Supporting Information

Photophysical Properties of Benzophenone Based TADF Emitters in Relation to Their Molecular Structure

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Ground State Geometry Optimization with Different Methods

Table S1. Ground state geometry optimizations of different TADF and non-TADF compounds calculated with M06-2X/6-31+G(d,p) and B3LYP-D3/6-31+G(d,p).

| Compound            | Computational Method |                          |                          |
|---------------------|----------------------|--------------------------|--------------------------|
|                     |                      | M06-2X/6-31+G(d,p)       | B3LYP-D3/6-31+G(d,p)     |
| CC2BP (Group 1)     | ![CC2BP M06-2X](image1) | ![CC2BP B3LYP](image2)  |                          |
| CP-BP-DMAC (Group 2)| ![CP-BP-DMAC M06-2X](image3) | ![CP-BP-DMAC B3LYP](image4) |                          |
| b1 (Group 3)        | ![b1 M06-2X](image5)  | ![b1 B3LYP](image6)      |                          |
| ACRXTN (Group 4)    | ![ACRXTN M06-2X](image7) | ![ACRXTN B3LYP](image8)  |                          |
| C1 (Non-TADF)       | ![C1 M06-2X](image9)  | ![C1 B3LYP](image10)     |                          |
**Table S2.** Torsion angles for the ground state geometry optimizations of different TADF and non-TADF compounds calculated with M06-2X/6-31+G(d,p) and B3LYP-D3/6-31+G(d,p).

| Compound       | Computational Method | M06-2X/6-31+G(d,p) | B3LYP-D3/6-31+G(d,p) |
|----------------|----------------------|---------------------|----------------------|
| ![CC2BP](image) | θ = 54.35            | θ = 54.32           |
| ![CP-BP-DMAC](image) | θ = 89.82            | θ = 89.60           |
| ![b1](image)   | θ = 36.16            | θ = 36.27           |
| ![ACRXTN](image) | θ₁ = 87.89          | θ₁ = 88.93          |
| ![C1](image)   | θ = 53.63            | θ = 55.13           |
**Investigation of the Conformational Effects**

**Table S3.** UV-Vis absorption spectra for the most stable conformation and weighted conformations of the emitters Px2BP, Cz2BP, DBT-BZ-PXZ and DBT-BZ-DMAC calculated at different levels of theory.

| Compound          | The Most Stable Conformation | Weighted Conformations |
|-------------------|------------------------------|------------------------|
| **Px2BP in toluene** | ![Px2BP (The Most Stable Conformation)](image) | ![Px2BP (All Conformations)](image) |
| **Cz2BP in toluene** | ![Cz2BP (The Most Stable Conformation)](image) | ![Cz2BP (All Conformations)](image) |
| **DBT-BZ-PXZ in THF** | ![DBT-BZ-PXZ (The Most Stable Conformation)](image) | ![DBT-BZ-PXZ (All Conformations)](image) |
| **DBT-BZ-DMAC in THF** | ![DBT-BZ-DMAC (The Most Stable Conformation)](image) | ![DBT-BZ-DMAC (All Conformations)](image) |
**Table S4.** $\Delta E_{ST}$ values (eV) and relative Gibbs free energies ($\Delta G_{rel}$ in kcal/mol) for all ground state conformations of Cz2BP and CC2BP, together with their Boltzmann weighted and experimental $\Delta E_{ST}$ values (eV).

| Compound | Conformation | $\Delta G_{rel}$ | $\Delta E_{ST}$ | Boltzmann Weighted $\Delta E_{ST}$ | Exp. $\Delta E_{ST}$ |
|----------|--------------|-----------------|----------------|----------------------------------|------------------|
| Cz2BP    | 1            | 0.00            | 0.23           |                                  | 0.21             |
|          | 2            | 0.12            | 0.21           |                                  |                  |
|          | 3            | 0.13            | 0.21           |                                  |                  |
|          | 4            | 0.28            | 0.18           |                                  |                  |
|          | 5            | 0.30            | 0.18           |                                  |                  |
|          | 6            | 0.51            | 0.23           | 0.21                            | 0.21             |
| CC2BP    | 1            | 0.00            | 0.08           |                                  |                  |
|          | 2            | 0.10            | 0.07           |                                  |                  |
|          | 3            | 0.17            | 0.07           |                                  |                  |
|          | 4            | 0.31            | 0.09           |                                  |                  |
|          | 5            | 0.40            | 0.08           |                                  |                  |
|          | 6            | 0.56            | 0.08           | 0.08                            | 0.14             |
Table S5. Absorption spectra for Px2BP, DMAC-BP and Cz2BP calculated at different levels of theory and experimental $\lambda_{\text{max}}$ values in nm.

| Compound          | Absorption Spectra | Exp. $\lambda_{\text{max}}$ |
|-------------------|--------------------|-----------------------------|
| Px2BP in toluene  | ![Px2BP Spectra](image) | 234, 413                    |
| DMAC-BP in DCM    | ![DMAC-BP Spectra](image) | 370                         |
| Cz2BP in toluene  | ![Cz2BP Spectra](image) | 340, 353                    |
Table S6. Absorption spectra for CC2BP, A-BP-TA and OPDPO calculated at different levels of theory and experimental $\lambda_{\text{max}}$ values in nm.

| Compound      | Absorption Spectra          | Exp. $\lambda_{\text{max}}$ |
|---------------|-----------------------------|------------------------------|
| CC2BP in toluene | ![CC2BP Spectrum](image) | 345                          |
| A-BP-TA in THF  | ![A-BP-TA Spectrum](image) | 265, 285                     |
| OPDPO in THF   | ![OPDPO Spectrum](image)   | 348                          |
Table S7. Absorption spectra for DBT-BZ-PXZ, DBT-BZ-PTZ and DBT-BZ-DMAC calculated at different levels of theory and experimental $\lambda_{\text{max}}$ values in nm.

| Compound         | Method | $\Delta E_{\text{S1-T1}}$ | Exp. $\Delta E_{\text{ST}}$ |
|------------------|--------|----------------------------|-----------------------------|
| DBT-BZ-PXZ in THF |        |                           |                             |
| DBT-BZ-PTZ in THF |        |                           |                             |
| DBT-BZ-DMAC in THF |        |                           |                             |

**DBT-BZ-PXZ in THF**

![Absorption spectrum for DBT-BZ-PXZ](image)

Exp. $\lambda_{\text{max}}$: 394, 312

**DBT-BZ-PTZ in THF**

![Absorption spectrum for DBT-BZ-PTZ](image)

Exp. $\lambda_{\text{max}}$: 330

**DBT-BZ-DMAC in THF**

![Absorption spectrum for DBT-BZ-DMAC](image)

Exp. $\lambda_{\text{max}}$: 300
Table S8. \( \Delta E_{S1-T1} \) values (eV) calculated at different level of theories (BLYP, B3LYP, PBE0, M06-2X) for the geometries and Group 2 together with the experimental values.

| Theory | Px2BP | DMAC-BP | Cz2BP | CC2BP | A-BP-TA | OPDPO | DBT-BZ-PXZ | DBT-BZ-PTZ | DBT-BZ-DMAC |
|--------|-------|---------|-------|-------|---------|-------|------------|------------|------------|
| BLYP   | 0.004 | 0.04    | 0.099 | 0.017 | 0.004   | 0.033 | 0.004      | 0.004      | 0.004      |
| B3LYP  | 0.007 | 0.06    | 0.232 | 0.085 | 0.006   | 0.006 | 0.008      | 0.009      | 0.006      |
| PBE0   | 0.010 | 0.009   | 0.321 | 0.165 | 0.008   | 0.010 | 0.011      | 0.015      | 0.009      |
| M06-2X | 0.162 | 0.178   | 0.496 | 0.484 | 0.215   | 0.361 | 0.241      | 0.402      | 0.235      |

\( \Delta E_{S1-T1} \) calculated at level of (BLYP, PBE0, M06-2X) of Group 1 emitters with the
Figure S1. Histogram chart including $\Delta E_{S_1-T_1}$ values calculated at different level of theories for the $S_0$ geometries of Group 1 emitters together with the experimental values (The basis set is 6-31+G(d,p)).

Figure S2. Histogram chart including $\Delta E_{S_1-T_1}$ values calculated at different level of theories for the $S_0$ geometries of three molecules from Group 2 emitters together with the experimental values (The basis set is 6-31+G(d,p)).

Table S9. $\Delta E_{S_1-T_1}$ values (eV) calculated at different level of theories (BLYP, B3LYP, PBE0, CAM-B3LYP, LC-ωPBE) for the $S_0$ and $T_1$ geometries of selected emitters chosen from each group together with the experimental values.
| Compound | Method | $\Delta E_{S_{1}-T_{1}}$ (S$_0$ Geometry) | $\Delta E_{S_{1}-T_{1}}$ (T$_1$ Geometry) | Exp. $\Delta E_{ST}$ |
|----------|--------|----------------------------------------|----------------------------------------|---------------------|
| CC2BP    | BLYP   | 0.017                                  | 0.015                                  | 0.14                |
|          | B3LYP  | 0.085                                  | 0.284                                  |                     |
|          | PBE0   | 0.165                                  | 0.406                                  |                     |
|          | CAM-B3LYP | 0.660                                  | 0.889                                  |                     |
|          | LC-ωPBE | 0.692                                  | 1.079                                  |                     |
| CP-BP-DMAC | BLYP   | 0.004                                  | 0.006                                  | 0.016               |
|          | B3LYP  | 0.007                                  | 0.008                                  |                     |
|          | PBE0   | 0.010                                  | 0.011                                  |                     |
|          | CAM-B3LYP | 0.456                                  | 0.121                                  |                     |
|          | LC-ωPBE | 0.740                                  | 0.646                                  |                     |
| b1       | BLYP   | 0.085                                  | 0.088                                  | 0.24                |
|          | B3LYP  | 0.104                                  | 0.110                                  |                     |
|          | PBE0   | 0.124                                  | 0.097                                  |                     |
|          | CAM-B3LYP | 0.506                                  | 0.641                                  |                     |
|          | LC-ωPBE | 0.595                                  | 0.989                                  |                     |
| ACRXTN   | BLYP   | 0.006                                  | 0.006                                  | 0.06                |
|          | B3LYP  | 0.010                                  | 0.008                                  |                     |
|          | PBE0   | 0.013                                  | 0.011                                  |                     |
|          | CAM-B3LYP | 0.083                                  | 0.017                                  |                     |
|          | LC-ωPBE | 0.647                                  | 0.606                                  |                     |
| C1       | BLYP   | 0.060                                  | 0.101                                  | -                   |
|          | B3LYP  | 0.123                                  | 0.283                                  |                     |
|          | PBE0   | 0.161                                  | 0.343                                  |                     |
|          | CAM-B3LYP | 0.562                                  | 0.651                                  |                     |
|          | LC-ωPBE | 0.650                                  | 0.780                                  |                     |
| Compound          | Method | \( \Delta E_{S_1-T_1} \) (S\(_0\) Geometry) | \( \Delta E_{S_1-T_1} \) (S\(_1\) Geometry) | \( \Delta E_{S_1-T_1} \) (T\(_1\) Geometry) | Exp. \( \Delta E_{ST} \) |
|-------------------|--------|---------------------------------------------|---------------------------------------------|---------------------------------------------|-------------------------|
| Px2BP (Group 1)   | BLYP   | 0.004                                       | 0.005                                       | 0.165                                       | 0.03                    |
|                   | B3LYP  | 0.007                                       | 0.007                                       | 0.104                                       |                         |
|                   | PBE0   | 0.010                                       | 0.010                                       | 0.106                                       |                         |
| DBT-BZ-PXZ (Group 2) | BLYP  | 0.004                                       | 0.009                                       | 0.026                                       | 0.09                    |
|                   | B3LYP  | 0.008                                       | 0.012                                       | 0.018                                       |                         |
|                   | PBE0   | 0.011                                       | 0.014                                       | 0.020                                       |                         |
| a1 (Group 3)      | BLYP   | 0.254                                       | 0.005                                       | 0.309                                       | 0.29                    |
|                   | B3LYP  | 0.284                                       | 0.007                                       | 0.302                                       |                         |
|                   | PBE0   | 0.317                                       | 0.010                                       | 0.324                                       |                         |
| MCz-XT (Group 4)  | BLYP   | 0.006                                       | 0.006                                       | 0.009                                       | 0.011                   |
|                   | B3LYP  | 0.009                                       | 0.009                                       | 0.011                                       |                         |
|                   | PBE0   | 0.012                                       | 0.011                                       | 0.014                                       |                         |
| p-Cz (Non-TADF)   | BLYP   | 0.164                                       | 0.188                                       | 0.443                                       | 0.61                    |
|                   | B3LYP  | 0.275                                       | 0.325                                       | 0.613                                       |                         |
|                   | PBE0   | 0.358                                       | 0.442                                       | 0.697                                       |                         |

**Table S10.** \( \Delta E_{S_1-T_1} \) values (eV) calculated at different level of theories (BLYP, B3LYP, PBE0) for the \( S_0, S_1 \) and \( T_1 \) geometries of selected emitters chosen from each group together with the experimental values.
Figure S3. The 3D representations for the $S_0$ and $S_1$ optimized geometries of the compounds given in Table S10.

UV-Vis Absorption Spectra
Figure S4. Absorption spectra of Group 1 emitters calculated at different levels of theory. Full-width half maximum values (nm) are given as follows, Px2BP (51 for B3LYP, 61 for PBE0, 46 for BLYP), DMAC-BP (39 for B3LYP, 50 for PBE0, 61 for BLYP), Cz2BP (165 for B3LYP, 140 for PBE0, 109 for BLYP), CC2BP (70 for B3LYP, 31 for PBE0, 120 for BLYP), A-BP-TA (35 for B3LYP, 62 for PBE0, 48 for BLYP), OPDPO (44 for B3LYP, 48 for PBE0, 61 for BLYP)
Figure S5. Absorption spectra of Group 2 emitters calculated at different levels of theory. Full-width half maximum values (nm) are given as follows, DBT-BZ-PXZ (39 for B3LYP, 45 for PBE0, 38 for BLYP), DBT-BZ-PTZ (36 for B3LYP, 33 for PBE0, 77 for BLYP), DBT-BZ-DMAC (45 for B3LYP, 46 for PBE0, 35 for BLYP), CP-BP-PXZ (47 for B3LYP, 63 for PBE0, 42 for BLYP), CP-BP-DMAC (34 for B3LYP, 41 for PBE0, 105 for BLYP)
Figure S6. Absorption spectra of Group 3 emitters calculated at different level of theories. Full-width half maximum values (nm) are given as follows, a1 (29 for B3LYP, 43 for PBE0, 71 for BLYP), a2 (79 for B3LYP, 83 for PBE0, 114 for BLYP), a3 (40 for B3LYP, 37 for PBE0, 120 for BLYP), a4 (103 for B3LYP, 87 for PBE0, 192 for BLYP), b1 (37 for B3LYP, 51 for PBE0, 102 for BLYP), b4 (59 for B3LYP, 71 for PBE0, 83 for BLYP)
Figure S7. Absorption spectra of Group 4 emitters calculated at different level of theories. Full-width half maximum values (nm) are given as follows, ACRXTN (36 for B3LYP, 34 for PBE0, 29 for BLYP), MCz-XT (30 for B3LYP, 32 for PBE0, 21 for BLYP), 3-PXZ-XO (77 for B3LYP, 74 for PBE0, 101 for BLYP), PTZ-XT (70 for B3LYP, 36 for PBE0, 106 for BLYP)
**Figure S8.** Absorption spectra of non-TADF emitters calculated at different level of theories. Full-width half maximum values (nm) are given as follows, MC2 (9 for B3LYP, 21 for PBE0, 80 for BLYP), OPM (49 for B3LYP, 39 for PBE0, 160 for BLYP), p-Cz (56 for B3LYP, 31 for PBE0, 70 for BLYP), ODFRCZ (33 for B3LYP, 47 for PBE0, 44 for BLYP), ODBTCZ (71 for B3LYP, 85 for PBE0, 32 for BLYP), C1 (52 for B3LYP, 51 for PBE0, 59 for BLYP), C2 (42 for B3LYP, 55 for PBE0, 70 for BLYP).

