.445779	-4.728200	1.044085
16	1.425086	-3.852249	-0.985769
6	2.756104	-4.731477	-0.224133
6	2.934589	-4.310799	1.074438
6	2.016338	-3.297276	1.466061
1	4.015413	2.393003	-0.036038
1	5.026354	4.760237	0.348068
1	-3.692370	4.726881	1.726516
1	-2.017275	2.840681	2.449791
1	-4.015413	-2.393003	-0.036038
1	-5.026354	-4.760237	0.348068
1	3.692370	-4.726881	1.726516
1	2.017275	-2.840681	2.449791
7	-3.220724	-6.814997	1.126110
6	-4.277562	-7.527667	0.474547
6	-2.257229	-7.558348	1.880345
6	-5.057323	-8.434500	1.209959
6	-6.066890	-9.159839	0.592171
6	-6.334196	-8.983216	-0.774315
6	-5.564767	-8.075531	-1.513260
6	-4.538649	-7.363611	-0.889152
6	-1.599601	-8.653007	1.296130
6	-0.650851	-9.367903	2.013193
6	-0.326103	-8.994330	3.327210
6	-0.983454	-7.909694	3.920524
6	-1.950818	-7.207678	3.198364
6	-7.664653	-9.596707	-2.667357
6	0.992195	-9.425392	5.280789
8	-7.353904	-9.733770	-1.283503
8	0.641359	-9.743308	3.934820
1	-4.863674	-8.570197	2.268970
1	-6.671284	-9.863031	1.155786
1	-5.741992	-7.923696	-2.570909
1	-1.835345	-8.936611	0.275766
1	-0.137583	-10.213463	1.567426
1	-0.761949	-7.608290	4.936755
1	-2.466771	-6.374567	3.664322
1	-8.498123	-10.273829	-2.856188
1	-7.968304	-8.571840	-2.911274
1	-6.815978	-9.882010	-3.300033
1	1.761755	-10.142423	5.567092
1	1.394682	-8.409199	5.360462
1	0.132263	-9.529125	5.952162
1	-3.940455	-6.670904	-1.471231
7	3.406756	-5.767843	-0.887686
6	3.702658	-5.662336	-2.280158
6	3.290075	-8.713839	1.423511
6	-2.910184	7.569825	0.718485
6	-3.433664	6.735815	-3.146548
6	-3.722051	6.638751	-4.500325
6	-4.269154	5.458663	-5.029050
6	-4.534129	4.381698	-4.174808
6	-4.262529	4.494954	-2.809615
6	-4.171224	11.052603	2.764202
6	-5.057323	4.288236	-6.962015
8	-5.033778	10.383627	1.849587

8	-4.504312	5.462041	-6.374006	6	-6.645937	-7.881948	-1.719518
1	-5.766537	7.018893	-1.034828	8	2.990038	-11.935807	-0.413460
1	-6.432462	9.076820	0.183934	8	-5.820753	-8.463501	-0.706456
1	-2.585520	9.164966	2.112331	1	-0.366785	-9.492903	-2.115987
1	-2.997979	7.647152	-2.750739	1	1.124745	-11.481252	-2.064847
1	-3.515925	7.464972	-5.172953	1	3.131755	-9.873497	1.387844
1	-4.962662	3.461026	-4.551441	1	-1.787678	-9.001553	1.190334
1	-4.487891	3.663126	-2.150296	1	-4.229179	-9.438111	1.008573
1	-4.734088	11.909160	3.136637	1	-4.437222	-6.800367	-2.387953
1	-3.897246	10.405006	3.605427	1	-2.018759	-6.401726	-2.226306
1	-3.256909	11.404893	2.272533	1	4.496519	-13.066255	0.313108
1	-5.154493	4.502725	-8.026670	1	4.761667	-11.313362	0.509261
1	-4.398990	3.422175	-6.825586	1	3.606137	-12.170422	1.572185
1	-6.046064	4.058366	-6.547534	1	-7.639229	-8.304999	-1.569666
1	-1.917551	7.159390	0.869875	1	-6.695323	-6.793503	-1.610923

E = -6220.7339793 au; all frequencies positive

TbT-2 (Radical Cation)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.402613	-2.288575	0.148429
16	-1.264511	-1.669603	0.171495
6	-0.697270	-0.017133	0.153429
6	0.697286	0.017246	0.153473
6	1.356266	-1.236491	0.210787
6	-1.356241	1.236631	0.210421
6	-0.402529	2.288695	0.147813
16	1.264589	1.669694	0.171142
6	-0.591504	3.690209	-0.021848
6	0.591630	-3.690163	-0.020763
6	2.791713	-1.399014	0.387244
6	-2.791640	1.399278	0.386818
6	-1.693718	4.391896	-0.519692
6	-1.477084	5.757339	-0.720056
6	-0.186510	6.168006	-0.379446
16	0.759353	4.812927	0.232142
16	-3.927479	0.231640	-0.288494
6	-5.281308	0.966209	0.573914
6	-4.860303	2.077808	1.278397
6	-3.470005	2.311158	1.173324
6	1.693963	-4.391994	-0.518079
6	1.477366	-5.757507	-0.718133
6	0.186703	-6.168057	-0.377796
16	-0.759305	-4.812797	0.233173
16	3.927525	-0.232025	-0.289172
6	5.281401	-0.965895	0.573799
6	4.860403	-2.076846	1.279247
6	3.470067	-2.310260	1.174457
1	-2.621572	3.900665	-0.778467
1	-2.216596	6.433940	-1.126699
1	-5.531829	2.679489	1.877823
1	-2.963484	3.099631	1.716469
1	2.621915	-3.900865	-0.776689
1	2.216999	-6.434226	-1.124355
1	5.531963	-2.678041	1.879130
1	2.963543	-3.098271	1.718275
7	-0.329705	-7.432755	-0.412188
6	0.547075	-8.569343	-0.392566
6	-1.744516	-7.659234	-0.499160
6	0.398592	-9.581999	-1.352522
6	1.227834	-10.692982	-1.326852
6	2.227876	-10.812113	-0.346557
6	2.377823	-9.802181	0.613943
6	1.532956	-8.692441	0.590045
6	-2.371886	-8.524328	0.410726
6	-3.732974	-8.770335	0.312536
6	-4.497093	-8.152410	-0.692973
6	-3.874069	-7.284259	-1.600089
6	-2.501851	-7.052781	-1.505432
6	4.018997	-12.117722	0.558485

1	-4.761881	11.313460	0.504975	1	-2.874496	3.207152	1.754483
1	-3.606589	12.170822	1.567911	1	2.665572	-3.819323	-0.714193
1	2.019584	6.401272	-2.227286	1	2.279528	-6.296796	-1.302687
7	-6.560164	0.457956	0.430422	1	5.416914	-2.815471	2.091490
6	-7.682712	1.337994	0.345783	1	2.873756	-3.207130	1.755707
6	-6.762633	-0.959366	0.456471	7	-0.303984	-7.324129	-0.827632
6	-8.856599	1.059823	1.065170	6	0.569590	-8.460000	-0.952319
6	-9.955534	1.902390	0.970958	6	-1.725033	-7.549457	-0.897721
6	-9.904825	3.053264	0.169137	6	0.396325	-9.350957	-2.022526
6	-8.734504	3.340491	-0.545143	6	1.219283	-10.458650	-2.137373
6	-7.639232	2.479758	-0.461047	6	2.228111	-10.699165	-1.186044
6	-7.523027	-1.591504	-0.540061	6	2.395370	-9.811706	-0.112791
6	-7.707498	-2.967103	-0.513257	6	1.562123	-8.700066	0.001369
6	-7.125160	-3.743449	0.502334	6	-2.325881	-8.472869	-0.029240
6	-6.368073	-3.117680	1.500831	6	-3.688771	-8.708301	-0.109414
6	-6.200801	-1.733003	1.476322	6	-4.473739	-8.030319	-1.060581
6	-11.040055	4.993339	-0.653529	6	-3.870087	-7.112109	-1.932683
6	-6.817025	-5.912751	1.467718	6	-2.497727	-6.882527	-1.852207
8	-11.034129	3.818249	0.152607	6	4.007846	-12.124597	-0.454772
8	-7.350151	-5.086963	0.432080	6	-6.646297	-7.697340	-2.016805
1	-8.904544	0.179660	1.697196	8	2.975620	-11.809946	-1.391749
1	-10.864860	1.691433	1.524060	8	-5.794098	-8.336458	-1.060170
1	-8.667120	4.216315	-1.178741	1	-0.377066	-9.168048	-2.760475
1	-7.965860	-0.999633	-1.334385	1	1.104240	-11.154308	-2.961285
1	-8.291695	-3.464310	-1.280552	1	3.152510	-9.982522	0.641766
1	-5.917932	-3.688648	2.303097	1	-1.723050	-8.996955	0.704482
1	-5.624973	-1.249503	2.258831	1	-4.171467	-9.415587	0.555941
1	-12.023283	5.444640	-0.518564	1	-4.449803	-6.587956	-2.681558
1	-10.268574	5.703618	-0.333694	1	-2.028168	-6.192243	-2.545082
1	-10.893801	4.754117	-1.713382	1	4.465080	-13.045344	-0.815762
1	-7.089208	-6.934745	1.207319	1	4.763986	-11.332947	-0.415720
1	-5.725029	-5.836377	1.516948	1	3.597244	-12.289649	0.547200
1	-7.244736	-5.651871	2.442447	1	-7.635372	-8.127768	-1.862769
1	-6.742225	2.702352	-1.029152	1	-6.688851	-6.617014	-1.844745
1	-6.315723	-7.902344	-3.040262	1	1.678357	-8.027431	0.844443
1	6.516816	-0.490979	0.876489	7	6.720712	0.926538	0.769658
6	7.653344	-1.352787	1.003290	6	7.509786	1.453569	-0.263701
6	7.700379	2.824306	-0.363346	6	7.102446	3.694592	0.564385
6	6.322245	3.169842	1.604018	6	6.142452	1.790793	1.703426
6	8.704751	-1.001706	1.865125	6	9.820173	-1.818034	1.975050
6	9.907385	-3.009112	1.234917	6	8.858973	-3.364091	0.374936
6	7.745632	-2.532085	0.257608	6	6.800515	5.946356	1.320550
6	6.1193245	-4.952450	0.684895	6	7.337186	5.021158	0.372900
8	7.337186	5.021158	0.372900	8	11.039664	-3.739390	1.419971
1	7.967452	0.785566	-0.985846	1	8.304429	3.245808	-1.159654
1	5.864686	3.816178	2.342190	1	8.643033	-0.088259	2.446530
1	8.643033	-0.088259	2.446530	1	10.637153	-1.555943	2.638801
1	8.903752	-4.269711	-0.216989	1	6.946724	-2.803310	-0.424220
1	7.090721	6.936000	0.970740	1	5.707265	5.887061	1.359497
1	7.212170	5.771309	2.320549	1	12.157426	-5.362935	0.984625
1	10.401718	-5.670444	0.928103	1	11.197327	-4.767305	-0.395221
1	5.550227	1.383571	2.516409	7	0.304338	7.324092	-0.827451
6	1.725418	7.549432	-0.896832	6	-0.569181	8.459944	-0.952715
6	2.325796	8.472994	-0.028186	6	3.688725	8.708437	-0.107687
6	4.474199	8.030313	-1.058336	6	3.871017	7.111947	-1.930599
6	2.498620	6.882363	-1.850806	6	-0.395410	9.350745	-2.022971

E = -6220.5794458 au; all frequencies positive

TbT-2 (Dication (Singlet))

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.388216	-2.289886	0.200456
16	-1.275127	-1.670939	0.274806
6	-0.700050	-0.016170	0.247716
6	0.699918	0.016156	0.248040
6	1.359909	-1.224583	0.313408
6	-1.360068	1.224568	0.312862
6	-0.388317	2.289872	0.200388
16	1.274992	1.670924	0.275485
6	-0.581475	3.654197	-0.057673
6	0.581479	-3.654212	-0.057533
6	2.772591	-1.410596	0.537251
6	-2.772837	1.410597	0.536093
6	-1.725394	4.327004	-0.551364
6	-1.523463	5.652701	-0.875639
6	-0.198329	6.086798	-0.642661
16	0.790851	4.784121	0.002154
16	-3.943837	0.190237	0.030398
6	-5.244437	0.999630	0.902023
6	-4.783053	2.169334	1.497582
6	-3.410721	2.385839	1.295207
6	1.725636	-4.327042	-0.550632
6	1.523854	-5.652745	-0.874983
6	0.198600	-6.086823	-0.642668
16	-0.790903	-4.784106	0.001572
16	3.943779	-0.190210	0.032061
6	5.244024	-0.999569	0.904252
6	4.782405	-2.169268	1.499626
6	3.410160	-2.385808	1.296658
1	-2.665233	3.819260	-0.715411
1	-2.278920	6.296733	-1.303756
1	-5.417801	2.815549	2.089174

6	-1.218290	10.458438	-2.138353	6	3.389091	3.267179	0.472759
6	-2.227545	10.699114	-1.187516	6	3.875029	4.513008	0.814012
6	-2.395322	9.811800	-0.114224	6	2.848979	5.421088	1.165414
6	-1.562154	8.700156	0.000474	16	1.261323	4.673612	1.052100
6	6.647236	7.697221	-2.013415	16	-1.131489	3.925082	-1.280115
6	-4.007509	12.124752	-0.457203	6	-2.593801	4.741134	-0.739609
8	5.794556	8.336461	-1.057289	6	-3.071509	4.193812	0.450056
8	-2.974917	11.809893	-1.393706	6	-2.275071	3.138020	0.920326
1	1.722565	8.997183	0.705134	6	-3.388419	-3.267636	0.482802
1	4.171062	9.415834	0.557808	6	-3.873767	-4.513331	0.825558
1	4.451138	6.587667	-2.679071	6	-2.847110	-5.421430	1.174908
1	0.378318	9.167711	-2.760535	16	-1.259585	-4.674176	1.057673
1	-1.102855	11.153978	-2.962308	16	1.129614	-3.925449	-1.279959
1	-3.152801	9.982735	0.639964	6	2.592658	-4.741504	-0.741535
1	-1.678799	8.027637	0.843582	6	3.071811	-4.194615	0.447682
1	7.636239	8.127649	-1.858920	6	2.275897	-3.138912	0.919214
1	6.689675	6.616915	-1.841214	1	4.034995	2.444484	0.186910
1	6.317187	7.902111	-3.037066	1	4.923423	4.775514	0.835648
1	-4.464531	13.045477	-0.818517	1	-3.967185	4.549406	0.941826
1	-4.763720	11.333161	-0.418343	1	-2.484001	2.592073	1.832672
1	-3.597309	12.289928	0.544913	1	-4.034843	-2.444969	0.198071
1	2.029434	6.191958	-2.543813	1	-4.922151	-4.775670	0.849549
7	-6.517211	0.491042	0.873731	1	3.968178	-4.550226	0.938187
6	-7.653810	1.352799	1.000250	1	2.485937	-2.593054	1.831349
6	-6.721037	-0.926474	0.766636	7	-2.971334	-6.720675	1.517702
6	-8.705551	1.001523	1.861595	6	-4.164531	-7.463011	1.224355
6	-9.821034	1.817807	1.971239	6	-1.866782	-7.412703	2.131187
6	-9.907980	3.009029	1.231309	6	-4.737775	-8.267386	2.222070
6	-8.859242	3.364196	0.371802	6	-5.874277	-9.006655	1.943544
6	-7.745835	2.532237	0.254753	6	-6.459771	-8.959777	0.664110
6	-7.509470	-1.453398	-0.267264	6	-5.880605	-8.162719	-0.335000
6	-7.699979	-2.824127	-0.367179	6	-4.733835	-7.423814	-0.052323
6	-7.102602	-3.694503	0.560828	6	-1.305597	-8.529614	1.493645
6	-6.323051	-3.169857	1.601001	6	-0.224296	-9.178052	2.067956
6	-6.143335	-1.790816	1.700666	6	0.306179	-8.728466	3.291615
6	-11.193643	4.952478	0.681215	6	-0.274364	-7.629674	3.941956
6	-6.801201	-5.946339	1.316992	6	-1.359361	-6.977779	3.358702
8	-11.040347	3.739247	1.416069	6	-8.212417	-9.725710	-0.777933
8	-7.337188	-5.021050	0.369043	6	1.917548	-9.066150	5.035705
1	-8.644048	0.087962	2.442846	8	-7.566995	-9.719552	0.497995
1	-10.638270	1.555569	2.634616	8	1.378344	-9.417847	3.756883
1	-8.903810	4.269926	-0.219971	1	-4.294116	-8.303092	3.210894
1	-7.966701	-0.785321	-0.989617	1	-6.334457	-9.627710	2.704027
1	-8.303536	-3.245554	-1.163900	1	-6.299588	-8.123978	-1.332283
1	-5.865934	-3.816267	2.339384	1	-1.711888	-8.874836	0.549205
1	-5.551605	-1.383671	2.514049	1	0.231186	-10.035370	1.584888
1	-12.157937	5.362893	0.980666	1	0.100110	-7.281289	4.895723
1	-10.402207	5.670411	0.924894	1	-1.816249	-6.135035	3.866656
1	-11.197313	4.767583	-0.398944	1	-9.067084	-10.393275	-0.673536
1	-7.091189	-6.935944	0.966897	1	-8.562312	-8.724117	-1.050085
1	-5.707978	-5.887076	1.356703	1	-7.544799	-10.107048	-1.558023
1	-7.213544	-5.771356	2.316719	1	2.734268	-9.764702	5.214010
1	-6.946671	2.803610	-0.426715	1	2.305474	-8.041983	5.034880

E = -6220.4080366 au; all frequencies positive

TbT-2 (Trication (Doblet))