**Table S11.** Oscillator strengths ($S_0 \rightarrow S_1$) for the $S_0$ and $T_1$ geometries of the investigated TADF and non-TADF calculated with B3LYP, PBE0 and BLYP functionals. (Basis set: 6-31+G(d,p))
| Group | Compound | S₀ Geometry | T₁ Geometry |
|-------|----------|-------------|-------------|
|       |          | B3LYP       | PBE0        | BLYP        | B3LYP       | PBE0        | BLYP        |
| Group 1 | Px2BP    | 0.0001      | 0.0001      | 0.0001      | 0.0833      | 0.0836      | 0.0074      |
|        | DMAC-BP  | 0.0000      | 0.0000      | 0.0000      | 0.0055      | 0.0056      | 0.0063      |
|        | Cz2BP    | 0.4329      | 0.4810      | 0.3080      | 0.6715      | 0.7240      | 0.5327      |
|        | CC2BP    | 0.2302      | 0.3003      | 0.0921      | 0.3716      | 0.4880      | 0.0608      |
|        | A-BP-TA  | 0.0006      | 0.0006      | 0.0006      | 0.0766      | 0.0854      | 0.0005      |
|        | OPDPO    | 0.0000      | 0.0000      | 0.0000      | 0.0001      | 0.0001      | 0.0001      |
| Group 2 | DBT-BZ-PXZ| 0.0004      | 0.0005      | 0.0004      | 0.0119      | 0.0121      | 0.0143      |
|        | DBT-BZ-PTZ| 0.0001      | 0.0001      | 0.0001      | 0.0000      | 0.0000      | 0.0000      |
|        | DBT-BZ-DMAC | 0.0002     | 0.0002      | 0.0003      | 0.0002      | 0.0002      | 0.0002      |
|        | CP-BP-PXZ | 0.0003      | 0.0004      | 0.0003      | 0.0042      | 0.0044      | 0.0044      |
|        | CP-BP-DMAC| 0.0002      | 0.0002      | 0.0002      | 0.0001      | 0.0001      | 0.0002      |
| Group 3 | a1       | 0.0000      | 0.0000      | 0.0000      | 0.0000      | 0.0000      | 0.0000      |
|        | a2       | 0.0000      | 0.0000      | 0.0000      | 0.0000      | 0.0000      | 0.0000      |
|        | a3       | 0.0000      | 0.0000      | 0.2612      | 0.0000      | 0.0000      | 0.3484      |
|        | a4       | 0.0000      | 0.0000      | 0.0000      | 0.0000      | 0.0000      | 0.0000      |
|        | b1       | 0.2969      | 0.2488      | 0.3055      | 0.3514      | 0.4725      | 0.2488      |
|        | b4       | 0.0000      | 0.0000      | 0.0004      | 0.0012      | 0.0012      | 0.0028      |
| Group 4 | ACRXTN   | 0.0001      | 0.0001      | 0.0001      | 0.0001      | 0.0000      | 0.0001      |
|        | MCz-XT   | 0.0001      | 0.0001      | 0.0001      | 0.0038      | 0.0040      | 0.0035      |
|        | PXZ-XO   | 0.0001      | 0.0001      | 0.0000      | 0.0554      | 0.0567      | 0.0609      |
|        | PTZ-XT   | 0.0000      | 0.0000      | 0.0000      | 0.0004      | 0.0004      | 0.0004      |
| Non-TADF | MC2     | 0.2864      | 0.3172      | 0.1991      | 0.7082      | 0.7434      | 0.5808      |
|        | OPM      | 0.4243      | 0.2618      | 0.1734      | 0.7383      | 0.4178      | 0.3451      |
|        | p-Cz     | 0.2581      | 0.2864      | 0.1810      | 0.6160      | 0.6530      | 0.4823      |
|        | ODFRCZ   | 0.2926      | 0.3295      | 0.1879      | 0.7291      | 0.7715      | 0.5642      |
|        | ODBTCZ   | 0.2895      | 0.3270      | 0.1904      | 0.3106      | 0.4829      | 0.1163      |
|        | C1       | 0.0042      | 0.0041      | 0.0048      | 0.0142      | 0.0167      | 0.0021      |
|        | C2       | 0.0010      | 0.0008      | 0.0013      | 0.0005      | 0.0005      | 0.0007      |

**Table S12.** Reorganization energies (kcal/mol) between the S₁ and S₀ geometries of selected compounds.
| Group   | Compound          | Reorganization Energy |
|---------|-------------------|-----------------------|
| Group 1 | Px2BP             | 12.63                 |
|         | Cz2BP             | 6.30                  |
|         | A-BP-TA           | 12.95                 |
|         | OPDPO             | 15.46                 |
| Group 2 | DBT-BZ-PXZ        | 10.84                 |
|         | DBT-BZ-PTZ        | 14.93                 |
|         | DBT-BZ-DMAC       | 10.42                 |
|         | CP-BP-PXZ         | 13.52                 |
|         | CP-BP-DMAC        | 12.94                 |
| Group 3 | a1                | 7.77                  |
|         | a4                | 8.45                  |
| Group 4 | ACRXTN           | 6.21                  |
|         | MCz-XT            | 6.99                  |
|         | PXZ-XO            | 8.66                  |
|         | PTZ-XT            | 12.27                 |
| Non-TADF | MC2               | 12.81                 |
|         | OPM               | 17.82                 |
|         | p-Cz              | 6.39                  |
|         | ODFRCZ            | 7.54                  |
|         | ODBTCZ            | 6.71                  |
|         | C1                | 6.13                  |
Table S13. 3D representations of the most stable ground state ($S_0$) and $T_1$ structures of Group 1 emitters along with the relative Gibbs free energies (kcal/mol) for the conformations, optimized at M06-2X/6-31+G(d,p) level of theory.

| Emitter           | Conf. | Rel. Gibbs Free Energy | Optimized Geometry at $S_0$ Level | Optimized Geometry at $T_1$ Level |
|-------------------|-------|------------------------|----------------------------------|----------------------------------|
| Px2BP in toluene  | 1     | 0.00                   | ![Image](image1)                  | ![Image](image2)                  |
|                   | 2     | 0.00                   | ![Image](image3)                  | ![Image](image4)                  |
|                   | 3     | 0.24                   | ![Image](image5)                  | ![Image](image6)                  |
|                   | 4     | 0.25                   | ![Image](image7)                  | ![Image](image8)                  |
|                   | 5     | 0.51                   | ![Image](image9)                  | ![Image](image10)                 |
|                   | 6     | 0.51                   | ![Image](image11)                 | ![Image](image12)                 |
| DMAC-BP in DCM    | 1     | 0.00                   | ![Image](image13)                 | ![Image](image14)                 |
|                   | 2     | 0.24                   | ![Image](image15)                 | ![Image](image16)                 |
| Cz2BP in toluene  | 1     | 0.00                   | ![Image](image17)                 | ![Image](image18)                 |
|                   | 2     | 0.01                   | ![Image](image19)                 | ![Image](image20)                 |
|                   | 3     | 0.12                   | ![Image](image21)                 | ![Image](image22)                 |
|                   | 4     | 0.13                   | ![Image](image23)                 | ![Image](image24)                 |
|                   | 5     | 0.28                   | ![Image](image25)                 | ![Image](image26)                 |
|                   | 6     | 0.30                   | ![Image](image27)                 | ![Image](image28)                 |
| CC2BP in toluene  | 1     | 0.00                   | ![Image](image29)                 | ![Image](image30)                 |
|                   | 2     | 0.10                   | ![Image](image31)                 | ![Image](image32)                 |
|                   | 3     | 0.17                   | ![Image](image33)                 | ![Image](image34)                 |
|                   | 4     | 0.31                   | ![Image](image35)                 | ![Image](image36)                 |
|                   | 5     | 0.40                   | ![Image](image37)                 | ![Image](image38)                 |
|                   | 6     | 0.56                   | ![Image](image39)                 | ![Image](image40)                 |
| A-BP-TA in THF    | 1     | 0.00                   | ![Image](image41)                 | ![Image](image42)                 |
|                   | 2     | 0.47                   | ![Image](image43)                 | ![Image](image44)                 |
|                   | 3     | 0.47                   | ![Image](image45)                 | ![Image](image46)                 |
|                   | 4     | 0.58                   | ![Image](image47)                 | ![Image](image48)                 |
|                   | 5     | 0.62                   | ![Image](image49)                 | ![Image](image50)                 |
|                   | 6     | 0.72                   | ![Image](image51)                 | ![Image](image52)                 |
|                   | 7     | 0.79                   | ![Image](image53)                 | ![Image](image54)                 |
|                   | 8     | 0.80                   | ![Image](image55)                 | ![Image](image56)                 |
| OPDPO in THF      | 1     | 0.00                   | ![Image](image57)                 | ![Image](image58)                 |
|                   | 2     | 0.14                   | ![Image](image59)                 | ![Image](image60)                 |
|                   | 3     | 0.26                   | ![Image](image61)                 | ![Image](image62)                 |
|                   | 4     | 0.47                   | ![Image](image63)                 | ![Image](image64)                 |
|                   | 5     | 0.53                   | ![Image](image65)                 | ![Image](image66)                 |
|                   | 6     | 0.92                   | ![Image](image67)                 | ![Image](image68)                 |
|                   | 7     | 0.95                   | ![Image](image69)                 | ![Image](image70)                 |
|                   | 8     | 2.84                   | ![Image](image71)                 | ![Image](image72)                 |

Table S14. 3D representations of the most stable ground state ($S_0$) and $T_1$ structures of Group 2 emitters along with the relative Gibbs free energies (kcal/mol) for the conformations, optimized at M06-2X/6-31+G(d,p) level of theory.

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Table S15. 3D representations of the most stable ground state (S\(_0\)) and T\(_1\) structures of Group 3 emitters along with the relative Gibbs free energies (kcal/mol) for the conformations, optimized at M06-2X/6-31+G(d,p) level of theory.

| Emitter          | Conf. | Rel. Gibbs Free Energy | Optimized Geometry at S\(_0\) Level | Optimized Geometry at T\(_1\) Level |
|------------------|-------|------------------------|-------------------------------------|-------------------------------------|
| DBT-BZ-PXZ in THF | 1     | 0.00                   | [Image]                             | [Image]                             |
|                  | 2     | 0.07                   | [Image]                             | [Image]                             |
|                  | 3     | 0.23                   | [Image]                             | [Image]                             |
|                  | 4     | 0.37                   | [Image]                             | [Image]                             |
| DBT-BZ-PTZ in THF| 1     | 0.00                   | [Image]                             | [Image]                             |
|                  | 2     | 0.15                   | [Image]                             | [Image]                             |
|                  | 3     | 0.25                   | [Image]                             | [Image]                             |
|                  | 4     | 0.57                   | [Image]                             | [Image]                             |
| DBT-BZ-DMAC in THF | 1 | 0.00                   | [Image]                             | [Image]                             |
|                  | 2     | 0.17                   | [Image]                             | [Image]                             |
| CP-BP-PXZ in THF | 1     | 0.00                   | [Image]                             | [Image]                             |
|                  | 2     | 0.10                   | [Image]                             | [Image]                             |
|                  | 3     | 0.10                   | [Image]                             | [Image]                             |
|                  | 4     | 0.15                   | [Image]                             | [Image]                             |
|                  | 5     | 0.18                   | [Image]                             | [Image]                             |
|                  | 6     | 0.23                   | [Image]                             | [Image]                             |
|                  | 7     | 0.35                   | [Image]                             | [Image]                             |
|                  | 8     | 0.44                   | [Image]                             | [Image]                             |
| CP-BP-DMAC in THF | 1 | 0.00                   | [Image]                             | [Image]                             |
|                  | 2     | 0.05                   | [Image]                             | [Image]                             |
|                  | 3     | 0.42                   | [Image]                             | [Image]                             |
|                  | 4     | 0.44                   | [Image]                             | [Image]                             |
|      | 1 |   |   |   |   |   |
|------|---|---|---|---|---|---|
| a1 in toluene | 1 | 0.00 |
| a2 in toluene | 1 | 0.00 |
| a3 in toluen | 1 | 0.00 | 0.04 | 0.05 |
| a4 in toluene | 1 | 0.00 |
| b1 in toluene | 1 | 0.00 | 0.02 | 0.37 | 0.47 | 0.69 | 0.87 |
| b4 in toluene | 1 | 0.00 | 0.45 | 0.49 |

**Table S16.** 3D representations of the most stable ground state ($S_0$) and $T_1$ structures of Group 4 emitters along with the relative Gibbs free energies (kcal/mol) for the conformations, optimized at M06-2X/6-31+G(d,p) level of theory.
| Emitter                  | Conf. | Rel. Gibbs Free Energy | Optimized Geometry at S₀ Level | Optimized Geometry at T₁ Level |
|-------------------------|-------|-----------------------|-------------------------------|-------------------------------|
| ACRXTN in DCM           | 1     | 0.00                  | ![Image](image1.png)          | ![Image](image2.png)          |
|                         | 2     | 0.63                  | ![Image](image3.png)          | ![Image](image4.png)          |
| MCz-XT in toluene       | 1     | 0.00                  | ![Image](image5.png)          | ![Image](image6.png)          |
|                         | 2     | 0.63                  | ![Image](image7.png)          | ![Image](image8.png)          |
| 3-PXZ-XO in toluene     | 1     | 0.00                  | ![Image](image9.png)          | ![Image](image10.png)         |
|                         | 2     | 0.10                  | ![Image](image11.png)         | ![Image](image12.png)         |
| PTZ-XT in THF           | 1     | 0.00                  | ![Image](image13.png)         | ![Image](image14.png)         |
|                         | 2     | 0.00                  | ![Image](image15.png)         | ![Image](image16.png)         |
|                         | 3     | 1.67                  | ![Image](image17.png)         | ![Image](image18.png)         |
|                         | 4     | 1.71                  | ![Image](image19.png)         | ![Image](image20.png)         |