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.231399	-1.966518	0.354430
16	-2.067860	-0.389173	0.355678
6	-0.538043	0.449933	0.404135
6	0.538486	-0.450388	0.403152
6	0.188762	-1.804824	0.309243
6	-0.188584	1.804293	0.307756
6	1.231817	1.965922	0.349408
16	2.068262	0.388544	0.349558
6	1.981545	3.138343	0.528640
6	-1.980823	-3.138916	0.535630
6	1.160684	-2.875674	0.134753
6	-1.160666	2.874981	0.134553
6	3.389091	3.267179	0.472759
6	3.875029	4.513008	0.814012
6	2.848979	5.421088	1.165414
16	1.261323	4.673612	1.052100
16	-1.131489	3.925082	-1.280115
6	-2.593801	4.741134	-0.739609
6	-3.071509	4.193812	0.450056
6	-2.275071	3.138020	0.920326
6	-3.388419	-3.267636	0.482802
6	-3.873767	-4.513331	0.825558
6	-2.847110	-5.421430	1.174908
16	-1.259585	-4.674176	1.057673
16	1.129614	-3.925449	-1.279959
6	2.592658	-4.741504	-0.741535
6	3.071811	-4.194615	0.447682
6	2.275897	-3.138912	0.919214
1	4.034995	2.444484	0.186910
1	4.923423	4.775514	0.835648
1	-3.967185	4.549406	0.941826
1	-2.484001	2.592073	1.832672
1	-4.034843	-2.444969	0.198071
1	-4.922151	-4.775670	0.849549
1	3.968178	-4.550226	0.938187
1	2.485937	-2.593054	1.831349
7	-2.971334	-6.720675	1.517702
6	-4.164531	-7.463011	1.224355
6	-1.866782	-7.412703	2.131187
6	-4.737775	-8.267386	2.222070
6	-5.874277	-9.006655	1.943544
6	-6.459771	-8.959777	0.664110
6	-5.880605	-8.162719	-0.335000
6	-4.733835	-7.423814	-0.052323
6	-1.305597	-8.529614	1.493645
6	-0.224296	-9.178052	2.067956
6	0.306179	-8.728466	3.291615
6	-0.274364	-7.629674	3.941956
6	-1.359361	-6.977779	3.358702
6	-8.212417	-9.725710	-0.777933
6	1.917548	-9.066150	5.035705
8	-7.566995	-9.719552	0.497995
8	1.378344	-9.417847	3.756883
1	-4.294116	-8.303092	3.210894
1	-6.334457	-9.627710	2.704027
1	-6.299588	-8.123978	-1.332283
1	-1.711888	-8.874836	0.549205
1	0.231186	-10.035370	1.584888
1	0.100110	-7.281289	4.895723
1	-1.816249	-6.135035	3.866656
1	-9.067084	-10.393275	-0.673536
1	-8.562312	-8.724117	-1.050085
1	-7.544799	-10.107048	-1.558023
1	2.734268	-9.764702	5.214010
1	2.305474	-8.041983	5.034880
1	1.164962	-9.174678	5.823276
1	-4.273987	-6.830204	-0.835127
7	3.106991	-5.821812	-1.420046
6	2.961220	-5.936233	-2.830644
6	3.755663	-6.864156	-0.698678
6	2.590285	-7.170109	-3.401039
6	2.450769	-7.283051	-4.770726
6	2.682667	-6.171617	-5.606658
6	3.061822	-4.942251	-5.040455
6	3.201944	-4.831668	-3.662157
6	4.961129	-7.408237	-1.182025
6	5.572497	-8.442300	-0.499012
6	4.992385	-8.963946	0.675825
6	3.785775	-8.425822	1.157209
6	3.177901	-7.382062	0.470701
6	2.745363	-5.312647	-7.842867
6	5.137369	-10.558693	2.456872
8	2.519202	-6.390151	-6.927272
8	5.663800	-9.977888	1.258301
1	2.397576	-8.024416	-2.762066
1	2.152176	-8.221194	-5.224907
1	3.266948	-4.080861	-5.662881
1	5.414362	-7.004655	-2.080589

1 6.507581 -8.865270 -0.848548
 1 3.302240 -8.828745 2.038626
 1 2.231965 -6.988851 0.825184
 1 2.539773 -5.719540 -8.832021
 1 2.068271 -4.475972 -7.642394
 1 3.783731 -4.968427 -7.797133
 1 5.835650 -11.347892 2.732339
 1 5.084021 -9.817911 3.261432
 1 4.145666 -10.988747 2.284319
 1 3.529864 -3.892148 -3.231272
 7 2.973678 6.720406 1.507556
 6 1.870162 7.412136 2.123281
 6 4.165869 7.463128 1.211158
 6 1.306303 8.527887 1.486082
 6 0.225747 9.175729 2.062458
 6 -0.301251 8.726712 3.287829
 6 0.282060 7.629156 3.937796
 6 1.366269 6.977820 3.352463
 6 4.741092 8.268101 2.207248
 6 5.876591 9.007791 1.925781
 6 6.459056 8.960754 0.644968
 6 5.877900 8.163088 -0.352504
 6 4.732135 7.423764 -0.066865
 6 -1.909099 9.063849 5.035248
 6 8.207872 9.727010 -0.801520
 8 -1.372998 9.415372 3.755066
 8 7.565488 9.721032 0.475943
 1 1.709894 8.872599 0.540302
 1 -0.231860 10.032104 1.579730
 1 -0.089714 7.281280 4.892806
 1 4.299750 8.303921 3.197106
 1 6.338285 9.629329 2.684947
 1 6.294525 8.124241 -1.350775
 1 4.270617 6.829770 -0.848400
 1 -2.726212 9.761604 5.214893
 1 -2.295889 8.039252 5.035827
 1 -1.154958 9.173660 5.821148
 1 9.062173 10.395416 -0.699562
 1 8.558026 8.725561 -1.073867
 1 7.538049 10.107239 -1.580258
 1 1.825300 6.135984 3.860007
 7 -3.108730 5.821683 -1.417013
 6 -3.757390 6.863454 -0.694535
 6 -2.963365 5.937413 -2.827653
 6 -4.963635 7.406941 -1.176423
 6 -5.575007 8.440399 -0.492387
 6 -4.994133 8.961879 0.682093
 6 -3.786671 8.424432 1.161949
 6 -3.178744 7.381360 0.474331
 6 -2.591940 7.171577 -3.396984
 6 -2.452923 7.285803 -4.766659
 6 -2.685769 6.175359 -5.603582
 6 -3.065391 4.945702 -5.038437
 6 -3.205090 4.833873 -3.660145
 6 -5.139053 10.554708 2.464819
 6 -2.750070 5.318608 -7.840568
 8 -5.665744 9.975101 1.265840
 8 -2.522691 6.395093 -6.924140
 1 -5.417432 7.003505 -2.074774
 1 -6.510686 8.862924 -0.840881
 1 -3.302434 8.827329 2.042993
 1 -2.398626 8.025192 -2.757260
 1 -2.154065 8.224257 -5.220031
 1 -3.271204 4.085004 -5.661592
 1 -3.533317 3.894088 -3.230054
 1 -5.838046 11.342652 2.742095
 1 -5.084143 9.812751 3.268199
 1 -4.147991 10.986259 2.292261
 1 -2.544718 5.726221 -8.829481
 1 -2.073471 4.481246 -7.641234
 1 -3.788648 4.975022 -7.794628
 1 -2.232179 6.988675 0.827737

E = -6220.2159061 au; all frequencies positive

TbT-2 (Tetracation (Triplet))

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.253925	-1.946123	0.654304
16	-2.075072	-0.355581	0.642270
6	-0.541203	0.464018	0.659857
6	0.540422	-0.464343	0.659431
6	0.176337	-1.798864	0.631181
6	-0.177087	1.798538	0.631106
6	1.253209	1.945720	0.652956
16	2.074295	0.355160	0.640336
6	2.018283	3.103332	0.736028
6	-2.018774	-3.103829	0.738178
6	1.146252	-2.901805	0.523311
6	-1.146982	2.901597	0.524079
6	3.439224	3.182402	0.663878
6	3.957243	4.438928	0.836262
6	2.951606	5.420581	1.060933
16	1.339354	4.714804	1.053021
16	-1.436847	3.679257	-1.020095
6	-2.715585	4.655984	-0.312325
6	-2.889633	4.374630	1.034384
6	-2.004754	3.376578	1.497050
6	-3.439782	-3.183145	0.667629
6	-3.957418	-4.439701	0.840986
6	-2.951371	-5.421136	1.064806
16	-1.339228	-4.715167	1.054669
16	1.434677	-3.679381	-1.021156
6	2.714320	-4.655871	-0.314735
6	2.889696	-4.374505	1.031816
6	2.005117	-3.376623	1.495404
1	4.058404	2.311115	0.484553
1	5.011860	4.674880	0.827890
1	-3.643093	4.851601	1.647271
1	-1.995498	3.007151	2.515338
1	-4.059289	-2.311994	0.488772
1	-5.012011	-4.675809	0.833902
1	3.643887	-4.851325	1.643920
1	1.996834	-3.007205	2.513704
7	-3.129480	-6.738787	1.238241
6	-4.360166	-7.382925	0.877091
6	-2.069016	-7.552993	1.775770
6	-4.961643	-8.272151	1.783166
6	-6.142164	-8.904813	1.440787
6	-6.740822	-8.670095	0.186535
6	-6.126705	-7.795555	-0.724955
6	-4.938515	-7.159335	-0.377305
6	-1.579619	-8.635624	1.029798
6	-0.562721	-9.418946	1.548873
6	-0.037647	-9.145946	2.826500
6	-0.545332	-8.075687	3.578895
6	-1.559663	-7.282518	3.049017
6	-8.569550	-9.138387	-1.288336
6	1.431821	-9.842221	4.588392
8	-7.891215	-9.336059	-0.043383
8	0.955309	-9.969087	3.242267
1	-4.509261	-8.449149	2.752446
1	-6.630281	-9.584120	2.130416
1	-6.550919	-7.620753	-1.705288
1	-1.990845	-8.848739	0.049244
1	-0.162859	-10.256102	0.987885
1	-0.171934	-7.862056	4.572075
1	-1.967578	-6.467037	3.636574
1	-9.464141	-9.757586	-1.237745
1	-8.856039	-8.089725	-1.418819
1	-7.949252	-9.460458	-2.130869
1	2.163276	-10.638444	4.718127
1	1.913206	-8.872253	4.747986
1	0.615966	-9.973899	5.305652
1	-4.449918	-6.508586	-1.094271
7	3.392155	-5.601968	-1.071962
6	3.650055	-5.356154	-2.446852