**Table S17.** 3D representations of the most stable ground state (S₀) and T₁ structures of non-TADF emitters along with the relative Gibbs free energies (kcal/mol) for the conformations, optimized at M06-2X/6-31+G(d,p) level of theory.
| Emitter          | Conf. | Rel. Gibbs Free Energy | Optimized Geometry at S<sub>0</sub> Level | Optimized Geometry at T<sub>1</sub> Level |
|------------------|-------|------------------------|------------------------------------------|------------------------------------------|
| MC2 in toluene   | 1     | 0.00                   |                                          |                                          |
|                  | 2     | 0.03                   |                                          |                                          |
|                  | 3     | 0.03                   |                                          |                                          |
|                  | 4     | 0.16                   |                                          |                                          |
| OPM in toluene   | 1     | 0.00                   |                                          |                                          |
|                  | 2     | 0.03                   |                                          |                                          |
|                  | 3     | 0.13                   |                                          |                                          |
|                  | 4     | 0.27                   |                                          |                                          |
| p-Cz in THF      | 1     | 0.00                   |                                          |                                          |
|                  | 2     | 0.17                   |                                          |                                          |
|                  | 3     | 0.00                   |                                          |                                          |
|                  | 4     | 0.17                   |                                          |                                          |
| ODFRCZ in DCM    | 1     | 0.00                   |                                          |                                          |
|                  | 2     | 0.30                   |                                          |                                          |
|                  | 3     | 0.37                   |                                          |                                          |
|                  | 4     | 0.42                   |                                          |                                          |
| ODBTCZ in DCM    | 1     | 0.00                   |                                          |                                          |
|                  | 2     | 0.04                   |                                          |                                          |
|                  | 3     | 0.27                   |                                          |                                          |
|                  | 4     | 0.32                   |                                          |                                          |
| C1 in THF        | 1     | 0.00                   |                                          |                                          |
|                  | 2     | 0.03                   |                                          |                                          |
|                  | 3     | 0.50                   |                                          |                                          |
| C2 in THF        | 1     | 0.00                   |                                          |                                          |
|                  | 2     | 0.21                   |                                          |                                          |
|                  | 3     | 0.58                   |                                          |                                          |

Investigated Donor-Acceptor Torsion Angles
Figure S9. Group 1 emitters together with their analyzed torsion angles (For A-BP-TA, $\theta_1$ has been taken for the $S_0$ optimized geometry, $\theta_2$ has been taken for the $T_1$ optimized geometry).

Figure S10. Group 2 emitters with together their analyzed torsion angles.
Figure S11. Group 3 emitters together with their analyzed torsion angles (For b1, $\theta_1$ has been taken for the $S_0$ optimized geometry, $\theta_2$ has been taken for the $T_1$ optimized geometry).

Figure S12. Group 4 emitters together with their analyzed torsion angles.
Figure S13. Non-TADF emitters together with their analyzed torsion angles.
Table S18. Measured torsion angles of the $S_0$ and $T_1$ optimized geometries of the investigated compounds.

| Group | Compound   | Torsion Angle ($\theta$) from the $S_0$ Optimized Geometry | Torsion Angle ($\theta$) from the $T_1$ Optimized Geometry |
|-------|------------|------------------------------------------------------------|------------------------------------------------------------|
|       |            |                                                             |                                                             |
| Group 1|            |                                                             |                                                             |
|       | Px2BP      | 76.41                                                      | 107.90                                                     |
|       | DMAC-BP    | 90.29                                                      | 90.91                                                      |
|       | Cz2BP      | 51.43                                                      | 48.19                                                      |
|       | CC2BP      | 54.35                                                      | 43.33                                                      |
|       | A-BP-TA    | 89.41                                                      | 38.90                                                      |
|       | OPDPO      | 76.93                                                      | 90.06                                                      |
| Group 2|            |                                                             |                                                             |
|       | DBT-BZ-PXZ | 76.10                                                      | 83.84                                                      |
|       | DBT-BZ-PTZ | 101.79                                                     | 90.21                                                      |
|       | DBT-BZ-DMAC| 90.14                                                      | 90.11                                                      |
|       | CP-BP-PXZ  | 77.26                                                      | 93.80                                                      |
|       | CP-BP-DMAC | 89.82                                                      | 88.90                                                      |
| Group 3|            |                                                             |                                                             |
|       | a1         | 28.01                                                      | 30.54                                                      |
|       | a2         | 28.81                                                      | 33.32                                                      |
|       | a3         | 47.84                                                      | 45.42                                                      |
|       | a4         | 90.95                                                      | 90.67                                                      |
|       | b1         | 36.16                                                      | 39.68                                                      |
|       | b4         | 89.40                                                      | 91.00                                                      |
| Group 4|            |                                                             |                                                             |
|       | ACRXTN     | 87.79                                                      | 90.21                                                      |
|       | MCz-XT     | 106.62                                                     | 92.89                                                      |
|       | 3-PXZ-XO   | 75.81                                                      | 74.04                                                      |
|       | PTZ-XT     | 101.64                                                     | 91.49                                                      |
| Non-TADF|            |                                                             |                                                             |
|       | MC2        | 52.06                                                      | 41.45                                                      |
|       | OPM        | 21.76                                                      | 10.05                                                      |
|       | p-Cz       | 51.59                                                      | 43.66                                                      |
|       | ODFRCZ     | 51.45                                                      | 43.69                                                      |
|       | ODBTCZ     | 52.73                                                      | 54.20                                                      |
|       | C1         | 53.63                                                      | 41.19                                                      |
|       | C2         | 79.38                                                      | 95.14                                                      |
### Occupied and Virtual NTOs

**Table S19.** Hole and electron NTOs for Px2BP, DMAC-BP and Cz2BP (TDA: B3LYP/6-31+G(d,p)).

| Compound | Hole | Electron |
|----------|------|----------|
|          | ![S0 Optimization](image1) | ![S0 Optimization](image2) |
| Px2BP    | ![T1 Optimization](image3) | ![T1 Optimization](image4) |
|          | ![S0 Optimization](image5) | ![S0 Optimization](image6) |
| DMAC-BP  | ![T1 Optimization](image7) | ![T1 Optimization](image8) |
|          | ![S0 Optimization](image9) | ![S0 Optimization](image10) |
| Cz2BP    | ![T1 Optimization](image11) | ![T1 Optimization](image12) |
Table S20. Hole and electron NTOs for CC2BP, A-BP-TA and OPDPO (TDA: B3LYP/6-31+G(d,p)).

| Compound | Hole | Electron |
|----------|------|----------|
|          | ![CC2BP Hole S0 Optimization](image) | ![CC2BP Electron S0 Optimization](image) |
|          | ![CC2BP Hole T1 Optimization](image) | ![CC2BP Electron T1 Optimization](image) |
|          | ![A-BP-TA Hole S0 Optimization](image) | ![A-BP-TA Electron S0 Optimization](image) |
|          | ![A-BP-TA Hole T1 Optimization](image) | ![A-BP-TA Electron T1 Optimization](image) |
|          | ![OPDPO Hole S0 Optimization](image) | ![OPDPO Electron S0 Optimization](image) |
|          | ![OPDPO Hole T1 Optimization](image) | ![OPDPO Electron T1 Optimization](image) |
**Table S21.** Hole and electron NTOs for DBT-BZ-PXZ, DBT-BZ-PTZ and DBT-BZ-DMAC (TDA: B3LYP/6-31+G(d,p)).

| Molecule     | Hole | Electron |
|--------------|------|----------|
| **S0 Optimization** | ![Hole S0 DBT-BZ-PXZ](image) | ![Electron S0 DBT-BZ-PXZ](image) |
| **T1 Optimization** | ![Hole T1 DBT-BZ-PXZ](image) | ![Electron T1 DBT-BZ-PXZ](image) |
| **S0 Optimization** | ![Hole S0 DBT-BZ-PTZ](image) | ![Electron S0 DBT-BZ-PTZ](image) |
| **T1 Optimization** | ![Hole T1 DBT-BZ-PTZ](image) | ![Electron T1 DBT-BZ-PTZ](image) |
| **S0 Optimization** | ![Hole S0 DBT-BZ-DMAC](image) | ![Electron S0 DBT-BZ-DMAC](image) |
| **T1 Optimization** | ![Hole T1 DBT-BZ-DMAC](image) | ![Electron T1 DBT-BZ-DMAC](image) |
Table S22. Hole and electron NTOs for CP-BP-PXZ and CP-BP-DMAC. (TDA: B3LYP/6-31+G(d,p)).

| Molecule   | Hole     | Electron     |
|------------|----------|--------------|
|            | $S_0$ Optimization | $T_1$ Optimization |
| CP-BP-PXZ  | ![Hole](image1) ![Electron](image2) | ![Hole](image3) ![Electron](image4) |
| CP-BP-DMAC | ![Hole](image5) ![Electron](image6) | ![Hole](image7) ![Electron](image8) |
Table S23. Hole and electron NTOs for a1, a2 and a3. (TDA: B3LYP/6-31+G(d,p)).

| Molecule | Hole | Electron |
|----------|------|----------|
| a1       | ![Hole Image] | ![Electron Image] |
| a2       | ![Hole Image] | ![Electron Image] |
| a3       | ![Hole Image] | ![Electron Image] |
Table S24. Hole and electron NTOs for a4, b1 and b4. (TDA: B3LYP/6-31+G(d,p)).

| Molecule | Hole | Electron |
|----------|------|----------|
| **S₂ Optimization** | ![Image] | ![Image] |
| a4       | ![Image] | ![Image] |
| **T₁ Optimization** | ![Image] | ![Image] |
| b1       | ![Image] | ![Image] |
| **S₂ Optimization** | ![Image] | ![Image] |
| b4       | ![Image] | ![Image] |
Table S25. Hole and electron NTOs for ACRXTN, MCz-XT and 3-PXZ-XO (TDA: B3LYP/6-31+G(d,p)).

| Molecule  | Hole | Electron |
|-----------|------|----------|
| ACRXTN    | ![Hole Optimization](image1) | ![Electron Optimization](image2) |
|           | ![S0 Optimization](image3) | ![T1 Optimization](image4) |
| MCz-XT    | ![Hole Optimization](image5) | ![Electron Optimization](image6) |
|           | ![S0 Optimization](image7) | ![T1 Optimization](image8) |
| 3-PXZ-XO  | ![Hole Optimization](image9) | ![Electron Optimization](image10) |
|           | ![S0 Optimization](image11) | ![T1 Optimization](image12) |
Table S26. Hole and electron NTOs for PTZ-XT, MC2 and OPM (TDA: B3LYP/6-31+G(d,p)).

| Molecule | Hole | Electron |
|----------|------|----------|
| PTZ-XT   | ![Hole](image1) | ![Electron](image2) |
|          | ![S₂ Optimization](image3) | ![T₁ Optimization](image4) |
| MC2      | ![Hole](image5) | ![Electron](image6) |
|          | ![S₂ Optimization](image7) | ![T₁ Optimization](image8) |
| OPM      | ![Hole](image9) | ![Electron](image10) |
|          | ![S₂ Optimization](image11) | ![T₁ Optimization](image12) |
Table S27. Hole and electron NTOs for \( p \)-Cz, ODFRCZ and ODBTCZ (TDA: B3LYP/6-31+G(d,p)).

| Molecule | Hole | Electron |
|----------|------|----------|
| \( p \)-Cz | ![Hole](image1) | ![Electron](image2) |
|           | ![S\(_0\) Optimization](image3) | ![T\(_1\) Optimization](image4) |
| ODFRCZ   | ![Hole](image5) | ![Electron](image6) |
|           | ![S\(_0\) Optimization](image7) | ![T\(_1\) Optimization](image8) |
| ODBTCZ   | ![Hole](image9) | ![Electron](image10) |
|           | ![S\(_0\) Optimization](image11) | ![T\(_1\) Optimization](image12) |
Table S28. Hole and electron NTOs for C1 and C2 (TDA: B3LYP/6-31+G(d,p)).

| Molecule | Hole | Electron |
|----------|------|----------|
|          | ![Hole S0 Optimization](image1) | ![Electron S0 Optimization](image2) |
|          | ![Hole T1 Optimization](image3) | ![Electron T1 Optimization](image4) |

**C1**

**C2**
Φ, Indices

**Table S29.** Φ indices for Group 1 emitters in Lowdin (L) and Mulliken (M) charge distributions for the excitations from S₀ to S₁ calculated with different functionals.

| Compound  | Transition | Method | S₀ Geometry | T₁ Geometry |
|-----------|------------|--------|-------------|-------------|
|           |            |        | L           | M           | L           | M           |
| Px2BP     | S₀ → S₁    | BLYP   | 0.2055      | 0.3682      | 0.3708      | 0.4718      |
|           |            | B3LYP  | 0.2191      | 0.3793      | 0.6097      | 0.7479      |
|           |            | PBE0   | 0.2594      | 0.4034      | 0.5827      | 0.7093      |
| DMAC-BP   | S₀ → S₁    | BLYP   | 0.2250      | 0.3392      | 0.1939      | 0.2765      |
|           |            | B3LYP  | 0.2488      | 0.3519      | 0.1991      | 0.2920      |
|           |            | PBE0   | 0.2515      | 0.3240      | 0.2169      | 0.2911      |
| Cz2BP     | S₀ → S₁    | BLYP   | 0.3584      | 0.4066      | 0.4085      | 0.4703      |
|           |            | B3LYP  | 0.4209      | 0.4763      | 0.4603      | 0.5073      |
|           |            | PBE0   | 0.4596      | 0.5099      | 0.4904      | 0.5269      |
| CC2BP     | S₀ → S₁    | BLYP   | 0.1807      | 0.2195      | 0.2586      | 0.2972      |
|           |            | B3LYP  | 0.3059      | 0.3566      | 0.5206      | 0.6021      |
|           |            | PBE0   | 0.3703      | 0.4126      | 0.5681      | 0.6363      |
| A-BP-TA   | S₀ → S₁    | BLYP   | 0.0642      | 0.1109      | 0.1226      | 0.1942      |
|           |            | B3LYP  | 0.0943      | 0.1396      | 0.4509      | 0.5170      |
|           |            | PBE0   | 0.1208      | 0.1489      | 0.4743      | 0.5342      |
| OPDPO     | S₀ → S₁    | BLYP   | 0.2336      | 0.2336      | 0.1213      | 0.1477      |
|           |            | B3LYP  | 0.2019      | 0.2609      | 0.1009      | 0.1265      |
|           |            | PBE0   | 0.2183      | 0.2777      | 0.1255      | 0.1427      |
Table S30. $\Phi_s$ indices for Group 2 emitters in Lowdin (L) and Mulliken (M) charge distributions for the excitations from $S_0$ to $S_1$ calculated with different functionals.

| Compound     | Transition | Method  | $S_0$ Geometry | $T_1$ Geometry |
|--------------|------------|---------|----------------|----------------|
|              |            |         | L              | M              | L              | M              |
| DBT-BZ-PXZ   | $S_0 \rightarrow S_1$ | BLYP    | 0.1763         | 0.2764         | 0.1633         | 0.2490         |
|              |            | B3LYP   | 0.1667         | 0.2660         | 0.1279         | 0.2146         |
|              |            | PBE0    | 0.1774         | 0.2641         | 0.1318         | 0.2060         |
| DBT-BZ-PTZ   | $S_0 \rightarrow S_1$ | BLYP    | 0.1991         | 0.3187         | 0.1372         | 0.1827         |
|              |            | B3LYP   | 0.2825         | 0.4175         | 0.1480         | 0.2004         |
|              |            | PBE0    | 0.3762         | 0.4940         | 0.1531         | 0.1988         |
| DBT-BZ-DMAC  | $S_0 \rightarrow S_1$ | BLYP    | 0.1057         | 0.1781         | 0.1359         | 0.1978         |
|              |            | B3LYP   | 0.1080         | 0.1814         | 0.1967         | 0.2656         |
|              |            | PBE0    | 0.1274         | 0.1767         | 0.1998         | 0.2473         |
| CP-BP-PXZ    | $S_0 \rightarrow S_1$ | BLYP    | 0.1743         | 0.2630         | 0.1425         | 0.2189         |
|              |            | B3LYP   | 0.1994         | 0.2907         | 0.1494         | 0.2357         |
|              |            | PBE0    | 0.2185         | 0.2949         | 0.1695         | 0.2403         |
| CP-BP-DMAC   | $S_0 \rightarrow S_1$ | BLYP    | 0.1162         | 0.1958         | 0.1163         | 0.1753         |
|              |            | B3LYP   | 0.1618         | 0.2473         | 0.1514         | 0.2138         |
|              |            | PBE0    | 0.1634         | 0.2198         | 0.1639         | 0.2136         |
Table S31. Φ_s indices for Group 3 emitters in Lowdin (L) and Mulliken (M) charge distributions for the excitations from S_0 to S_1 calculated with different functionals.

| Compound | Transition | Method | \( S_0 \) Geometry | \( T_1 \) Geometry |
|----------|------------|--------|-----------------|-----------------|
|          |            |        | \( L \) | \( M \) | \( L \) | \( M \) |
| a1       | \( S_0 \to S_1 \) | BLYP   | 0.6604 | 0.7240 | 0.6843 | 0.7351 |
|          |            | B3LYP  | 0.6685 | 0.7327 | 0.6839 | 0.7329 |
|          |            | PBE0   | 0.6625 | 0.7143 | 0.6833 | 0.7260 |
| a2       | \( S_0 \to S_1 \) | BLYP   | 0.6932 | 0.7263 | 0.6253 | 0.7404 |
|          |            | B3LYP  | 0.6704 | 0.7094 | 0.6992 | 0.7284 |
|          |            | PBE0   | 0.6780 | 0.7128 | 0.7124 | 0.7476 |
| a3       | \( S_0 \to S_1 \) | BLYP   | 0.4419 | 0.4952 | 0.4780 | 0.5468 |
|          |            | B3LYP  | 0.5299 | 0.5520 | 0.5689 | 0.5896 |
|          |            | PBE0   | 0.5827 | 0.5973 | 0.6219 | 0.6335 |
| a4       | \( S_0 \to S_1 \) | BLYP   | 0.0444 | 0.0475 | 0.0497 | 0.0552 |
|          |            | B3LYP  | 0.0607 | 0.0634 | 0.0546 | 0.0591 |
|          |            | PBE0   | 0.0611 | 0.0601 | 0.0597 | 0.0614 |
| b1       | \( S_0 \to S_1 \) | BLYP   | 0.4099 | 0.4517 | 0.3369 | 0.3588 |
|          |            | B3LYP  | 0.3682 | 0.3996 | 0.3627 | 0.3784 |
|          |            | PBE0   | 0.4419 | 0.4656 | 0.5492 | 0.5688 |
| b4       | \( S_0 \to S_1 \) | BLYP   | 0.0262 | 0.0549 | 0.0408 | 0.0730 |
|          |            | B3LYP  | 0.0929 | 0.1262 | 0.0544 | 0.0862 |
|          |            | PBE0   | 0.1075 | 0.1335 | 0.0817 | 0.1082 |
**Table S32.** $\Phi_s$ indices for Group 4 emitters in Lowdin (L) and Mulliken (M) charge distributions for the excitations from $S_0$ to $S_1$ calculated with different functionals.

| Compound | Transition | Method | $S_0$ Geometry | $T_1$ Geometry |
|----------|------------|--------|----------------|----------------|
|          |            |        | L   | M   | L   | M   |
| ACRXTN   | $S_0 \rightarrow S_1$ | BLYP   | 0.0460 | 0.0622 | 0.0516 | 0.0628 |
|          |            | B3LYP  | 0.0610 | 0.0820 | 0.0595 | 0.0711 |
|          |            | PBE0   | 0.0803 | 0.1056 | 0.0665 | 0.0767 |
| MCz-XT   | $S_0 \rightarrow S_1$ | BLYP   | 0.0682 | 0.1062 | 0.1272 | 0.1371 |
|          |            | B3LYP  | 0.1038 | 0.1531 | 0.1199 | 0.1294 |
|          |            | PBE0   | 0.1117 | 0.1402 | 0.1244 | 0.1323 |
| 3-PXZ-XO | $S_0 \rightarrow S_1$ | BLYP   | 0.0507 | 0.0885 | 0.3427 | 0.4065 |
|          |            | B3LYP  | 0.0767 | 0.1311 | 0.3243 | 0.3972 |
|          |            | PBE0   | 0.0918 | 0.1535 | 0.2937 | 0.3537 |
| PTZ-XT   | $S_0 \rightarrow S_1$ | BLYP   | 0.0776 | 0.1619 | 0.0706 | 0.0757 |
|          |            | B3LYP  | 0.1028 | 0.1755 | 0.0721 | 0.0760 |
|          |            | PBE0   | 0.1178 | 0.1796 | 0.0810 | 0.0841 |
Table S33. \( \Phi \) indices for non-TADF emitters in Lowdin (L) and Mulliken (M) charge distributions for the excitations from \( S_0 \) to \( S_1 \) calculated with different functionals.

| Compound | Transition | Method | \( S_0 \) Geometry | \( T_1 \) Geometry |
|----------|------------|--------|--------------------|-------------------|
|          |            |        | L      | M      | L      | M      |
| MC2      | \( S_0 \rightarrow S_1 \) | BLYP   | 0.4323 | 0.4719 | 0.5595 | 0.5967 |
|          |            | B3LYP  | 0.4643 | 0.5079 | 0.5879 | 0.6259 |
|          |            | PBE0   | 0.4913 | 0.5304 | 0.6026 | 0.6384 |
| OPM      | \( S_0 \rightarrow S_1 \) | BLYP   | 0.4026 | 0.4926 | 0.4907 | 0.5580 |
|          |            | B3LYP  | 0.5535 | 0.6354 | 0.6566 | 0.7241 |
|          |            | PBE0   | 0.5611 | 0.6271 | 0.6043 | 0.6658 |
| \( p\)-Cz | \( S_0 \rightarrow S_1 \) | BLYP   | 0.3970 | 0.4344 | 0.5410 | 0.5907 |
|          |            | B3LYP  | 0.4389 | 0.4847 | 0.5675 | 0.6088 |
|          |            | PBE0   | 0.4885 | 0.5292 | 0.5923 | 0.6335 |
| ODFRCZ   | \( S_0 \rightarrow S_1 \) | BLYP   | 0.3811 | 0.4128 | 0.5612 | 0.6112 |
|          |            | B3LYP  | 0.4664 | 0.5039 | 0.5936 | 0.6435 |
|          |            | PBE0   | 0.4965 | 0.5273 | 0.6101 | 0.6540 |
| ODBTCZ   | \( S_0 \rightarrow S_1 \) | BLYP   | 0.4692 | 0.4929 | 0.4296 | 0.4722 |
|          |            | B3LYP  | 0.5648 | 0.5846 | 0.4911 | 0.5257 |
|          |            | PBE0   | 0.5989 | 0.6107 | 0.5548 | 0.5862 |
| C1       | \( S_0 \rightarrow S_1 \) | BLYP   | 0.3273 | 0.3846 | 0.2953 | 0.3449 |
|          |            | B3LYP  | 0.3624 | 0.4358 | 0.4369 | 0.5282 |
|          |            | PBE0   | 0.4214 | 0.4902 | 0.4764 | 0.5549 |
| C2       | \( S_0 \rightarrow S_1 \) | BLYP   | 0.5548 | 0.6764 | 0.3857 | 0.4607 |
|          |            | B3LYP  | 0.5380 | 0.6559 | 0.4208 | 0.5038 |
|          |            | PBE0   | 0.4828 | 0.5937 | 0.4114 | 0.4866 |
Figure S14. $\Phi_s$ indices for the TADF emitters calculated from $S_0$ and $T_1$ geometries with PBE0/6-31+G(d,p).

Figure S15. $\Phi_s$ indices for the TADF emitters calculated from $S_0$ and $T_1$ geometries with BLYP/6-31+G(d,p).
Low Lying Singlet-Triplet Energy Gaps

Table S34. Low lying singlet-triplet energy gaps ($\Delta E_{S1-T1}$, $\Delta E_{S1-T2}$) in eV for Group 1 emitters together with the experimental values.

| Compound | Method | $S_0$ Geometry | $T_1$ Geometry | Exp. $\Delta E_{ST}$ |
|----------|--------|----------------|----------------|---------------------|
|          |        | $\Delta E_{S1-T1}$ | $\Delta E_{S1-T2}$ | $\Delta E_{S1-T1}$ | $\Delta E_{S1-T2}$ |         |
| Px2BP    | BLYP   | 0.004          | 0.002          | 0.165               | -                   | 0.03    |
|          | B3LYP  | 0.007          | 0.005          | 0.104               | -                   |         |
|          | PBE0   | 0.010          | 0.007          | 0.106               | -                   |         |
| DMAC-BP  | BLYP   | 0.004          | 0.001          | 0.014               | -                   | 0.07    |
|          | B3LYP  | 0.006          | 0.003          | 0.013               | -                   |         |
|          | PBE0   | 0.009          | 0.006          | 0.017               | -                   |         |
| Cz2BP    | BLYP   | 0.099          | 0.090          | 0.149               | 0.138               | 0.21    |
|          | B3LYP  | 0.232          | 0.165          | 0.278               | 0.224               |         |
|          | PBE0   | 0.321          | 0.216          | 0.366               | 0.271               |         |
| CC2BP    | BLYP   | 0.017          | 0.013          | 0.015               | -                   | 0.14    |
|          | B3LYP  | 0.085          | 0.069          | 0.284               | 0.013               |         |
|          | PBE0   | 0.165          | 0.114          | 0.406               | 0.025               |         |
| A-BP-TA  | BLYP   | 0.004          | -              | 0.066               | 0.002               | 0.06    |
|          | B3LYP  | 0.006          | -              | 0.225               | -                   |         |
|          | PBE0   | 0.008          | -              | 0.275               | -                   |         |
| OPDPO    | BLYP   | 0.003          | -              | 0.003               | -                   | 0.02    |
|          | B3LYP  | 0.006          | -              | 0.004               | -                   |         |
|          | PBE0   | 0.010          | -              | 0.005               | -                   |         |
Table S35. Low lying singlet-triplet energy gaps ($\Delta E_{S1-T1}$) in eV for Group 2 emitters together with the experimental values.

| Compound   | Method | $S_0$ Geometry $\Delta E_{S1-T1}$ | $T_1$ Geometry $\Delta E_{S1-T1}$ | Exp. $\Delta E_{ST}$ |
|------------|--------|-------------------------------|-------------------------------|-------------------|
| DBT-BZ-PXZ | BLYP   | 0.004                         | 0.026                         | 0.09              |
|            | B3LYP  | 0.008                         | 0.018                         |                   |
|            | PBE0   | 0.011                         | 0.020                         |                   |
| DBT-BZ-PTZ | BLYP   | 0.004                         | 0.004                         | 0.05              |
|            | B3LYP  | 0.009                         | 0.005                         |                   |
|            | PBE0   | 0.015                         | 0.007                         |                   |
| DBT-BZ-DMAC| BLYP   | 0.004                         | 0.002                         | 0.08              |
|            | B3LYP  | 0.006                         | 0.004                         |                   |
|            | PBE0   | 0.009                         | 0.009                         |                   |
| CP-BP-PXZ  | BLYP   | 0.005                         | 0.011                         | 0.024             |
|            | B3LYP  | 0.009                         | 0.011                         |                   |
|            | PBE0   | 0.013                         | 0.013                         |                   |
| CP-BP-DMAC | BLYP   | 0.004                         | 0.006                         | 0.016             |
|            | B3LYP  | 0.007                         | 0.008                         |                   |
|            | PBE0   | 0.010                         | 0.011                         |                   |
Table S36. Low lying singlet-triplet energy gaps ($\Delta E_{S1-T1}$, $\Delta E_{S1-T2}$) in eV for Group 3 emitters together with the experimental values.

| Compound | Method | $S_0$ Geometry | $T_1$ Geometry | Exp. $\Delta E_{ST}$ |
|----------|--------|----------------|----------------|---------------------|
|          |        | $\Delta E_{S1-T1}$ | $\Delta E_{S1-T2}$ | $\Delta E_{S1-T1}$ | $\Delta E_{S1-T2}$ |
| a1       | BLYP   | 0.375           | 0.254           | 0.440         | 0.309         | 0.29 |
|          | B3LYP  | 0.443           | 0.284           | 0.481         | 0.302         |
|          | PBE0   | 0.483           | 0.317           | 0.513         | 0.324         |
| a2       | BLYP   | 0.338           | 0.238           | 0.376         | 0.277         | 0.27 |
|          | B3LYP  | 0.398           | 0.258           | 0.428         | 0.280         |
|          | PBE0   | 0.435           | 0.286           | 0.455         | 0.295         |
| a3       | BLYP   | 0.182           | 0.138           | 0.239         | 0.183         | 0.17 |
|          | B3LYP  | 0.211           | 0.138           | 0.272         | 0.177         |
|          | PBE0   | 0.234           | 0.151           | 0.291         | 0.184         |
| a4       | BLYP   | 0.005           | 0.004           | 0.005         | 0.004         | 0.08 |
|          | B3LYP  | 0.008           | 0.004           | 0.007         | 0.004         |
|          | PBE0   | 0.010           | 0.005           | 0.008         | 0.004         |
| b1       | BLYP   | 0.107           | 0.085           | 0.127         | 0.088         | 0.24 |
|          | B3LYP  | 0.150           | 0.104           | 0.346         | 0.110         |
|          | PBE0   | 0.179           | 0.124           | 0.400         | 0.097         |
| b4       | BLYP   | 0.001           | 0.001           | 0.002         | 0.002         | 0.07 |
|          | B3LYP  | 0.001           | 0.001           | 0.001         | 0.001         |
|          | PBE0   | 0.001           | 0.001           | 0.001         | 0.001         |
Table S37. Low lying singlet-triplet energy gaps ($\Delta E_{S1-T1}$) in eV for Group 4 emitters together with the experimental values.