6	3.837103	-6.804603	-0.485359	8	-4.380654	4.755747	-6.470484
6	3.442640	-6.381428	-3.394255	1	-5.687750	6.841579	-1.613482
6	3.690457	-6.142934	-4.729897	1	-6.467509	8.971024	-0.617279
6	4.162156	-4.881695	-5.155003	1	-2.870661	9.173081	1.764535
6	4.379623	-3.861157	-4.208915	1	-3.064878	7.344849	-3.072065
6	4.122535	-4.100703	-2.867458	1	-3.522093	6.910466	-5.472319
6	5.073708	-7.359588	-0.892167	1	-4.771313	2.896323	-4.504347
6	5.514471	-8.540097	-0.338548	1	-4.328977	3.327447	-2.131535
6	4.735456	-9.210435	0.632503	1	-5.156382	11.983595	2.292854
6	3.501312	-8.662396	1.041513	1	-4.499249	10.502221	3.041837
6	3.062256	-7.472043	0.485966	1	-3.554324	11.374137	1.792702
6	4.850533	-3.506179	-6.994130	1	-4.937661	3.648829	-8.065937
6	4.563304	-11.089184	2.117521	1	-4.151338	2.698887	-6.775577
8	4.373584	-4.755507	-6.474620	1	-5.841688	3.262548	-6.576851
8	5.253346	-10.355732	1.093630	1	-2.095135	7.074111	0.776301
1	3.061747	-7.344706	-3.074748				
1	3.516532	-6.910375	-5.475483				
1	4.765418	-2.895765	-4.509008				
1	5.686331	-6.839636	-1.618781				
1	6.468594	-8.968425	-0.623141				
1	2.874201	-9.172785	1.762241				
1	2.096174	-7.074579	0.774438				
1	4.929084	-3.648657	-8.070645				
1	4.143926	-2.698667	-6.779610				
1	5.834471	-3.262282	-6.582410				
1	5.162344	-11.982065	2.287965				
1	4.505358	-10.501230	3.038096				
1	3.559410	-11.373275	1.789829				
1	4.325445	-3.326814	-2.135766				
7	3.130183	6.738256	1.233757				
6	2.070644	7.552795	1.772580				
6	4.360620	7.382018	0.871030				
6	1.580636	8.635605	1.027268				
6	0.564728	9.419298	1.547722				
6	0.041299	9.146497	2.826067				
6	0.549555	8.076016	3.577755				
6	1.562874	7.282485	3.046494				
6	4.963371	8.271272	1.776232				
6	6.143640	8.903595	1.432362				
6	6.740790	8.668494	0.177464				
6	6.125417	7.793910	-0.733138				
6	4.937476	7.158041	-0.383986				
6	-1.425143	9.843690	4.590145				
6	8.568036	9.135960	-1.299514				
8	-0.950790	9.970005	3.243202				
8	7.891055	9.334172	-0.053914				
1	1.990608	8.848600	0.046164				
1	0.164459	10.256632	0.987292				
1	0.177409	7.862503	4.571435				
1	4.512170	8.448558	2.746011				
1	6.632714	9.582922	2.121295				
1	6.548447	7.618804	-1.713933				
1	4.447936	6.507263	-1.100271				
1	-2.156171	10.640153	4.720821				
1	-1.906535	8.873909	4.750843				
1	-0.608073	9.975373	5.306020				
1	9.462779	9.755032	-1.250086				
1	8.854216	8.087208	-1.429925				
1	7.946916	9.457834	-2.141514				
1	1.971280	6.466839	3.633477				
7	-3.393903	5.602337	-1.068817				
6	-3.837470	6.805279	-0.481816				
6	-3.653304	5.356562	-2.443433				
6	-5.074066	7.361135	-0.887483				
6	-5.513423	8.542027	-0.333567				
6	-4.732971	9.211888	0.636656				
6	-3.498840	8.662984	1.044541				
6	-3.061203	7.472242	0.488712				
6	-3.446435	6.381685	-3.391116				
6	-3.695586	6.143150	-4.726504				
6	-4.168051	4.882015	-5.151062				
6	-4.384973	3.861630	-4.204681				
6	-4.126566	4.101217	-2.863488				
6	-4.557976	11.090465	2.121498				
6	-4.858127	3.506407	-6.989487				
8	-5.249536	10.357616	1.098193				

E = -6220.0169449 au; all frequencies positive

TbT-3 (Neutral)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.204465	-1.978308	0.283473
16	-2.046947	-0.417735	0.322655
6	-0.532528	0.443074	0.376438
6	0.532528	-0.443074	0.376438
6	0.178487	-1.828041	0.305067
6	-0.178487	1.828041	0.305067
6	1.204465	1.978308	0.283473
16	2.046947	0.417735	0.322655
6	2.021609	3.177243	0.321295
6	-2.021609	-3.177243	0.321295
6	1.183248	-2.890263	0.205656
6	-1.183248	2.890263	0.205656
6	3.211895	3.410852	-0.337284
6	3.808662	4.656132	-0.019367
6	3.093978	5.401061	0.897603
16	1.656159	4.523734	1.392387
16	-1.126699	4.108722	-1.055663
6	-2.631222	4.838015	-0.519994
6	-3.135622	4.137577	0.555837
6	-2.327642	3.040595	0.956795
6	-3.211895	-3.410852	-0.337284
6	-3.808662	-4.656132	-0.019367
6	-3.093978	-5.401061	0.897603
16	-1.656159	-4.523734	1.392387
16	1.126699	-4.108722	-1.055663
6	2.631222	-4.838015	-0.519994
6	3.135622	-4.137577	0.555837
6	2.327642	-3.040595	0.956795
1	3.626337	2.713132	-1.056516
1	4.719916	5.012732	-0.484761
1	-4.046341	4.422766	1.069350
1	-2.563242	2.398614	1.798323
1	-3.626337	-2.713132	-1.056516
1	-4.719916	-5.012732	-0.484761
1	4.046341	-4.422766	1.069350
1	2.563242	-2.398614	1.798323
6	-3.403024	-6.724931	1.437554
6	-2.412280	-7.564635	1.981275
6	-2.717459	-8.822209	2.483823
6	-4.041537	-9.303196	2.471619
6	-5.040547	-8.466685	1.933454
6	-4.725249	-7.212454	1.431243
7	-4.358327	-10.575284	2.981735
6	-5.448294	-11.326083	2.446480
6	-3.596054	-11.148796	4.043867
6	-6.397823	-11.909889	3.301939
6	-7.446139	-12.661587	2.788885
6	-7.585342	-12.834672	1.402987
6	-6.649098	-12.250573	0.540881
6	-5.585180	-11.514723	1.066779
6	-3.129106	-12.470739	3.950660
6	-2.409072	-13.042818	4.990650
6	-2.118537	-12.301463	6.146437
6	-2.572050	-10.980318	6.246369
6	-3.315084	-10.420370	5.205118
6	-8.839150	-13.793184	-0.396612
6	-1.078612	-12.245441	8.301588
8	-8.655114	-13.581691	1.000043
8	-1.396248	-12.951621	7.105914
1	-1.923980	-9.446885	2.877772
1	-6.071824	-8.800794	1.926863
1	-5.526929	-6.584395	1.055407
1	-6.305954	-11.773077	4.374455
1	-8.179788	-13.115121	3.447455
1	-6.724993	-12.372798	-0.532682
1	-4.854822	-11.079073	0.392696
1	-3.338361	-13.049343	3.056884
1	-2.049148	-14.064284	4.921792
1	-2.370215	-10.384965	7.128438
1			
1	-3.676467	-9.401335	5.297562
1	-9.738067	-14.402902	-0.492259
1	-8.985100	-12.846899	-0.930935
1	-7.990096	-14.328778	-0.837540
1	-0.505342	-12.939361	8.917062
1	-0.469809	-11.357386	8.094489
1	-1.983146	-11.943991	8.843073
1	-1.374638	-7.242841	1.982460
6	3.192622	-6.011152	-1.192132
6	4.572330	-6.287355	-1.122240
6	5.124715	-7.397028	-1.746085
6	4.318190	-8.292780	-2.476764
6	2.938063	-8.021953	-2.553873
6	2.395173	-6.907620	-1.928171
7	4.874826	-9.419032	-3.111068
6	4.299544	-9.941985	-4.308318
6	6.027900	-10.065579	-2.572691
6	4.041537	-11.317651	-4.431815
6	3.504484	-11.835638	-5.602591
6	3.191650	-10.988487	-6.677012
6	3.437720	-9.614742	-6.561875
6	3.998972	-9.105479	-5.389064
6	7.117782	-10.382142	-3.401217
6	8.232433	-11.031838	-2.888642
6	8.297130	-11.366135	-1.527042
6	7.219598	-11.049043	-0.690788
6	6.092882	-10.415740	-1.219432
6	2.325257	-10.779772	-8.898567
6	9.555929	-12.357165	0.251475
8	2.657302	-11.594370	-7.778175
8	9.440972	-11.991957	-1.120554
1	6.193511	-7.567633	-1.684287
1	2.288614	-8.699031	-3.096900
1	1.321852	-6.750171	-1.987237
1	4.268744	-11.980115	-3.602984
1	3.305816	-12.897987	-5.700836
1	3.214607	-8.936423	-7.376315
1	4.200835	-8.041900	-5.314094
1	7.083428	-10.117861	-4.453080
1	9.074603	-11.278735	-3.526978
1	7.235875	-11.301634	0.362403
1	5.255720	-10.187991	-0.567618
1	1.917712	-11.455488	-9.651101
1	1.569832	-10.028336	-8.639860
1	3.209872	-10.275999	-9.305818
1	10.531893	-12.832258	0.355224
1	9.509496	-11.479097	0.906545
1	8.774495	-13.067839	0.545607
1	5.230252	-5.602264	-0.596607
6	3.403024	6.724931	1.437554
6	4.725249	7.212454	1.431243
6	5.040547	8.466685	1.933454
6	4.041537	9.303196	2.471619
6	2.717459	8.822209	2.483823
6	2.412280	7.564635	1.981275
7	4.358327	10.575284	2.981735
6	3.596054	11.148796	4.043867
6	5.448294	11.326083	2.446480
6	3.129106	12.470739	3.950660
6	2.409072	13.042818	4.990650
6	2.118537	12.301463	6.146437
6	2.572050	10.980318	6.246369
6	3.315084	10.420370	5.205118
6	6.397823	11.909889	3.301939
6	7.446139	12.661587	2.788885
6	7.585342	12.834672	1.402987
6	6.649098	12.250573	0.540881
6	5.585180	11.514723	1.066779
6	1.078612	12.245441	8.301588
6	8.839150	13.793184	-0.396612
8	1.396248	12.951621	7.105914
8	8.655114	13.581691	1.000043
1	6.071824	8.800794	1.926863
1	1.923980	9.446885	2.877772
1	1.374638	7.242841	1.982460
1	3.338361	13.049343	3.056884

1	2.049148	14.064284	4.921792	6	-1.017015	2.952761	0.842570
1	2.370215	10.384965	7.128438	6	3.558964	3.064168	0.741872
1	3.676467	9.401335	5.297562	6	4.151143	4.314018	0.948674
1	6.305954	11.773077	4.374455	6	3.258148	5.300549	1.366661
1	8.179788	13.115121	3.447455	16	1.641639	4.629103	1.506112
1	6.724993	12.372798	-0.532682	16	-1.183559	3.903627	-0.624039
1	4.854822	11.079073	0.392696	6	-2.458204	4.886157	0.076003
1	0.505342	12.939361	8.917062	6	-2.735310	4.455937	1.357872
1	0.469809	11.357386	8.094489	6	-1.933735	3.363688	1.783057
1	1.983146	11.943991	8.843073	6	-3.558978	-3.064170	0.741876
1	9.738067	14.402902	-0.492259	6	-4.151153	-4.314023	0.948675
1	8.985100	12.846899	-0.930935	6	-3.258155	-5.300552	1.366660
1	7.990096	14.328778	-0.837540	16	-1.641648	-4.629101	1.506111
1	5.526929	6.584395	1.055407	16	1.183529	-3.903640	-0.624020
6	-3.192622	6.011152	-1.192132	6	2.458184	-4.886158	0.076019
6	-2.395173	6.907620	-1.928171	6	2.735290	-4.455936	1.357887
6	-2.938063	8.021953	-2.553873	6	1.933714	-3.363688	1.783071
6	-4.318190	8.292780	-2.476764	1	4.108988	2.196759	0.395225
6	-5.124715	7.397028	-1.746085	1	5.201921	4.504128	0.770206
6	-4.572330	6.287355	-1.122240	1	-3.474085	4.932089	1.991488
7	-4.874826	9.419032	-3.111068	1	-2.005365	2.910410	2.765412
6	-6.027900	10.065579	-2.572691	1	-4.109004	-2.196762	0.395230
6	-4.299544	9.941985	-4.308318	1	-5.201930	-4.504136	0.770207
6	-7.117782	10.382142	-3.401217	1	3.474067	-4.932085	1.991503
6	-8.232433	11.031838	-2.888642	1	2.005346	-2.910406	2.765424
6	-8.297130	11.366135	-1.527042	6	-3.530374	-6.689847	1.659968
6	-7.219598	11.049043	-0.690788	6	-2.496350	-7.637190	1.847899
6	-6.092882	10.415740	-1.219432	6	-2.764542	-8.961888	2.131589
6	-4.041537	11.317651	-4.431815	6	-4.098168	-9.423084	2.242724
6	-3.504484	11.835638	-5.602591	6	-5.140847	-8.483783	2.055307
6	-3.191650	10.988487	-6.677012	6	-4.860912	-7.161079	1.775612
6	-3.437720	9.614742	-6.561875	7	-4.376105	-10.757542	2.526616
6	-3.998972	9.105479	-5.389064	6	-5.608247	-11.356852	2.117683
6	-9.555929	12.357165	0.251475	6	-3.441194	-11.571916	3.237830
6	-2.325257	10.779772	-8.898567	6	-6.379682	-12.083699	3.039746
8	-9.440972	11.991957	-1.120554	6	-7.563693	-12.686310	2.643193
8	-2.657302	11.594370	-7.778175	6	-8.011129	-12.570633	1.316023
1	-2.288614	8.699031	-3.096900	6	-7.246332	-11.847066	0.390673
1	-6.193511	7.567633	-1.684287	6	-6.049690	-11.254521	0.793892
1	-5.230252	5.602264	-0.596607	6	-3.099391	-12.844267	2.749630
1	-7.083428	10.117861	-4.453080	6	-2.213247	-13.649408	3.448651
1	-9.074603	11.278735	-3.526978	6	-1.639051	-13.199783	4.649918
1	-7.235875	11.301634	0.362403	6	-1.974544	-11.931098	5.142352
1	-5.255720	10.187991	-0.567618	6	-2.877124	-11.132122	4.440592
1	-4.268744	11.980115	-3.602984	6	-9.691236	-13.114097	-0.300698
1	-3.305816	12.897987	-5.700836	6	-0.172239	-13.666733	6.483369
1	-3.214607	8.936423	-7.376315	8	-9.186643	-13.193147	1.031475
1	-4.200835	8.041900	-5.314094	8	-0.779382	-14.063327	5.254765
1	-10.531893	12.832258	0.355224	1	-1.944922	-9.660709	2.246314
1	-9.509496	11.479097	0.906545	1	-6.171409	-8.801789	2.156092
1	-8.774495	13.067839	0.545607	1	-5.689695	-6.469145	1.673844
1	-1.917712	11.455488	-9.651101	1	-6.045575	-12.170072	4.068204
1	-1.569832	10.028336	-8.639860	1	-8.167249	-13.246352	3.349545
1	-3.209872	10.275999	-9.305818	1	-7.560056	-11.752077	-0.641367
1	-1.321852	6.750171	-1.987237	1	-5.452204	-10.711135	0.069334

E = -7145.0120779 au; All frequencies positive

TbT-3 (Radical Cation)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.324869	-1.897304	0.924136
16	-2.074830	-0.282093	0.939804
6	-0.508814	0.478117	0.965331
6	0.508797	-0.478114	0.965332
6	0.081058	-1.822804	0.922912
6	-0.081075	1.822806	0.922904
6	1.324852	1.897307	0.924128
16	2.074813	0.282095	0.939797
6	2.184529	3.035998	0.988012
6	-2.184543	-3.035996	0.988018
6	1.016995	-2.952760	0.842583

6	4.000995	-10.946701	-5.951982	6	-5.006277	7.425486	-1.072296
6	3.977558	-9.907845	-6.895754	6	-4.392924	6.397948	-0.371003
6	4.278593	-8.602280	-6.487753	7	-4.957794	9.119477	-2.842642
6	4.606962	-8.350059	-5.154255	6	-5.943737	9.948566	-2.225048
6	7.172682	-10.184991	-2.863261	6	-4.617120	9.378403	-4.205642
6	8.124655	-11.011142	-2.281908	6	-7.172683	10.185011	-2.863269
6	7.880574	-11.610104	-1.036006	6	-8.124651	11.011167	-2.281913
6	6.661422	-11.375126	-0.387975	6	-7.880564	11.610127	-1.036011
6	5.701091	-10.559690	-0.990144	6	-6.661412	11.375142	-0.387983
6	3.620925	-9.254804	-9.170891	6	-5.701087	10.559701	-0.990155
6	8.683735	-13.037498	0.709810	6	-4.307529	10.683246	-4.624046
8	3.653667	-10.269563	-8.171288	6	-4.001000	10.946703	-5.951998
8	8.883335	-12.396061	-0.546619	6	-3.977571	9.907847	-6.895769
1	6.018514	-7.716257	-0.816220	6	-4.278612	8.602283	-6.487767
1	2.488072	-8.146389	-3.243057	6	-4.606979	8.350065	-5.154268
1	1.411072	-6.346211	-1.995473	6	-8.683713	13.037525	0.709806
1	4.312877	-11.491741	-3.900343	6	-3.620947	9.254803	-9.170907
1	3.763260	-11.953728	-6.278984	8	-8.883320	12.396089	-0.546623
1	4.277265	-7.781201	-7.194178	8	-3.653682	10.269563	-8.171304
1	4.854763	-7.338541	-4.849203	1	-2.488086	8.146384	-3.243076
1	7.375024	-9.718937	-3.822049	1	-6.018523	7.716271	-0.816229
1	9.074183	-11.197395	-2.773070	1	-4.950859	5.895339	0.412877
1	6.440621	-11.829783	0.569983	1	-7.375030	9.718959	-3.822057
1	4.752298	-10.395693	-0.489565	1	-9.074179	11.197425	-2.773073
1	3.341494	-9.755768	-10.098135	1	-6.440607	11.829797	0.569975
1	2.876767	-8.484287	-8.937155	1	-4.752293	10.395698	-0.489577
1	4.602285	-8.782438	-9.296251	1	-4.312875	11.491745	-3.900357
1	9.594172	-13.604700	0.905246	1	-3.763261	11.953729	-6.279000
1	8.532169	-12.307931	1.514131	1	-4.277290	7.781204	-7.194192
1	7.829312	-13.723861	0.679331	1	-4.854784	7.338548	-4.849215
1	4.950845	-5.895330	0.412887	1	-9.594148	13.604732	0.905244
6	3.530372	6.689842	1.659971	1	-8.532150	12.307957	1.514127
6	4.860911	7.161071	1.775612	1	-7.829287	13.723884	0.679326
6	5.140850	8.483774	2.055308	1	-3.341517	9.755765	-10.098152
6	4.098174	9.423078	2.242729	1	-2.876793	8.484283	-8.937173
6	2.764547	8.961885	2.131598	1	-4.602310	8.782442	-9.296264
6	2.496350	7.637188	1.847907	1	-1.411091	6.346202	-1.995494
7	4.376115	10.757534	2.526621				
6	3.441209	11.571909	3.237839				
6	5.608257	11.356842	2.117684				
6	3.099407	12.844262	2.749641				
6	2.213267	13.649404	3.448665				
6	1.639074	13.199780	4.649934				
6	1.974566	11.931093	5.142365				
6	2.877142	11.132115	4.440602				
6	6.379696	12.083687	3.039745				
6	7.563708	12.686295	2.643189				
6	8.011140	12.570616	1.316018				
6	7.246339	11.847050	0.390671				
6	6.049697	11.254509	0.793893				
6	0.172269	13.666730	6.483390				
6	9.691245	13.114074	-0.300708				
8	0.779409	14.063325	5.254785				
8	9.186655	13.193127	1.031467				
1	6.171414	8.801777	2.156090				
1	1.944929	9.660707	2.246326				
1	1.459291	7.334105	1.739282				
1	3.531874	13.195374	1.818794				
1	1.942023	14.631873	3.077094				
1	1.556572	11.563306	6.071120				
1	3.148065	10.158927	4.836426				
1	6.045592	12.170062	4.068203				
1	8.167266	13.246336	3.349539				
1	7.560061	11.752060	-0.641371				
1	5.452208	10.711123	0.069336				
1	-0.468766	14.496539	6.781073				
1	-0.436794	12.764663	6.355389				
1	0.923292	13.490561	7.261860				
1	10.629164	13.669413	-0.298000				
1	9.884483	12.075958	-0.594072				
1	9.000312	13.571766	-1.017707				
1	5.689692	6.469135	1.673840				
6	-3.087319	5.968589	-0.681264				
6	-2.429623	6.624287	-1.739239				
6	-3.033728	7.654146	-2.446476				
6	-4.339610	8.080100	-2.129111				