| Compound  | Method | $S_0$ Geometry | $T_1$ Geometry | Exp. $\Delta E_{ST}$ |
|-----------|--------|----------------|----------------|----------------------|
| ACRXTN    | BLYP   | 0.006          | 0.006          | 0.06                 |
|           | B3LYP  | 0.010          | 0.008          |                      |
|           | PBE0   | 0.013          | 0.011          |                      |
| MCz-XT    | BLYP   | 0.006          | 0.009          | 0.011                |
|           | B3LYP  | 0.009          | 0.011          |                      |
|           | PBE0   | 0.012          | 0.014          |                      |
| 3-PXZ-XO  | BLYP   | 0.006          | 0.089          | 0.036                |
|           | B3LYP  | 0.011          | 0.066          |                      |
|           | PBE0   | 0.015          | 0.070          |                      |
| PTZ-XT    | BLYP   | 0.006          | 0.012          | 0.071                |
|           | B3LYP  | 0.013          | 0.018          |                      |
|           | PBE0   | 0.020          | 0.022          |                      |
**Table S38.** Low lying singlet-triplet energy gaps ($\Delta E_{S1-T1}$, $\Delta E_{S1-T2}$) in eV for non-TADF emitters together with the experimental values.

| Compound | Method | $S_0$ Geometry | $T_1$ Geometry | Exp. $\Delta E_{ST}$ |
|----------|--------|----------------|----------------|---------------------|
|          | $\Delta E_{S1-T1}$ | $\Delta E_{S1-T2}$ | $\Delta E_{S1-T1}$ | $\Delta E_{S1-T2}$ |
| MC2      | BLYP   | 0.152          | -              | 0.445              | 0.118              | 0.23          |
|          | B3LYP  | 0.289          | 0.037          | 0.651              | 0.152              |
|          | PBE0   | 0.392          | 0.170          | 0.743              | 0.241              |
| OPM      | BLYP   | 0.338          | -              | 0.595              | 0.220              | -             |
|          | B3LYP  | 0.667          | 0.307          | 0.944              | 0.350              |
|          | PBE0   | 0.755          | 0.436          | 1.019              | 0.422              |
| p-Cz     | BLYP   | 0.164          | -              | 0.443              | -                  | 0.61          |
|          | B3LYP  | 0.275          | -              | 0.613              | 0.011              |
|          | PBE0   | 0.358          | 0.053          | 0.697              | 0.127              |
| ODFRCZ   | BLYP   | 0.131          | -              | 0.372              | -                  |
|          | B3LYP  | 0.238          | 0.038          | 0.553              | 0.024              |
|          | PBE0   | 0.322          | 0.187          | 0.637              | 0.124              |
| ODBTCZ   | BLYP   | 0.124          | -              | 0.059              | -                  |
|          | B3LYP  | 0.218          | 0.048          | 0.591              | -                  |
|          | PBE0   | 0.292          | 0.179          | 0.765              | -                  |
| C1       | BLYP   | 0.060          | 0.057          | 0.101              | -                  |
|          | B3LYP  | 0.123          | 0.118          | 0.283              | -                  |
|          | PBE0   | 0.161          | 0.156          | 0.343              | -                  |
| C2       | BLYP   | 0.012          | -              | 0.011              | -                  | 0.57          |
|          | B3LYP  | 0.019          | -              | 0.016              | -                  |
|          | PBE0   | 0.026          | 0.004          | 0.019              | -                  |
Figure S16. $\Delta E_{ST}$ values for TADF emitters calculated from $S_0$ and $T_1$ geometries with PBE0/6-31+G(d,p). (Experimental $\Delta E_{ST}$ values also included)

Figure S17. $\Delta E_{ST}$ values for TADF emitters calculated from $S_0$ and $T_1$ geometries with BLYP/6-31+G(d,p). (Experimental $\Delta E_{ST}$ values also included)
### Spin-Orbit Coupling Values

**Table S39.** Spin-orbit coupling (SOC) values between different energy states for the $T_1$ geometries of Group 1 emitters.

| Compound | Method  | SOC       |
|----------|---------|-----------|
|          |         | $S_1-T_1$ | $S_1-T_2$ |
| Px2BP    | BLYP    | 0.060     | -         |
|          | B3LYP   | 0.073     | -         |
|          | PBE0    | 0.086     | -         |
| DMAC-BP  | BLYP    | 0.020     | -         |
|          | B3LYP   | 0.037     | -         |
|          | PBE0    | 0.045     | -         |
| Cz2BP    | BLYP    | 0.057     | 0.158     |
|          | B3LYP   | 0.465     | 0.105     |
|          | PBE0    | 0.565     | 0.117     |
| CC2BP    | BLYP    | 0.048     | -         |
|          | B3LYP   | 0.942     | 0.868     |
|          | PBE0    | 1.231     | 2.142     |
| A-BP-TA  | BLYP    | 0.764     | -         |
|          | B3LYP   | 0.999     | -         |
|          | PBE0    | 1.068     | 0.291     |
| OPDPO    | BLYP    | 0.003     | -         |
|          | B3LYP   | 0.004     | -         |
|          | PBE0    | 0.004     | -         |
Table S40. Spin-orbit coupling (SOC) values between S₁ and T₁ for the T₁ geometries of Group 2 emitters.

| Compound       | Method | SOC S₁-T₁ |
|----------------|--------|-----------|
| DBT-BZ-PXZ     | BLYP   | 0.040     |
|                | B3LYP  | 0.042     |
|                | PBE0   | 0.046     |
| DBT-BZ-PTZ     | BLYP   | 0.002     |
|                | B3LYP  | 0.002     |
|                | PBE0   | 0.002     |
| DBT-BZ-DMAC    | BLYP   | 0.005     |
|                | B3LYP  | 0.026     |
|                | PBE0   | 0.446     |
| CP-BP-PXZ      | BLYP   | 0.022     |
|                | B3LYP  | 0.026     |
|                | PBE0   | 0.028     |
| CP-BP-DMAC     | BLYP   | 0.004     |
|                | B3LYP  | 0.009     |
|                | PBE0   | 0.013     |
Table S41. Spin-orbit coupling (SOC) values between different energy states for the T\textsubscript{1} geometries of Group 3 emitters.

| Compound | Method | SOC   |
|----------|--------|-------|
|          |        | S\textsubscript{1}-T\textsubscript{1} | S\textsubscript{1}-T\textsubscript{2} |
| a1       | BLYP   | 0.216 | 0.000 |
|          | B3LYP  | 0.144 | 0.000 |
|          | PBE0   | 0.163 | 0.000 |
| a2       | BLYP   | 0.000 | 0.117 |
|          | B3LYP  | 0.120 | 0.000 |
|          | PBE0   | 0.109 | 0.000 |
| a3       | BLYP   | 0.000 | 0.079 |
|          | B3LYP  | 0.134 | 0.000 |
|          | PBE0   | 0.138 | 0.000 |
| a4       | BLYP   | 0.016 | 0.000 |
|          | B3LYP  | 0.025 | 0.000 |
|          | PBE0   | 0.031 | 0.000 |
| b1       | BLYP   | 0.057 | 0.023 |
|          | B3LYP  | 0.097 | 0.059 |
|          | PBE0   | 0.072 | 0.006 |
| b4       | BLYP   | 0.000 | 0.004 |
|          | B3LYP  | 0.000 | 0.004 |
|          | PBE0   | 0.000 | 0.005 |
Table S42. Spin-orbit coupling (SOC) values between $S_1$ and $T_1$ for the $T_1$ geometries of Group 4 emitters.

| Compound | Method | SOC $S_1$-$T_1$ |
|----------|--------|----------------|
| ACRXTN   | BLYP   | 0.016          |
|          | B3LYP  | 0.025          |
|          | PBE0   | 0.029          |
| MCz-XT   | BLYP   | 0.018          |
|          | B3LYP  | 0.026          |
|          | PBE0   | 0.029          |
| 3-PXZ-XO | BLYP   | 0.047          |
|          | B3LYP  | 0.060          |
|          | PBE0   | 0.065          |
| PTZ-XT   | BLYP   | 0.005          |
|          | B3LYP  | 0.022          |
|          | PBE0   | 0.033          |
Table S43. Spin-orbit coupling (SOC) values between different energy states for the $T_1$ geometries of non-TADF emitters.

| Compound | Method | SOC   |
|----------|--------|-------|
|          |        | $S_1$-$T_1$ | $S_1$-$T_2$ |
| MC2      | BLYP   | 1.390 | 2.878 |
|          | B3LYP  | 0.617 | 4.203 |
|          | PBE0   | 0.435 | 4.494 |
| OPM      | BLYP   | 1.581 | 4.635 |
|          | B3LYP  | 2.070 | 8.383 |
|          | PBE0   | 8.381 | 7.830 |
| p-Cz     | BLYP   | 0.335 | -     |
|          | B3LYP  | 0.246 | 5.306 |
|          | PBE0   | 0.274 | 5.500 |
| ODFRCZ   | BLYP   | 0.321 | -     |
|          | B3LYP  | 0.345 | 3.449 |
|          | PBE0   | 0.299 | 3.825 |
| ODBTCZ   | BLYP   | 0.314 | -     |
|          | B3LYP  | 1.078 | -     |
|          | PBE0   | 1.262 | -     |
| C1       | BLYP   | 0.121 | -     |
|          | B3LYP  | 0.202 | -     |
|          | PBE0   | 0.231 | -     |
| C2       | BLYP   | 0.011 | -     |
|          | B3LYP  | 0.015 | -     |
|          | PBE0   | 0.016 | -     |
S₀ and T₁ cartesian coordinates of the most stable conformations optimized at M06-2X/6-31+G(d,p) level of theory

**Px2BP-S₀ Geometry (Solvent: Toluene)**

| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| H     | -0.59472200 | 1.10720700 | 0.14573100 |
| C     | -1.44306100 | 0.61872900 | -0.32346600 |
| C     | -3.64281900 | -0.59585800 | -1.54508700 |
| C     | -1.29756300 | -0.00870600 | -1.56412400 |
| C     | -2.68862600 | 0.64760800 | 0.30237500 |
| C     | -3.78064200 | 0.03514500 | -0.30518500 |
| C     | -2.40674600 | -0.60615200 | -2.17693100 |
| H     | -2.82566800 | 1.14295300 | 1.25812800 |
| H     | -2.28136900 | -1.07290100 | -3.14857300 |
| H     | -4.50954400 | -1.06478400 | -2.00237100 |
| C     | 0.00007700 | -0.00224000 | -2.31428400 |
| O     | 0.00012400 | -0.00324000 | -3.53316900 |
| C     | 1.29766100 | 0.00545200 | -1.56404200 |
| C     | 3.78067300 | -0.03632800 | -0.30489300 |
| C     | 2.40689300 | 0.60184900 | -2.17779000 |
| C     | 1.44308200 | -0.61989900 | -0.32232900 |
| C     | 2.68862000 | -0.64776000 | 0.30362400 |
| C     | 3.64292500 | 0.59260600 | -1.54585800 |
| H     | 2.28156000 | 1.06697300 | -3.15021700 |
| H     | 0.59472900 | -1.10760300 | 0.14779000 |
| H     | 2.82560500 | -1.14151500 | 1.26020700 |
| H     | 4.50967700 | 1.06077400 | -2.00336800 |
| N     | 5.05243700 | -0.06709700 | 0.34835500 |
| C     | 6.02449700 | -0.97644400 | -0.11856500 |
| C     | 8.03039700 | -2.76883700 | -0.92791700 |
| C     | 5.75441000 | -1.96078100 | -1.07025000 |
| C     | 7.31741300 | -0.90767400 | 0.42140600 |
| C     | 8.31199200 | -1.78239300 | 0.01995700 |
| C     | 6.75205000 | -2.85461000 | -1.46656900 |
| H     | 4.76008200 | -2.03544600 | -1.49639100 |
| H     | 9.29517300 | -1.08389600 | 0.46799100 |
| H     | 6.51693000 | -3.61614700 | -2.02352000 |
| H     | 8.80758900 | -3.45982600 | -1.23522100 |
| C     | 5.51011200 | 1.10249500 | 0.98904000 |
| C     | 6.51594900 | 3.35321500 | 2.33659000 |
| C     | 6.81676700 | 1.11630500 | 1.50008800 |
| C     | 4.71647200 | 2.23656600 | 1.16699100 |
| C     | 5.21682500 | 3.35212100 | 1.84262100 |
| C     | 7.32059900 | 2.22551600 | 2.15700300 |
| H     | 3.70162700 | 2.24452600 | 0.78493800 |
| H     | 4.57893300 | 4.21943900 | 1.97571600 |
| H     | 8.33793100 | 2.18392100 | 2.53077500 |
| H     | 6.90814200 | 4.21836900 | 2.85966000 |
| O     | 7.62475900 | 0.00370000 | 1.40870200 |
| N     | -5.05246400 | 0.06713100 | 0.34786800 |
| C     | -6.02391200 | 0.97672200 | -0.11982700 |
| C     | -8.02855700 | 2.76978800 | -0.93081200 |
| C     | -5.75311100 | 1.96008600 | -1.07231900 |
| C     | -7.31694000 | 0.90920000 | 0.42004600 |
| C     | -8.31088600 | 1.78428300 | 0.01782300 |
| C     | -6.75012000 | 2.85421100 | -1.49945000 |
| H     | -4.75871600 | 2.03370600 | -1.49848500 |
| H     | -9.29418200 | 1.68678400 | 0.46582200 |
| H     | -6.51420700 | 3.61501500 | -2.02586200 |
| H     | -8.80526500 | 3.46105200 | -1.23871900 |
| C     | -5.51078900 | -1.10144400 | 0.98988200 |
| C     | -6.51776800 | -3.35076000 | 2.34008200 |
| C     | -6.81752300 | -1.11406300 | 1.50076600 |
| C     | -4.71765100 | -2.23562300 | 1.16938600 |
| C     | -5.21857200 | -3.35014200 | 1.84630000 |
| C     | -7.32156000 | -2.22224900 | 2.15899600 |
|    |        |          |          |          |          |
|----|--------|----------|----------|----------|----------|
| H  | -3.7023700 | -2.2446100 | 0.78753100 |          |          |
| H  | -4.58105600 | -4.21755700 | 1.98056200 |          |          |
| H  | -8.33926500 | -2.17974800 | 2.53257800 |          |          |
| H  | -6.91040900 | -4.21441700 | 2.86415800 |          |          |
| O  | -7.62510600 | -0.00129200 | 1.40789100 |          |          |

**Px2BP-T₁ Geometry (Solvent: Toluene)**

|    |        |          |          |          |          |
|----|--------|----------|----------|----------|----------|
| H  | 0.62351000 | -0.44345300 | 0.27766100 |          |          |
| C  | 1.46961300 | -0.09557400 | -0.30427100 |          |          |
| C  | 3.70578000 | 0.64189700 | -1.83205000 |          |          |
| C  | 1.27129300 | 0.39137300 | -1.63610300 |          |          |
| C  | 2.72808600 | -0.18694500 | 0.25053500 |          |          |