E = -7144.8465355 au; all frequencies positive

TbT-3 (Dication (Triplet))

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.314394	-1.910496	-0.106009
16	0.452598	-2.044571	-0.087585
6	0.622030	-0.308837	-0.024072
6	-0.622243	0.308158	-0.024013
6	-1.743309	-0.570920	-0.100720
6	1.743083	0.570250	-0.100856
6	1.314187	1.909814	-0.106100
16	-0.452790	2.043897	-0.087497
6	2.097650	3.111470	-0.030438
6	-2.097818	-3.112152	-0.030254
6	-3.122636	-0.129063	-0.239433
6	3.122420	0.128400	-0.239665
6	3.324949	3.318373	0.593532
6	3.772757	4.645410	0.536101
6	2.910894	5.513057	-0.131330
16	1.505268	4.625528	-0.701887
16	3.727671	-1.256743	0.650384
6	5.309865	-1.142690	-0.105382
6	5.326717	-0.074898	-0.994173
6	4.111998	0.631335	-1.068223
6	-3.325111	-3.319057	0.593777
6	-3.772864	-4.646093	0.536457
6	-2.910989	-5.513772	-0.130959
16	-1.505411	4.626228	-0.701626
16	-3.727699	1.256376	0.650323
6	-5.309996	1.142233	-0.105212
6	-5.327024	0.074213	-0.993720
6	-4.112359	-0.632122	-1.067743
1	3.863396	2.527313	1.098423

1	4.707976	4.966140	0.977432	1	-7.295438	8.712314	1.370847
1	6.197641	0.194557	-1.578377	1	-7.738684	6.514832	0.370687
1	3.950459	1.478504	-1.722692	1	-11.416637	6.248428	0.028681
1	-3.863558	-2.527977	1.098633	1	-13.786895	5.631653	-0.380571
1	-4.708044	-4.966825	0.977867	1	-13.071205	1.760751	1.365045
1	-6.198038	-0.195326	-1.577751	1	-10.735382	2.381869	1.787025
1	-3.950965	-1.479448	-1.722044	1	-7.710200	11.475269	3.699213
6	-3.071372	-6.929030	-0.382029	1	-6.657958	10.157179	3.118098
6	-2.159735	-7.661446	-1.178255	1	-7.859429	10.897939	2.018290
6	-2.326152	-9.010012	-1.424367	1	-16.496202	2.194832	0.218078
6	-3.427803	-9.713866	-0.881708	1	-14.942857	1.345236	0.000458
6	-4.342588	-8.992679	-0.076539	1	-15.400316	1.981471	1.609028
6	-4.165758	-7.644790	0.162391	1	-7.714699	1.384088	-1.347302
7	-3.606792	-11.071721	-1.131916	6	3.071286	6.928329	-0.382485
6	-4.906450	-11.664000	-1.093768	6	4.165421	7.644199	0.162258
6	-2.497652	-11.916400	-1.445559	6	4.342219	8.992105	-0.076677
6	-5.116415	-12.856066	-0.379492	6	3.427655	9.713180	-0.882177
6	-6.369105	-13.448213	-0.357026	6	2.326278	9.009196	-1.425199
6	-7.446677	-12.860826	-1.042756	6	2.159888	7.660615	-1.179077
6	-7.243751	-11.672370	-1.758619	7	3.606584	11.071069	-1.132337
6	-5.978070	-11.088159	-1.786328	6	2.497467	11.915617	-1.446431
6	-2.558829	-12.776555	-2.555250	6	4.906165	11.663498	-1.093708
6	-1.494843	-13.613078	-2.852891	6	2.558926	12.775678	-2.556175
6	-0.339343	-13.607239	-2.052278	6	1.494960	13.612084	-2.854252
6	-0.272476	-12.752823	-0.942625	6	0.339182	13.606188	-2.054050
6	-1.351202	-11.921746	-0.642677	6	0.272022	12.751863	-0.944352
6	-9.765728	-12.973543	-1.628659	6	1.350741	11.920930	-0.643950
6	1.847452	-14.500329	-1.661694	6	5.115785	12.855483	-0.379207
8	-8.632715	-13.517753	-0.952493	6	6.368398	13.447794	-0.356301
8	0.647384	-14.460714	-2.432923	6	7.446240	12.860636	-1.041790
1	-1.618275	-9.528956	-2.058869	6	7.243671	11.672251	-1.757863
1	-5.181401	-9.508975	0.374106	6	5.978062	11.087893	-1.786028
1	-4.878225	-7.138548	0.803927	6	-1.847866	14.499035	-1.664334
1	-4.292387	-13.310606	0.159863	6	9.765427	12.973737	-1.627059
1	-6.541395	-14.365473	0.195797	8	-0.647519	14.459530	-2.435120
1	-8.051892	-11.205036	-2.307239	8	8.632186	13.517705	-0.951095
1	-5.822254	-10.179462	-2.358221	1	5.180836	9.508488	0.374235
1	-3.443154	-12.780012	-3.183352	1	1.618566	9.528044	-2.059964
1	-1.531219	-14.276481	-3.710362	1	1.314123	7.156836	-1.637431
1	0.599071	-12.737986	-0.300265	1	3.443471	12.779176	-3.183968
1	-1.302233	-11.276476	0.228098	1	1.531573	14.275424	-3.711763
1	-10.592427	-13.651822	-1.418010	1	-0.599755	12.736976	-0.302304
1	-10.011448	-11.973390	-1.254258	1	1.301528	11.275721	0.226858
1	-9.600372	-12.927248	-2.710856	1	4.291540	13.309855	0.159961
1	2.486785	-15.240122	-2.143171	1	6.540405	14.365010	0.196686
1	2.353080	-13.528038	-1.660623	1	8.052033	11.205085	-2.306304
1	1.648686	-14.808672	-0.629195	1	5.822526	10.179244	-2.358075
1	-1.313754	-7.157767	-1.636318	1	-2.487146	15.238678	-2.146116
6	-6.380791	2.062725	0.225057	1	-2.353346	13.526665	-1.663342
6	-7.593120	2.057097	-0.505926	1	-1.649532	14.807514	-0.631790
6	-8.628189	2.918277	-0.198928	1	10.591991	13.652091	-1.416122
6	-8.508257	3.843459	0.864573	1	10.011192	11.973561	-1.252743
6	-7.299453	3.862319	1.597841	1	9.600340	12.927564	-2.709303
6	-6.271055	2.995171	1.282337	1	4.877703	7.138049	0.804077
7	-9.553411	4.713354	1.180359	6	6.380785	-2.062965	0.225024
6	-9.293426	5.986709	1.766609	6	6.271257	-2.995085	1.282629
6	-10.908880	4.351312	0.928089	6	7.299799	-3.861981	1.598317
6	-10.044999	6.420959	2.873512	6	8.508524	-3.843145	0.864922
6	-9.807717	7.663980	3.435867	6	8.628255	-2.918327	-0.198916
6	-8.810458	8.505091	2.910161	6	7.593038	-2.057412	-0.506112
6	-8.058846	8.078988	1.804964	7	9.553868	-4.712757	1.180942
6	-8.308123	6.830938	1.238150	6	10.909234	-4.350278	0.928978
6	-11.784153	5.271408	0.322838	6	9.294056	-5.986149	1.767097
6	-13.106611	4.931597	0.092331	6	11.785126	-5.270311	0.324483
6	-13.589927	3.661735	0.456336	6	13.107479	-4.930001	0.094218
6	-12.722684	2.739931	1.061649	6	13.590105	-3.659723	0.457742
6	-11.395573	3.090831	1.299090	6	12.722242	-2.737995	1.062323
6	-7.658391	10.599277	3.053024	6	11.395229	-3.089365	1.299490
6	-15.452423	2.158331	0.529118	6	10.045846	-6.420472	2.873846
8	-8.655817	9.699067	3.536368	6	9.808657	-7.663515	3.436147
8	-14.898527	3.428650	0.184069	6	8.811315	-8.504609	2.910527
1	-9.532505	2.902199	-0.795245	6	8.059510	-8.078435	1.805472
1	-7.188067	4.544928	2.431541	6	8.308649	-6.830345	1.238732
1	-5.371468	3.022948	1.889637	6	15.451898	-2.155422	0.530275
1	-10.807709	5.773433	3.292038	6	7.659271	-10.598806	3.053470
1	-10.376577	8.004497	4.294301	8	14.898646	-3.426194	0.185784