...
Px2BP-S$_1$ Geometry (Solvent: Toluene)

H  -0.70212000 -1.42801000 -0.54322000
C  -1.50172500 -1.00919800  0.06044900
C  -3.58964300 -0.01400200  1.61523800
C  -1.29343000 -0.78268600  1.42633200
C  -2.73648200 -0.73685300 -0.52753300
C  -3.77547800 -0.23037800  2.20886800
C  -2.36179700 -0.30144400  2.19823000
H  -2.90827700 -0.92244100 -1.58359000
H  -2.20765400 -0.16567300  3.26392900
H  -4.41445000  0.37175100  2.08868000
C  -0.00945400 -1.12455300  2.13067300
O  -0.09950400 -1.64589500  3.26772800
C   1.25977100 -0.84678500  1.51102600
C   3.83831400 -0.32937300  0.47435400
C   2.44186200 -1.35401700  2.14857800
C   1.44704500 -0.02752100  0.35255900
C   2.69827200  0.22806000 -0.15720600
C   3.69525500 -1.11554500  1.64583700
H   2.31284800 -1.94533600  3.04869800
H   0.59165900  0.44012000 -1.23305000
H   2.82296000  0.86595400 -1.02836000
H   4.57893800 -1.51950900  2.13292600
N   5.13780900 -0.06976400 -0.05320200
C   5.85557800  1.03539400  0.36859500
C   7.36757100  3.24486800  1.16987000
C   5.33910700  1.93085500  1.32638900
C   7.13987300  1.27689600 -0.17060100
C   7.89332200  2.37544500  0.22635700
C   6.09215400  3.01987500  1.71740500
H   4.35574100  1.74263600  1.73887900
H   8.87328200  2.52254700 -0.21278400
H   5.69288100  3.70617000  2.45484000
H   7.94809700  4.10386600  1.48617800
C   5.69422900 -0.92064900 -0.99167600
C   6.88475000 -2.59023900 -2.89031800
C   6.98115000 -0.64222300 -1.50557400
C   5.00928800 -2.06293000 -1.45179900
C   5.60390700 -2.88308500 -2.38977300
C   7.57495900 -1.47127700 -2.45022600
H   4.02398400 -2.27328000 -1.05496100
H   5.07519600 -3.76126500 -2.74122900
H   8.56340500 -1.22001100 -2.81717000
H   7.34017400 -3.24289900 -3.62423200
O   7.68010700  0.44409600 -1.09407700
N  -5.03862100  0.05374400 -0.36606000
C  -6.09867000 -0.85600000 -0.19811500
C  -8.28040200 -2.61345000  0.03873800
C  -5.94994300 -2.09245100  0.43302400
C  -7.36135400 -0.51859000 -0.71016300
C  -8.44102900 -1.37539100 -0.58863800
C  -7.03477900 -2.96592800  0.54386400
H  -4.98133500 -2.37315700  0.83145400
H  -9.39481600 -1.06284100 -1.00886100
H  -6.89184500 -3.92387300  1.03285600
H  -9.12460200 -3.28865500  0.12585700

C 6.85612600  0.89678900  1.60651400
C 4.72932300  2.06092000  1.47212900
C 5.17416900  2.93499500  2.44276800
C 7.29992800  1.78168700  2.58599000
H 3.74864100  2.16537600  1.02410200
H 4.52705200  3.74141800  2.76821000
H 8.29843800  1.65423300  2.98827100
H 6.79147300  3.49093400  3.76708000
O 7.71774900 -0.06796200  1.20176400
DMAC-BP-S\(_0\) Geometry (Solvent: DCM)

C -5.36516900   1.38826200   -0.66478000
C -6.11471000   4.01352800   -1.16572400
C -6.64578100   1.67180600   -1.16572400
C -4.46709200   2.44612100   -0.51028400
C -4.83981800   3.74830800   -0.85233100
C -7.02286600   2.96288200   -1.49098900
H -3.47239100   2.24610300   -0.12776000
H -4.12168100   4.55232600   -0.72947800
H -8.02583000   5.03381000   -1.60346000
O -7.55402000   0.66101700   -1.39895300

DMAC-BP-S\(_0\) Geometry (Solvent: DCM)

H  2.24990800 -1.23741800  3.57061900
C  2.38447400 -0.74418300  2.61343400
C  2.69696900  0.56367200  0.16672900
C  1.29510700 -0.09077200  2.02504100
C  3.61732900 -0.76341200  1.97225400
C  3.77053300 -0.10698800  0.74986800
C  1.45631300  0.56451400  0.79895200
H  4.46784600 -1.27892500  2.40795700
H  0.62376400  1.09455800  0.34709700
H  2.84193600  1.07845900 -0.77811900
C -0.00026700  0.06140900  2.77597700
H  0.00093800 -0.09003000  3.99658100
C -1.29475200  0.00218100  2.02575100
C -3.76931200  0.07308300  0.75088100
C -1.45412100 -0.59669500  0.77098700
C -2.38531000  0.62701100  2.64239300
C -3.61774700  0.67374600  2.00181100
C -2.69444000 -0.56887800  0.13856000
H -0.62046500 -1.10467400  0.29637800
H -2.52158000  1.07586800  3.62139400
H -4.46937500  1.16745800  2.46004500
H -2.83832000 -1.04069900 -0.82858600
N  5.03961000 -0.12066400  0.09215600
C  5.95965400  0.90034300  0.36792800
C  7.76743800  2.96886600  0.95555800
C  5.62557500  1.91244400  1.28718500
C  7.21477100  0.92209700 -0.26643300
C  8.09152500  1.96556100  0.04796600
C  6.52076500  2.93389700  1.57648600
C  4.66013600  1.98717000  1.77884800
H  9.06435900  1.99421100 -0.43471800
H  6.23731000  3.70128300  2.28996800
H  8.47589500  3.76110500  1.17247500
C  5.32526900 -1.14893900 -0.81629900
C  5.84847800 -3.23228200 -2.62717200
C  6.56164000 -1.18843800 -1.48585600
C  4.36797500 -2.15142000 -1.06098900
C  4.62856700 -3.18035900 -1.95643000
C  6.79052100 -2.23864000 -2.38031000
H  3.41479000 -2.12507100 -0.54641200
H  3.87242700 -3.94059200 -2.12566400
H  7.74145000 -2.28135200 -2.90436200
H  6.06492300 -4.03485000 -3.32901300
H  7.65223200 -1.04005700 -1.27326300
H  8.92545800 -0.83782900 -0.74728100
H  9.73318700 -1.11469100 -0.60284400
H  9.27560500 -1.59327300 -1.45645100
H  8.72535900 -1.32836400  0.20960000
C  7.96546300  0.54284100 -2.62232900
H  8.75810700  1.28740100 -2.50636400
H  7.07515600  1.04385100 -3.01366000
H  8.30196500 -0.19057300 -3.36049100
N -5.03809900  0.11372400  0.09371400
DMAC-BP-T Geometry (Solvent: DCM)

H  2.20786000 0.12612300 3.64274500
C  2.37183300 0.24825900 2.57710500
C  2.77824900 0.62447000 -0.14946700
C  1.28609400 0.65553400 1.77805400
C  3.62355100 0.00483300 2.02425400
C  3.82948000 0.18709000 0.65598100
C  1.52286500 0.85614600 0.40466800
H  4.45243000 -0.32557800 2.64490400
H  0.72816100 1.23308200 -0.23143900
H  2.95696900 0.79340000 -1.20810600
C -0.01146400 0.94178000 2.44634500
O  0.01536900 1.36229800 3.64941500
C -1.27176400 0.73383600 1.77048200
C -3.82909700 0.33909900 0.63640400
H -1.44924100 -0.02524000 0.57356900
C -2.45698200 1.24565500 2.38590600
C -3.70640000 1.05935100 1.82869600
C -2.69947500 -0.21966200 0.01744000
H -0.59826100 -0.50268500 0.10108800
H -2.34951300 1.79873500 3.31203100
H -4.59456600 1.48664300 2.30367200
H -2.81690300 -0.81296800 -0.88565900
N  5.11868200 -0.06130000 0.08267000
C  6.05432900 0.97981000 0.02849100
C  7.89221200 3.10684100 -0.05211000
C  5.71638800 2.24895000 0.53702400
C  7.33019200 0.77315600 -0.52870800
C  8.22093100 1.85146700 -0.55351800
C  6.62529200 3.29768600 0.49635300
C  4.73499900 2.40930600 0.96709700
H  9.20893200 1.70365200 -0.98070200
H  6.33710200 4.26473200 0.89683200
H  8.61179500 3.91777200 -0.08943300
C  5.41239100 -1.33671100 -0.40979800
C  5.94340100 -3.92086900 -1.38498100
C  6.66662600  -1.61746400   -0.98352900
C  4.44240000  -2.35492500  -0.33041800
C  4.70657500  -3.62993000  -0.81242600
C  6.89862600  -2.91208000  -1.45968400
H  3.47760000  -2.14089900   0.11368600
H  3.93984500  -4.39488600  -0.73688000
H  7.86311400  -3.14012800  -1.90495500
H  6.16254600  -4.91282400  -1.76552400
C  7.77368400  -0.57156800  -1.10196200
C  9.01689100  -1.06427800  -0.32965100
H  9.83636700  -0.34438000   0.11368600
H  9.36969400  -2.01947500  -0.72917500
H  8.77989100  -1.19920400   0.72980000
C  8.13930400  -0.38940800  -2.59114000
H  8.94528700  -0.29604400  -2.70725200
H  7.27149000  -0.03916200  -3.15783700
H  8.82582300  -1.33603000  -3.06292100
N  -5.13558300   0.12558100   0.05468400
C  -5.90654100  -0.93804300   0.50328100
C  -7.40734600  -3.08430500   1.45094500
C  -7.19308200  -1.16980000  -0.03840100
C  -5.37963100  -1.78990800   1.50724900
C  -6.12842400  -2.84854200   1.97320300
C  -7.91929100  -2.25086400   0.46037500
H  -4.38934000  -1.60414500  -1.90168500
H  -5.72246200  -3.49678800  -2.74133400
H  -8.89979500  -2.45365400   0.06714000
H  -8.00115800  -3.91411100   1.81439100
C  -5.57526000   0.99427900  -0.93358800
C  -6.39490800  -2.63620200  -2.92023500
C  -4.73342000  -2.06394000  -1.32777500
C  -6.48530500  -0.81529100  -1.53198900
C  -7.22353600   1.71998500  -2.52677700
C  -5.14425600   2.93646100  -2.31286700
H  -3.77108700  -2.18968600  -0.84856100
H  -8.18968000  -1.60701900  -3.00742900
H  -4.49738000  -3.75354200  -2.61313000
H  -6.72321300   3.44651300  -3.69634200
C  -7.78704100  -0.29667000  -1.12696100
C  -8.08611700  -1.18143600  -2.36495100
H  -7.16780200  -1.63441100  -2.74744600
H  -8.53746800  -0.58126500  -3.15814900
H  -8.78723200  -1.97729500  -2.10378800
C  -9.10577400  -0.32530600  -0.60689100
H  -9.56821900   0.93782800  -1.38428800
H  -8.91690000   0.95290500   0.26787600
H  -9.81347000 -0.45910500  -0.32922200

Cz2BP-S\textsubscript{0} Geometry (Solvent: Toluene)

H  -0.61977500  0.14075200  -1.08635800
C  -1.45502600  0.61053500  -0.57636600
C  -3.62852600  1.83638900   0.67597900
C  -1.29445900  1.85934000   0.03415200
C  -2.69704500  -0.01548900  -0.58052200
C  -3.78275900   0.59039500  -0.05727200
C  -2.39532000  2.47231500   0.64390500
H  -2.83692600  -0.96408200  -1.08896500
H  -2.26327900   3.44548400  -1.10569300
H  -4.47406400   2.28917900   1.18382900
C  -0.00000200  2.60913100  -0.00004800
O  -0.00000200  3.82959600  -0.00001500
C  1.29445800  1.85934200  -0.03422300
C  3.78275800   0.59039700  -0.05729600
C  1.45501200  0.61053500   0.57629300
C  2.39533100  2.47232000  -0.64395000

Cz2BP-S\textsubscript{0} Geometry (Solvent: Toluene)
C                  3.62853800   1.83639400   -0.67581800
C                  2.69703100   -0.01548900    0.58047300
H                  0.61974900    0.14075000    1.08626500
H                  2.26329900    3.44549100   -1.10573700
H                  4.47408700    2.28918600   -1.18383200
H                  2.83690200   -0.96408400    1.08891500
N                 -5.03897700   -0.05414700    0.07398400
C                 -5.27527100   -1.36709500    0.48172100
C                 -6.25965000   -3.85067200    1.21808900
C                 -4.37994600   -2.31249000    0.98870400
C                 -6.65487000   -1.64337000    0.35976400
C                 -7.14586100   -2.89872200    0.72942300
C                 -4.89271900   -3.55339400   1.34964600
H                 -3.32514200   -2.08865700   1.10607000
H                 -8.20478200   -3.12257400    0.64001400
H                 -4.21942600   -4.30707000    1.74553100
H                 -6.62418300   -4.83037700    1.50828000
C                 -6.25277400    0.51719400   -0.30953700
C                 -8.86107300   1.16216700   -0.98605900
C                 -7.27984200   -0.43839200   -0.14820000
C                 -6.50862500   1.78977600    0.82691700
C                 -7.82422300    2.09499200   -1.15707000
C                 -5.71377500   -0.10708800   -0.48792700
H                 -5.71374800    2.51277300   -0.97533100
H                 -8.05176600   3.07909900   -1.55965800
H                 -9.39292400   -0.83686800   -0.36815600
H                 -9.87623100   1.43615600   -1.25313600
C                  5.03897700  -0.05144400   -0.07398400
C                  6.25276500    0.51719700    0.30956400
C                  8.86104800   1.16216900    0.98614600
C                  7.27983800   -0.43838700    0.14824500
C                  6.50860300   1.78977700    0.82695600
C                  7.82419400    2.09499300   -1.15713800
C                  8.59470200   -0.10708300    0.48800200
C                  5.71374800    2.51277300    0.97533100
C                  8.05172700   3.07908800   1.55973600
C                  9.39291500   -0.83686200    0.36824500
C                  9.87620000   1.43615800   1.25324600
C                  5.27528100   -1.36708800   -0.48172500
C                  6.25967800   -3.85066100   -1.21808400
C                  4.37996800   -2.31248300   -0.98873200
C                  6.65487700   -1.64336300   -0.35973900
C                  7.14587700   -2.89876300   -0.72939400
C                  4.89274900   -3.55338400   -1.34967000
H                  3.32516500   -2.08865000  -1.10612000
H                  8.20479600   -3.12256500   -0.63996300
H                  4.21946600   -4.30705800   -1.74557300
H                  6.62421800  -4.83036400   -1.50827300

Cz2BP-T, Geometry (Solvent: Toluene)