8	8.656802	-9.698597	3.536653
1	7.188629	-4.544309	2.432276
1	9.532508	-2.902368	-0.795334
1	7.714414	-1.384687	-1.347740
1	11.418150	-6.247633	0.030668
1	13.788231	-5.629969	-0.378137
1	13.070230	-1.758516	1.365356
1	10.734570	-2.380468	1.786885
1	10.808588	-5.772953	3.292319
1	10.377635	-8.004083	4.294479
1	7.296063	-8.711756	1.371418
1	7.739084	-6.514194	0.371371
1	16.495782	-2.191662	0.219560
1	14.942129	-1.342866	0.000994
1	15.399398	-1.977990	1.610068
1	7.711229	-11.474815	3.699620
1	6.658861	-10.156703	3.118776
1	7.860121	-10.897416	2.018690
1	5.371738	-3.022759	1.890029

E = -7144.6709112 au; all frequencies positive

TbT-3 (Trication (Quadruplet))

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.244307	-1.953617	0.310828
16	-2.057600	-0.375318	0.330434
6	-0.527464	0.453665	0.368108
6	0.527508	-0.453658	0.368101
6	0.150629	-1.823473	0.320015
6	-0.150586	1.823481	0.320044
6	1.244350	1.953626	0.310859
16	2.057644	0.375328	0.330442
6	2.074950	3.125115	0.384714
6	-2.074907	-3.125106	0.384678
6	1.139921	-2.901848	0.240178
6	-1.139880	2.901854	0.240221
6	3.380759	3.256836	-0.076443
6	3.968172	4.496307	0.221851
6	3.137673	5.358283	0.930848
16	1.590760	4.584797	1.235737
16	-1.152028	4.059782	-1.071140
6	-2.607820	4.827850	-0.463850
6	-3.049235	4.178337	0.675866
6	-2.229704	3.094438	1.065991
6	-3.380721	-3.256823	-0.076470
6	-3.968135	-4.496292	0.221827
6	-3.137634	-5.358271	0.930817
16	-1.590711	-4.584794	1.235685
16	1.152084	-4.059740	-1.071214
6	2.607846	-4.827849	-0.463906
6	3.049249	-4.178367	0.675832
6	2.229729	-3.094461	1.065963
1	3.880799	2.480371	-0.644049
1	4.965163	4.768218	-0.101465
1	-3.919798	4.492983	1.237949
1	-2.410494	2.488801	1.946238
1	-3.880765	-2.480354	-0.644067
1	-4.965131	-4.768196	-0.101477
1	3.919792	-4.493043	1.237929
1	2.410508	-2.488849	1.946228
6	-3.417872	-6.702511	1.391609
6	-2.399941	-7.560971	1.868502
6	-2.676465	-8.838348	2.315301
6	-4.001038	-9.334918	2.305430
6	-5.027504	-8.486283	1.827458
6	-4.740199	-7.208811	1.388910
7	-4.285981	-10.624340	2.754665
6	-5.392621	-11.356140	2.231651
6	-3.475759	-11.246691	3.750046
6	-6.262366	-12.038098	3.101596
6	-7.326193	-12.767436	2.597381
6	7.552411	-12.831897	1.210645
6	-6.688329	-12.154464	0.337422
6	-5.614643	-11.429646	0.850368
6	-3.032866	-12.569964	3.574929
6	-2.259629	-13.183188	4.546728
6	-1.904924	-12.489448	5.717758
6	-2.346742	-11.170612	5.900246
6	-3.131193	-10.562123	4.922662
6	-8.898854	-13.688384	-0.574633
6	-0.745865	-12.530956	7.812915
8	-8.621762	-13.570919	0.821310
8	-1.140756	-13.178365	6.602804
1	-1.868022	-9.476051	2.651717
1	-6.054063	-8.832134	1.833544
1	-5.560043	-6.575766	1.068368
1	-6.101427	-11.984835	4.172790
1	-8.005981	-13.291287	3.260658
1	-6.830856	-12.198250	-0.735070
1	-4.937294	-10.924886	0.169809
1	-3.293095	-13.108276	2.670061
1	-1.907509	-14.200998	4.417575
1	-2.103381	-10.618849	6.799547
1	-3.487771	-9.549492	5.077941
1	-9.784179	-14.319304	-0.649908
1	-9.109015	-12.7110978	-1.022838
1	-8.066879	-14.163133	-1.106409
1	-0.143800	-13.258704	8.356463
1	-0.143298	-11.638890	7.608783
1	-1.615664	-12.253553	8.418274
1	-1.366019	-7.229571	1.860232
6	3.195052	-5.986411	-1.121661
6	4.531106	-6.364180	-0.851522
6	5.098644	-7.474313	-1.448498
6	4.350763	-8.251566	-2.357739
6	3.022742	-7.879264	-2.650188
6	2.461830	-6.772934	-2.038193
7	4.923253	-9.387682	-2.961997
6	4.623683	-9.705585	-4.304989
6	5.794727	-10.217816	-2.222244
6	4.427888	-11.050020	-4.691541
6	4.133513	-11.356843	-6.003897
6	4.030772	-10.335051	-6.971813
6	4.230825	-8.994165	-6.593149
6	4.522832	-8.687951	-5.272186
6	6.945862	-10.764941	-2.830944
6	7.795115	-11.573392	-2.103718
6	7.520102	-11.866071	-0.750808
6	6.371396	-11.327489	-0.141302
6	5.521444	-10.511749	-0.873228
6	3.593356	-9.768092	-9.260034
6	8.213451	-12.999096	1.245170
8	3.739074	-10.743682	-8.220009
8	8.410864	-12.664024	-0.134510
1	6.133013	-7.727128	-1.247197
1	2.427850	-8.485484	-3.323035
1	1.424065	-6.534213	-2.246605
1	4.480744	-11.838160	-3.949494
1	3.960277	-12.381789	-6.311646
1	4.177314	-8.194581	-7.320731
1	4.702166	-7.657159	-4.988986
1	7.176268	-10.525682	-3.862617
1	8.693253	-11.983865	-2.551216
1	6.129466	-11.552520	0.889217
1	4.623804	-10.120054	-0.408504
1	3.351719	-10.333029	-10.159148
1	2.780125	-9.071539	-9.033071
1	4.525446	-9.215518	-9.413163
1	9.054862	-13.635708	1.514722
1	8.215932	-12.101568	1.871553
1	7.277633	-13.548989	1.385318
1	5.139949	-5.759758	-0.189041
6	3.417909	6.702528	1.391631
6	4.740233	7.208834	1.388916
6	5.027535	8.486312	1.827450
6	4.001071	9.334947	2.305424
6	2.676501	8.838370	2.315312

6	2.399978	7.560987	1.868528	1	-1.424029	6.534295	-2.246466
7	4.286013	10.624378	2.754638				
6	3.475788	11.246747	3.750006	E = -7144.4905488 au; all frequencies positive			
6	5.392656	11.356168	2.231615	-----			
6	3.032889	12.570015	3.574861				
6	2.259652	13.183258	4.546648				
6	1.904951	12.489544	5.717694				
6	2.346773	11.170714	5.900211				
6	3.131226	10.562205	4.922639				
6	6.262402	12.038137	3.101551				
6	7.326231	12.767465	2.597326				
6	7.552452	12.831905	1.210590				
6	6.688368	12.154461	0.337375				
6	5.614679	11.429654	0.850331				
6	0.745897	12.531096	7.812853				
6	8.898900	13.688359	-0.574700				
8	1.140782	13.178479	6.602727				
8	8.621807	13.570918	0.821244				
1	6.054094	8.832170	1.833520				
1	1.868057	9.476072	2.651730				
1	1.366057	7.229582	1.860270				
1	3.293117	13.108308	2.669982				
1	1.907530	14.201065	4.417474				
1	2.103415	10.618969	6.799524				
1	3.487807	9.549578	5.077940				
1	6.101461	11.984891	4.172745				
1	8.006020	13.291325	3.260596				
1	6.830897	12.198230	-0.735117				
1	4.937331	10.924883	0.169779				
1	0.143832	13.258854	8.356388				
1	0.143332	11.639023	7.608743				
1	1.615699	12.253708	8.418216				
1	9.784227	14.319276	-0.649985				
1	9.109059	12.710946	-1.022890				
1	8.066927	14.163103	-1.106485				
1	5.560077	6.575791	1.068369				
6	-3.195040	5.986408	-1.121600				
6	-2.461810	6.772976	-2.038088				
6	-3.022737	7.879301	-2.650080				
6	-4.350785	8.251546	-2.357677				
6	-5.098674	7.474246	-1.448483				
6	-4.531117	6.364124	-0.851504				
7	-4.923296	9.387647	-2.961943				
6	-5.794863	10.217717	-2.222227				
6	-4.623657	9.705598	-4.304908				
6	-6.945985	10.764797	-2.830994				
6	-7.795330	11.573186	-2.103807				
6	-7.520425	11.865847	-0.750872				
6	-6.371731	11.327312	-0.141299				
6	-5.521687	10.511633	-0.873186				
6	-4.427926	11.050053	-4.691419				
6	-4.133478	11.356922	-6.003749				
6	-4.030598	10.335157	-6.971678				
6	-4.230588	8.994250	-6.593054				
6	-4.522668	8.687990	-5.272117				
6	-8.213967	12.998790	1.245085				
6	-3.592969	9.768273	-9.259877				
8	-8.411271	12.663740	-0.134616				
8	-3.738836	10.743833	-8.219843				
1	-2.427842	8.485555	-3.322893				
1	-6.133060	7.727018	-1.247220				
1	-5.139965	5.759666	-0.189061				
1	-7.176307	10.525549	-3.862689				
1	-8.693459	11.983621	-2.551357				
1	-6.129884	11.552331	0.889242				
1	-4.624059	10.119974	-0.408409				
1	-4.480887	11.838175	-3.949360				
1	-3.960289	12.381886	-6.311464				
1	-4.176968	8.194683	-7.320648				
1	-4.701949	7.657180	-4.988950				
1	-9.055430	13.635352	1.514596				
1	-8.216445	12.101248	1.871447				
1	-7.278187	13.548728	1.385309				
1	-3.351306	10.333245	-10.158962				
1	-2.779705	9.071774	-9.032867				
1	-4.525008	9.215634	-9.413085				