H                 -0.67668900   -0.23354000   -0.80457200
C                 -1.49401200    0.34369900   -0.38918300
C                 -3.68090400   1.86645000    0.46554800
C                 -1.27724100   1.68399100    0.03865200
C                 -2.75241000   -0.22240100   -0.37192500
C                 -3.86308700    0.52559300    0.06713300
C                 -2.42404100    2.42831000    0.44055900
H                 -2.90534100   -1.22886000   -0.75060700
H                 -2.62684290    3.45607100    0.74770300
H                 -4.53210200    2.43553100    0.82792300
C                  0.00000000    2.39733400   -0.00000700
O                  0.00000000    3.66647100    0.00000000
C                  1.27724100   1.68399200   -0.03866400
C                  3.86308600    0.52559400   -0.06713700
C                  1.49401000    0.34369800    0.38917000
C                  2.42404200    2.42831100   -0.44056500
| Atom | x          | y          | z          |
|------|------------|------------|------------|
| C    | 3.68090600 | 1.86645200 | -0.46555000|
| C    | 2.75240800 | -0.22240200| 0.82792000 |
| H    | 0.67668600 | -0.23354100| 0.80455500 |
| H    | 2.26843200 | 3.45607300  | -0.74770700|
| H    | 4.53210500 | 2.43553300  | -0.82792000|
| H    | 2.90533800 | -1.22886100| 0.75059600 |
| N    | -5.14198000| -0.05612300| 0.09115300 |
| C    | -5.45911000| -1.30198600| 0.63065500 |
| C    | -6.57971900| -3.63725200| 1.59566200 |
| C    | -4.63083000| -2.20360100| 1.30474300 |
| C    | -6.84304600| -1.53839500| 0.46248000 |
| C    | -7.40498500| -2.71574700| 0.94958900 |
| C    | -5.21339600| -3.37674500| 1.77502400 |
| C    | -3.58030600| -1.99216100| 1.46045900 |
| H    | -8.46667200| -2.91054200| 0.83442100 |
| C    | -4.59689400| -4.09893800| 2.29975400 |
| N    | -7.00184300| -4.56088400| 1.97706100 |
| C    | -6.30759200| 0.51602400  | -0.41938900|
| C    | -8.83435800| 1.18849600  | -1.31494600|
| C    | -7.38836300| -0.36927500| -0.20555000|
| C    | -6.46506600| 1.72121400  | -1.10927700|
| C    | -7.74701300| 2.04425200  | -1.54398100|
| C    | -8.66054400| -0.02795000| -0.65396200 |
| C    | -5.62289500| 2.37298900  | -1.31216800|
| H    | -7.90336600| 2.97502800  | -2.07887600|
| C    | -9.50046100| -0.69846900| -0.50032300|
| N    | -9.82004700| 1.47107900  | -1.66896600|
| C    | 5.14198000 | -0.05612200| -0.09115400|
| C    | 6.30759000 | 0.51602400  | 0.41939400 |
| C    | 8.83435300 | 1.18849500  | 1.31496100 |
| C    | 7.38836200 | -0.36927400| 0.20556200 |
| C    | 6.46506200 | 1.72121300  | 1.10926400 |
| C    | 7.74700700 | 2.04425100  | 1.54399400 |
| C    | 8.66054100 | -0.02795000| 0.65397400 |
| C    | 5.62289000 | 2.37298800  | 1.31217300 |
| C    | 7.90335800 | 2.97502600  | 2.07889000 |
| C    | 9.50045900 | -0.69846900| 0.50033800 |
| C    | 9.82004100 | 1.47107800  | 1.66896600 |
| C    | 5.45911200 | -1.30198500| -0.63056500|
| C    | 6.57972500 | -3.63724900| -1.59566200|
| C    | 4.63083400 | -2.03539800| -1.30474900|
| C    | 6.84304800 | -1.53839300| -0.46624400|
| C    | 7.40489800 | -2.71574400| -0.94958600|
| C    | 5.21340300 | -3.37674100| -1.77502900|
| H    | 3.58031100 | -1.99260700| -1.46946800|
| C    | 8.46667500 | -2.91053900| -0.83441400|
| C    | 4.59690200 | -4.09893400| -2.29976200|
| C    | 7.00185100 | -4.56088000| -1.97706200|

**CzBP-S$_1$ Geometry (Solvent: Toluene)**

| Atom | x          | y          | z          |
|------|------------|------------|------------|
| H    | -0.67025600| -0.06722400| -0.96213200|
| C    | -1.49787700| 0.45876700  | -0.49858500|
| C    | -3.67355300| 1.84773300  | 0.57271720 |
| C    | -1.30807800| 1.74982000  | 0.03122800 |
| C    | -2.75342400| -0.12949000| -0.47602800|
| C    | -3.84674900| 0.55713500  | 0.06555100 |
| C    | -2.42041900| 2.44433900  | 0.54679200 |
| H    | -2.90260700| -1.11618700| -0.90404000|
| H    | -2.28720200| 3.43908900  | 0.95876300 |
| H    | -4.52171400| 2.37153000  | 1.00197400 |
| C    | 0.00002400 | 2.40356400  | 0.00041100 |
| O    | 0.00003200 | 3.69953500  | 0.00043300 |
| C    | 1.30811100 | 1.74980500  | -0.03061900|
| C    | 3.84673800 | 0.55704200  | -0.06542900|
| C    | 1.49797200 | 0.45874900  | 0.49916600 |
| C    | 2.42037100 | 2.44428600  | -0.54640400|
| Atoms | X        | Y        | Z        |
|--------|----------|----------|----------|
| C      | 3.673276  | 1.847630 | -0.572051 |
| C      | 2.753500  | -0.067211| 0.962883  |
| H      | 0.670426  | 0.962883 | -0.868680 |
| H      | 2.902742  | -0.116225| 0.904403  |
| C      | -5.121605 | -0.052963| 0.088868  |
| C      | -5.417733 | -1.296643| 0.643194  |
| C      | -6.506207 | -3.649884| 1.619128  |
| C      | -4.575654 | -2.190566| 1.309864  |
| C      | -6.796128 | -1.557679| 0.477062  |
| C      | -7.339166 | -2.747907| 0.968787  |
| C      | -5.140222 | -3.369088| 1.789734  |
| H      | -3.522636 | -1.974260| 1.455683  |
| H      | -8.397622 | -2.960354| 0.847301  |
| H      | -4.509723 | -4.080224| 2.311066  |
| C      | -6.911959 | -4.578817| 2.005691  |
| C      | -6.294179 | 0.491494 | -0.430963 |
| C      | -8.841834 | 1.111432 | -1.324486 |
| C      | -7.357615 | -0.412313| -0.210751 |
| C      | -6.483200 | 1.697948 | -0.113095 |
| C      | -7.769450 | 1.991803 | -1.548750 |
| C      | -8.641696 | -0.093150| -0.661281 |
| H      | -5.658559 | 2.377745 | -1.296810 |
| H      | -7.946110 | 2.922451 | -2.078362 |
| C      | -9.467736 | -0.779104| -0.498920 |
| H      | -9.382664 | 1.374851 | -1.679275 |
| N      | 5.121594  | -0.050480| 0.088903  |
| C      | 6.294271  | 0.491505 | 0.430598  |
| C      | 8.842117  | 1.111624 | 1.323474  |
| C      | 7.357671  | -0.412144| 0.210273  |
| C      | 6.483423  | 1.698077 | 1.109785  |
| C      | 7.769762  | 1.992022 | 1.547540  |
| C      | 8.641843  | -0.093058| 0.660516  |
| H      | 5.658814  | 2.377896 | 1.296329  |
| H      | 7.946525  | 2.922763 | 2.077229  |
| H      | 9.467855  | -0.779045| 0.497268  |
| H      | 9.833011  | 1.375115 | 1.678007  |
| C      | 5.417622  | -1.296812| -0.643095 |
| C      | 6.505913  | -3.650215| -1.618844 |
| C      | 4.575413  | -2.190855| -1.309420 |
| C      | 6.796052  | -1.557811| -0.477197 |
| C      | 7.339348  | -2.748119| -0.968830 |
| C      | 5.139891  | -3.367278| -1.789222 |
| C      | 3.522365  | -1.974582| -1.455085 |
| C      | 8.397480  | -2.960538| -0.847524 |
| C      | 4.509290  | -0.806890| -2.310301 |
| C      | 6.911593  | -4.579213| -2.005328 |

**CC2BP-S8 Geometry (Solvent: Toluene)**

| Atoms | X        | Y        | Z        |
|--------|----------|----------|----------|
| C      | 0.716884  | -2.601649| 0.206748 |
| C      | 1.529159  | -2.313638| -0.453375 |
| C      | 3.631035  | -1.610410| -2.151953 |
| C      | 1.260876  | -1.911559| -1.766144 |
| C      | 2.838934  | -2.361920| 0.012766 |
| C      | 3.889879  | -2.005322| -0.835313 |
| C      | 2.321884  | -1.570074| -2.612354 |
| C      | 3.052973  | -2.663360| 1.033260 |
| C      | 2.105269  | -1.286760| -3.637303 |
| C      | 4.458882  | -1.358793| -2.807465 |
| C      | -0.125117 | -1.906884| -2.332660 |
| C      | -0.302800 | -2.137312| -3.517257 |
| C      | -1.291445 | -1.618335| -1.440345 |
| C      | -3.551484 | -1.045197| 0.094805  |
| C      | -2.530400 | -2.179141| -1.770658 |
| C      | -1.196704 | -0.758710| -0.340466 |
CC2BP-T$_1$ Geometry (Solvent: Toluene)

H 0.64471400 -1.71440900 -0.86254000
C 1.48884000 -1.13137600 -1.21061900
C 3.68411900 0.37831100 -2.17444500
C 1.25569300 0.10935600 -1.92985000
C 2.74984700 -1.57969100 -0.97569700
C 3.89561800 -0.82630800 -1.42259200
C 2.42614300 0.81150200 -2.44184400
H 2.58741800 -2.48311200 -0.39525900
C -0.03893300 0.64447600 -2.24157400
O -0.14271200 0.64447600 -2.24157400
C -1.28449900 0.10995900 -1.61242200
H -3.71083200 -0.74778400 -0.50234600
H -2.44526200 0.04406800 -2.39466600
C -1.36655000 -0.23887600 -0.25787900
C -2.57207800 -0.65453400 0.29940100
C -3.64539400 -0.40066700 -1.85430000
C -2.38695600 0.34168000 -3.46363200
H -0.49374200 -0.14118400 0.38142400
C -2.64288300 -0.88661800 1.35747000
H -4.53534600 -0.48448800 -2.47108800
N 5.17436200 -1.26532200 -1.13268300
C 5.63207700 -2.59306900 -1.21965200
C 7.00019900 -4.99081600 -1.28912100
C 4.96229200 -3.71840600 -1.69882400
C 6.98565900 -2.64056800 -0.82913700
C 7.67503400 -3.84814900 -0.85920100
C 5.66632800 -4.92079400 -1.71368800
C 3.94604900 -3.66394200 -2.07147600
C 8.71947200 -3.89281800 -0.56779970
H 5.17229000 -5.81682700 -2.07151300
H 7.52013600 -5.94226200 -0.31827600
H 6.23950700 -0.46529200 -0.69934000
C 8.58568700 0.65375600 0.23638200
C 7.37575700 -1.27699900 -0.49810400
C 6.24642400 0.89676300 -0.39272100
C 7.43532000 1.44471700 0.07197500
C 8.56037900 -0.71666600 -0.04037800
H 5.35394800 1.50616100 -0.47535400
H 7.47863000 2.49451400 0.34301800
H 9.45402900 -1.31694100 0.10155000
N -4.93924600 -1.18137200 0.05962000

N -9.82052300 1.02691600 -0.33790700
C -10.75640300 0.37828400 -1.13437300
C -12.93659300 -0.52476700 -2.58324100
C -11.94769100 1.13875900 -1.16046300
C -10.64194700 -0.83680800 -1.81525400
C -11.74657700 -1.27231500 -2.53773700
C -13.04441100 0.67782900 -1.89539000
H -9.72698900 -1.41913000 -1.77669100
H -11.68792700 -2.21255400 -3.07706400
H -13.96651100 1.25104100 -1.92479800
H -13.77855400 -0.89521100 -3.15887700
C -10.38971500 2.19599100 0.15335000
C -11.93692400 4.38634100 0.84475800
C -9.82304600 3.17462900 0.97440500
C -11.71279700 2.30493200 -0.33281600
C -12.48916300 3.41274200 0.02147300
C -10.61591100 4.26545800 1.31109500
H -8.80189800 3.08733000 1.33118600
H -13.50718100 3.51031900 -0.34439000
H -10.20316100 5.04212400 1.94733500
H -12.52680000 5.25127700 1.12946800
A-BP-TA-S\textsubscript{6} Geometry (Solvent: THF)

H  2.09922900  -1.17642800  -3.18748500
C  2.39359500  -1.00728100  -2.15676400
C  3.12077300  -0.61701300  0.50979900
### A-BP-TA-T\textsubscript{1} Geometry (Solvent: THF)

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 9.46559400| 0.58816500| 2.13438800|
| H    | 7.82682900| 1.03565800| 2.64743400|
| H    | 8.93406600| 2.26946800| 2.01445100|

2.00693600 -2.69205400 -1.75813800

1.47145400 -1.49640800 -0.05956300

3.67783600 -1.51602800 -1.07232000

4.12580800 -0.60288200 -0.11741200

1.93888800 -0.58560900 0.89927600

4.36803900 -1.86814100 -1.83386300

1.27440100 -0.24078600 1.68583700

3.63053700 0.55022600 1.62199800

0.08036900 -2.05924900 -0.03172200

-0.05704800 -3.27937900 -0.28374700

-1.04988800 -1.21003000 0.27060500

-3.40737100 0.35175800 0.77704700

-1.01403500 0.21638100 0.27883300

-2.31196100 -1.82041900 0.52788500

-3.43928100 -1.07620200 0.77580100

-2.14108700 0.96146800 0.53047200

-0.09194700 0.73499300 0.03667600

-2.35626900 -2.90413500 0.55978100

-4.35728900 -1.59214100 1.04325800

2.07618700 2.04514500 0.48282800

-4.56586800 1.15536100 1.08924800

-6.85195100 2.62803200 1.98795200

-9.07802400 0.81237900 0.65058000

-4.44560500 2.33409000 1.84557400

-5.55308800 3.04888800 2.28509800

-7.03119600 1.52203400 1.15805300

-3.45563500 2.64684500 2.16063300

-5.40951500 3.92649500 2.90655300

-7.71379200 3.15646600 2.38080000

-8.69126900 1.12635700 0.87048100

-5.96875100 -0.28174900 -0.67023500

-7.61940000 -0.59085800 -1.04744600

-10.19843900 -1.36495300 -1.80534200

-7.80894400 -1.50321800 -2.10932300

-8.74033800 -0.05756400 -0.38311100

-10.03218700 -0.46682700 -0.77134200

-9.07932800 -1.88280400 -2.45446600

-6.93868200 -1.90830900 -2.61680200

-10.89400000 -0.05864700 -0.25232900

-9.21285800 -2.58573500 -3.29881300

-11.19830500 -1.66779700 -2.09576100

5.48147900 -0.14362000 -0.14820700

6.45732100 -0.84912300 0.56720500

8.37394600 -2.30205200 2.02240700

6.09468000 -1.99817800 1.29554500

7.79786500 -0.42188100 0.56604300

8.72671400 -1.16636300 1.30048600

7.04301100 -2.71414800 2.01353500

5.06355600 -2.33068900 1.29689700

9.76469200 -0.84547300 1.30818200

6.73465200 -3.59683100 2.56556800

9.12453900 -2.85246000 2.57953000

5.79716000 0.99916800 -0.89283600

6.37375900 3.29915900 -2.40337600

7.11732100 1.48379700 -0.94038900

4.78415400 1.67215600 -1.60251100

5.07106900 2.80782600 -2.34803800

7.37068600 2.63027000 -1.70038500

3.76705600 1.30031500 -1.56867800
A-BP-TA-S\textsubscript{4} Geometry (Solvent: THF)