TbT-3 (Tetracation (Quintuplet))

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-1.231043	-1.958331	0.255915
16	-2.053366	-0.389432	0.280674
6	-0.529034	0.449107	0.317492
6	0.529201	-0.448944	0.317470
6	0.157406	-1.825655	0.267795
6	-0.157241	1.825818	0.267815
6	1.231207	1.958495	0.255884
16	2.053531	0.389595	0.280607
6	2.062803	3.141421	0.319028
6	-2.062637	-3.141258	0.319070
6	1.151798	-2.900975	0.195914
6	-1.151639	2.901136	0.195981
6	3.332862	3.299390	-0.214695
6	3.930419	4.534905	0.101392
6	3.136315	5.355758	0.888011
16	1.616808	4.556488	1.253092
16	-1.167037	4.070342	-1.104535
6	-2.628835	4.824689	-0.493676
6	-3.067196	4.164579	0.640416
6	-2.241689	3.081817	1.023040
6	-3.332706	-3.299223	-0.214631
6	-3.930250	-4.534748	0.101443
6	-3.136128	-5.355608	0.888037
16	-1.616625	-4.556330	1.253118
16	1.167131	-4.070177	-1.104605
6	2.628920	-4.824570	-0.493781
6	3.067357	-4.164442	0.640272
6	2.241890	-3.081657	1.022918
1	3.804241	2.548845	-0.838454
1	4.905125	4.828667	-0.268160
1	-3.940995	4.468969	1.203139
1	-2.420588	2.467338	1.897527
1	-3.804097	-2.548673	-0.838375
1	-4.904957	-4.828512	-0.268103
1	3.941171	-4.468847	1.202963
1	2.420840	-2.467173	1.897390
6	-3.433956	-6.690665	1.377949
6	-2.426457	-7.542594	1.886881
6	-2.720814	-8.809054	2.355893
6	-4.048986	-9.285028	2.327339
6	-5.066508	-8.447933	1.820550
6	-4.762099	-7.180227	1.364173
7	-4.355577	-10.573555	2.798362
6	-5.359959	-11.342434	2.167650
6	-3.664278	-11.110422	3.908547
6	-6.249895	-12.119442	2.941549
6	-7.228938	-12.870205	2.324248
6	-7.346269	-12.874791	0.917895
6	-6.457943	-12.106568	0.141959
6	-5.477382	-11.349071	0.765406
6	-3.281713	-12.469718	3.916524
6	-2.611322	-12.993745	5.002581
6	-2.307927	-12.180951	6.115462
6	-2.691467	-10.826788	6.114395
6	-3.362045	-10.301526	5.019441
6	-8.532573	-13.687470	-1.000266
6	-1.296442	-12.031533	8.283016
8	-8.332537	-13.640909	0.418433
8	-1.653299	-12.790384	7.120495
1	-1.925346	-9.452322	2.712807
1	-6.095769	-8.786352	1.828753
1	-5.569484	-6.542946	1.023343
1	-6.180477	-12.102370	4.023031
1	-7.932713	-13.455024	2.905597
1	-6.515444	-12.110215	-0.938714

1	-4.778126	-10.779346	0.164285	1	6.096004	8.786433	1.828835
1	-3.492286	-13.094320	3.056194	1	1.925580	9.452456	2.712847
1	-2.294414	-14.030417	5.015190	1	1.391333	7.218128	1.884834
1	-2.487304	-10.188835	6.964609	1	3.492602	13.094428	3.056324
1	-3.682049	-9.266031	5.034688	1	2.294660	14.030503	5.015287
1	-9.385113	-14.347328	-1.153943	1	2.487342	10.188859	6.964606
1	-8.760286	-12.693284	-1.397162	1	3.682156	9.266075	5.034718
1	-7.654073	-14.098768	-1.507190	1	6.180707	12.102416	4.023213
1	-0.776677	-12.727985	8.939254	1	7.933003	13.455056	2.905856
1	-0.629361	-11.204105	8.021346	1	6.515852	12.110310	-0.938521
1	-2.187482	-11.646340	8.788312	1	4.778474	10.779454	0.164402
1	-1.391126	-7.217970	1.884848	1	0.776669	12.727986	8.939228
6	3.226404	-5.981947	-1.146399	1	0.629348	11.204148	8.021250
6	4.568583	-6.339806	-0.880781	1	2.187442	11.646294	8.788324
6	5.147832	-7.446757	-1.473059	1	9.385559	14.347385	-1.153622
6	4.404901	-8.239577	-2.372037	1	8.760713	12.693354	-1.396883
6	3.071009	-7.887617	-2.660505	1	7.654526	14.098858	-1.506931
6	2.498455	-6.784186	-2.053029	1	5.569690	6.543052	1.023367
7	4.989724	-9.373982	-2.971250	6	-3.226399	5.982018	-1.146306
6	4.698403	-9.696927	-4.313693	6	-2.498527	6.784260	-2.052996
6	5.866584	-10.190840	-2.225479	6	-3.071165	7.887636	-2.660492
6	4.521830	-11.044772	-4.699564	6	-4.405063	8.239538	-2.371983
6	4.234992	-11.356225	-6.011981	6	-5.147915	7.446717	-1.472940
6	4.122072	-10.336264	-6.981409	6	-4.568584	6.339818	-0.880644
6	4.303160	-8.991957	-6.603321	7	-4.989976	9.373880	-2.971227
6	4.586081	-8.680832	-5.282096	6	-5.866866	10.190717	-2.225470
6	7.022329	-10.734776	-2.829669	6	-4.698727	9.696772	-4.313699
6	7.879893	-11.525783	-2.093995	6	-7.022661	10.734553	-2.829655
6	7.609147	-11.804798	-0.736848	6	-7.880255	11.525540	-2.093994
6	6.454502	-11.271599	-0.132585	6	-7.609490	11.804634	-0.736867
6	5.596724	-10.472413	-0.872465	6	-6.454794	11.271537	-0.132610
6	3.683451	-9.778787	-9.272400	6	-5.596986	10.472371	-0.872477
6	8.323944	-12.896214	1.275190	6	-4.522281	11.044610	-4.699652
8	3.839674	-10.749832	-8.228849	6	-4.235516	11.356013	-6.012098
8	8.508863	-12.583894	-0.112066	6	-4.122546	10.336005	-6.981471
1	6.186778	-7.684080	-1.276344	6	-4.303507	8.991705	-6.603300
1	2.480933	-8.506413	-3.326164	6	-4.586355	8.680632	-5.282047
1	1.456754	-6.560352	-2.258389	6	-8.324307	12.896089	1.275143
1	4.582153	-11.831481	-3.956629	6	-3.683968	9.778432	-9.272446
1	4.075608	-12.383382	-6.319655	8	-8.509238	12.583702	-0.112097
1	4.242265	-8.193919	-7.332000	8	-3.840230	10.749526	-8.228945
1	4.751354	-7.647682	-4.999139	1	-2.481151	8.506435	-3.326204
1	7.250415	-10.504029	-3.863734	1	-6.186865	7.683993	-1.276193
1	8.782324	-11.931625	-2.536962	1	-5.172853	5.722438	-0.225997
1	6.215222	-11.488600	0.900216	1	-7.250759	10.503745	-3.863703
1	4.695423	-10.084260	-0.411877	1	-8.782722	11.931306	-2.536955
1	3.453435	-10.349982	-10.170513	1	-6.215498	11.488603	0.900174
1	2.859192	-9.094050	-9.049742	1	-4.695647	10.084296	-0.411896
1	4.608085	-9.213538	-9.423413	1	-4.582646	11.831356	-3.956760
1	9.175517	-13.516358	1.550851	1	-4.076231	12.383165	-6.319836
1	8.318223	-11.986906	1.884174	1	-4.242573	8.193631	-7.331936
1	7.396635	-13.456051	1.430692	1	-4.751532	7.647484	-4.999025
1	5.172910	-5.722433	-0.226180	1	-9.175916	13.516184	1.550801
6	3.434161	6.690801	1.377949	1	-8.318508	11.986805	1.884162
6	4.762312	7.180340	1.364200	1	-7.397032	13.455996	1.430600
6	5.066737	8.448031	1.820610	1	-3.454035	10.349592	-10.170601
6	4.049223	9.285132	2.327402	1	-2.859644	9.093776	-9.049780
6	2.721041	8.809181	2.355928	1	-4.608561	9.213098	-9.423388
6	2.426669	7.542736	1.886887	1	-1.456825	6.560471	-2.258392
7	4.355827	10.573642	2.798460				
6	3.664499	11.110501	3.908631				
6	5.360244	11.342514	2.167793				
6	3.281972	12.469808	3.916627				
6	2.611542	12.993822	5.002665				
6	2.308067	12.181005	6.115508				
6	2.691570	10.826831	6.114421				
6	3.362187	10.301582	5.019486				
6	6.250163	12.119499	2.941733				
6	7.229239	12.870255	2.324476				
6	7.346620	12.874854	0.918126				
6	6.458311	12.106652	0.142150				
6	5.477716	11.349164	0.765554				
6	1.296445	12.031541	8.282993				
6	8.533003	13.687539	-0.999983				
8	1.653399	12.790424	7.120523				
8	8.332918	13.640964	0.418709				

E = -7144.3067876 au; all frequencies positive