H  2.26134400  0.83832600  -3.37956200
C  2.50375100  0.50543900  -2.37570700
C  3.07482200 -0.40688200   0.21744100
C  1.42886000  0.33731000  -1.54712600
C  3.79888400  0.55290200  -1.92753300
C  4.10157200  0.10795000  -0.61542400
C  1.77939800  0.43920000  -0.24124000
H  4.59842400  0.92668500  -2.56185200
H  1.01793000 -0.87060400   0.39992900
H  3.32512600 -0.78421700  1.20504000
O  0.10734200  0.19894000  -3.32931900
C  0.11362700 -0.00758000  -2.10606800
C  -0.10791600  0.31030000  -1.26835000
C  -3.42076800  0.83427200   0.25761200
C  -1.25044800  0.23151800   0.04397500
C  -2.10940000 -1.10151500  -1.76478500
C  -3.25526100 -1.37102700  -1.02634600
C  -2.40319200 -0.28028000   0.78077000
H  -0.48897300  0.88630100   0.45733000
H  -1.99231500 -1.50675000  -2.76541900
H  -4.02488100 -2.01652600  -1.44265600
H  -2.52797900  0.41808600  1.76384200
C  -4.62931900 -1.13146100  1.07051600
C  -6.84855900 -1.75336300  2.68528200
C  -5.93745200 -0.91171800  0.59390900
C  -4.46514100 -1.66671900  2.35429700
C  -5.55869300 -1.97414300  3.15775300
C  -7.03739600 -1.24008400  1.40999200
H  -3.45712400 -1.85115200  2.71378800
H  -5.40768300 -2.38607100  4.14999400
H  -7.71272500 -1.97940200  3.30167200
S  -8.69675200 -1.06704000  0.80851900
S  -6.20165200 -0.20874300 -1.01440600
C  -7.52290100  0.91841900  -0.68632600
C  -9.65202200  2.68907900  -0.32846800
C  -7.48546300  2.18679000  -1.27210700
C  -8.62065800  0.54691800  -0.97372200
C  -9.67565100  1.44185100  0.29115900
C  -8.55700000  3.06158100  -1.10910300
H  -6.61984400  2.47675000  -1.89627200
H  -10.51229700  1.15242400  0.91947800
H  -8.52888700  4.03832900  -1.58056200
H  -10.48192500  3.37388700  -0.18886700
N  5.44400800  0.14690800  -0.14235900
C  6.25862400 -0.96531400  -0.32626100
C  7.82349400  0.23139500  -0.72806300
C  5.71965700  0.20962700  -0.98549900
C  7.59669100  0.96607500  0.13527000
C  8.35184000  2.11588500  -0.08105100
C  6.50138100  2.31778000  1.31844400
H  4.69511000  2.07128600  -1.33230900

H                  4.27000900    3.30575700   -2.88556900
H                  8.38597900    3.01451600   -1.74358400
C                  6.61405000    4.18544000   -2.91819570
C                  8.27160700    0.81308700   -0.19800100
C                  9.35103400    0.39167200  -1.21864000
H                  10.20216400  -0.07509300   -0.71469000
H                  8.93963300  -0.32404500  -1.93644200
C                  8.80957000   1.82053700   -0.80120700
C                  9.72334600   1.37442000   1.33764700
H                  8.13127900  2.13035400   1.53412600
H                  9.24803000  2.71033100   0.28150700
H  9.38096600  -2.14974300  0.26092600
H  6.08457700  -4.08114000  -1.68751300
H  8.44367600  -4.10829900  -0.87821400
C  5.90497100   1.29622700   0.49138200
C  6.75319300   3.63280700   1.74277900
C  7.23297700   1.37264400   0.97454000
C  5.01604300   2.38741200   0.64179900
C  5.44290100   3.54428300   1.26382500
C  7.62549900   2.55617600   1.59489900
H  4.00489900   2.30396100   0.26590700
H  4.75884900   4.37746100   1.37680600
H  8.63730000   2.64809900   1.97548900
H  7.09615700   4.53804600   2.23174500
C  8.21545000   0.22513400   0.84104300
C  9.44998000   0.70744700   0.02808100
H 10.17635000  -0.09517800  -0.06431600
H  9.92267100   1.55016800   0.52945700
H  9.13949800   1.02243600  -0.97425300
C  8.66910100  -0.21170200   2.25520800
H  9.39893400  -1.02181100   2.18722900
H  7.81581200  -0.55812300   2.84417600
H  9.13934100   0.62374200   2.77895000

OPDPO-S<sub>0</sub> Geometry (Solvent: THF)

H  2.24983900  -3.17102800  -2.53066800
C  2.44812600  -2.23607600  -2.01665900
C  2.92521900  -1.92871900  -1.56867500
C  1.39561300  -1.33727000  -1.80798000
C  3.72701900  -1.92871900  -1.56867500
C  3.96953900  -0.70717500  -0.92793500
C  1.63794600  -0.11605200  -1.17125600
H  4.54667800  -2.62348600  -1.72671100
H  0.83358800  -0.59764000  -1.03360600
H  3.11144700  1.16584100  -0.27615500
C  0.04528900  -1.68966200  -2.35544000
C  -1.18919800  -1.90623000  -1.67086100
C  -3.56128600  -0.36242800  -0.46800100
C  -2.33325300  -0.97281500  -2.44973000
C  -1.24428200  -1.00155400  -0.28714900
C  -2.43484700  -0.59654100  0.31473200
C  -3.51254700  -0.54803000  -1.85350000
H  -2.28112300  -1.13525300  -3.52137200
H  -0.36984300  -1.19087300  0.32749900
H  -2.49982600  -0.45803700  1.38898500
H  -4.40117000  -0.36016500  -2.44976000
O  -0.04599300  -2.37853900  -3.35843200
N  -4.76711400  0.07331400  0.17536700
C  -5.79302900  -0.88771000  0.36067500
C  -7.85918300  -2.76425400  0.76811500
C  -5.72036100  -2.16955100  -0.19997200
C  -6.91014500  -0.57282800  1.15337400
C  -7.94232500  -1.49149600  1.32948200
C  -6.73838200  -3.09817900  0.01409600
H  -4.86280700  -2.45528700  -0.79648900
H  -8.80057500  -1.20783000  1.93137300
H  -6.64839900  -0.48398000  -0.42497200
H  -8.65720200  -3.48172100  0.92475900
C  -5.08289900  1.45305900  0.09519700
C  -5.74496800  4.19275400  -0.01956700
C  -6.13552300  1.97565600  0.86615700
C  -4.35536700  2.33510800  -0.71452600
C  -4.67807700  3.69118100  -0.75874700
C  -6.47794800  3.32357400  0.78623100
H  -3.52482200  1.97069600  -1.30606000
H  -4.08920700  4.35083100  -1.38757700
H  -7.30987000   3.69012800   1.38028000
H  -6.00445400   5.24488300  -0.30266100
S   -6.95171200   0.94819300   2.04215900
P    5.66480500  -0.38142000  -0.36578400
C    5.81669500   1.42007700  -0.30266100
C    6.04068000   4.20117900  -0.35818700
C    5.59133300   2.16366300   0.86010100
C    6.16276600   2.07315400  -1.49250000
C    6.27323100   3.46102200  -1.51884200
C    5.70175900   3.55383800   0.82927200
H    5.33612600   1.66298600   1.79004200
H    6.35212100   1.49100500  -2.39017500
H    6.54404200   3.96443300  -2.44126600
H    5.52930500   4.12856600   1.73344500
H    6.12936800   5.28278000  -0.37889400
C    5.74271400  -0.96604300   1.34387100
C    6.01326800  -1.83708300   3.98090400
C    4.62101300  -1.03417400   2.17740400
C    6.99884000  -1.34412400   1.83216500
C    7.13228100  -1.77823600   3.94529000
H     3.63975800  -0.75634800   1.80197000
H    10.60544000  -2.07383400   3.52490900
H    8.38748500  -1.52056800   4.13968000
H    11.17515000  -2.17763600   5.06238000
O     6.68291000   -1.02271700  -1.24566000

OPDPO-T1 Geometry (Solvent: THF)

H    2.26209200  -1.94597400  -3.48817900
C    2.46425100  -1.27399100  -2.66090200
C    2.96093300  -0.51167900  -0.58444900
C    1.37682400  -0.56754100  -2.09732600
C    3.75373900  -1.12236200  -2.17700600
C    4.02178000  -0.23436900  -1.12131600
C    1.66715600   0.34874100  -1.06094400
H    4.57108200  -1.68537900  -2.62063200
H    0.88171300   0.97986800  -0.65874100
H    3.15018600   1.24155800   0.19908400
C    0.04412500  -0.75720300  -2.69762800
C    1.18142900  -0.07205000  -1.94964900
C    -3.66261600  -0.14251600  -0.60662800
C    -2.39881500  -0.42441800  -2.68310400
C    -1.27867900  -0.43986900  -0.52318500
C    -2.49654700  -0.25749100   0.10187000
C    -3.61641500  -0.23541400  -2.05441600
H    -2.34682800  -0.51069200  -3.76241100
H    -0.39618100  -0.57909500   0.08140300
H    -2.55595400  -0.22344500   1.18660400
H    -4.53518700  -0.15950300  -2.63053800
O    -0.03148000  -1.16429300  -3.90355000
N    -4.93596600   0.04257900   0.00361500
C    -5.63786200  -1.09536100   0.37637300
C    -7.02100200  -3.44339700   1.11516000
C    -5.10098500  -2.37441400   0.09304300
C    -6.88828200  -1.03303300   1.03992900
C    -7.56659200  -2.21103700   1.40232400
C    -5.78025100  -3.51704400   0.45574900
H    -4.14855500  -2.44891900  -0.41468700
H    -8.52331800  -2.13218500  -1.90901400
H    -5.34611900  -4.48362500   0.22588000
H    -7.54771500  -4.34821300   1.39595300
C    -5.36863900   1.34387900   0.21643100
C    -6.20157600   0.41162600   0.61592800
C    -6.59555300   1.64129300   0.85977500
C    -4.56865000   2.42746400  -0.21916300
OPDPO-S$_1$ Geometry (Solvent: THF)

H  -2.19391000 -1.83562100  3.50939000
C  -2.41772500 -1.15504700  2.69416000
C  -2.97631100  0.65756100  0.65470000
C  -1.38533500 -0.34611000  2.19642500
C  -3.69856400 -1.08900200  2.16140200
C  -3.98800500 -0.18581000  1.12933400
C  -1.68978400  0.57508900  1.18134100
H  -4.48632400 -1.72891300  2.54994900
H  -0.92405200  1.25619600  0.82311300
H  -3.19255800  1.39159300 -0.11703000
C  -0.03904300 -0.42669000  2.85221100
C  1.16395100 -0.29030600  2.07593900
C  3.62968400 -0.08372600  0.70546600
C  2.41092800 -0.18398900  2.78053000
C  1.23000400 -0.33663900  0.64823400
C  2.42656800 -0.23519600 -0.02359400
C  3.60916400 -0.07328500  2.11921600
H  2.38224700 -0.18113800  3.86467500
H  0.32661700 -0.49305600  0.06857000
C  2.46000200 -0.28559600 -1.10845700
C  4.54288800  0.02507600  2.66694300
O  -0.01585600 -0.62522000  4.09747000
N  4.87199000  0.04113450  0.00837400
C  5.56320400 -1.12511500 -0.30213300
C  6.90476000 -3.53063700 -0.90154200
C  5.01918600 -2.37421500  0.07951800
C  6.80071300 -1.11930400 -0.99429200
C  7.45718500 -2.32447500 -1.28560100
C  5.67915100 -3.54878500 -0.21513000
H  4.07641700 -2.39736300  0.60896500
H  8.40388200 -2.29314500 -1.81577500
H  5.24168900 -4.49251900  0.08969100
H  7.41881400 -4.45719500 -1.13046100
DBT-BZ-PXZ-S₈ Geometry (Solvent: THF)

H  3.92316900  -1.67065400  1.10561900
C  3.82402400  -0.68012500  0.67148500
C  3.50681600  1.90651300  -0.40749100
C  2.57455800  -0.06132800  0.67381500
C  4.92151500  -0.25876000  0.11339000
C  4.74991100  1.25840900  -0.42408000
C  2.42309100  1.23143900  0.13451600
H  1.45516300  1.72101500  0.16435000
H  3.39027800  2.90806700  -0.80739700
C  1.44010200  -0.78644100  1.32092700
O  1.64951100  -1.59241500  2.21511700
C  0.03392000  -0.52971900  0.86814500
C  -2.61766500  -0.18740000  0.09309500
C  -0.27493800  -0.24880800  -0.46513900
C  -0.99524200  -0.65406300  1.81044300
C  -2.31763900  -0.47192000  1.42831700
C  -1.60389500  -0.08210600  -0.85438600
H  0.51445300  -0.17177800  -1.20666400
H  -0.74319700  -0.89049900  2.83914000
H  -3.12464300  -0.55186700  2.15116400
H  -1.86321100  0.12542900  -1.88750900
N  -3.97778700  -0.00781200  -0.31450400
C  -4.62155300  1.20466500  0.00446100
C  -6.00338700  3.59122200  0.54867800
C  -3.95260800  2.30621500  0.54115800
C  -5.99511900  1.32278600  -0.25729100
C  -6.68291400  2.49222300  0.01721900
C  -4.64050600  3.49327000  0.80516100
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DBT-BZ-PXZ-T, Geometry (Solvent: THF)

| Atoms | X          | Y          | Z          |
|-------|------------|------------|------------|
| H     | 3.86943700 | -0.91241600| 1.69796700 |
| C     | 3.79007100 | -0.18472500| 0.89543300 |
| C     | 3.55495800 | 1.75590300 | -1.12762800|
| C     | 2.56133900 | 0.45005800 | 0.68967400 |
| C     | 4.89098600 | 0.11523100 | 0.08840800 |
| C     | 4.76319300 | 1.08349700 | -0.92558000|
| C     | 2.47167000 | 1.43344700 | -0.32230700|
| H     | 1.54229600 | 1.97896000 | -0.45358400|
| H     | 3.46729600 | 2.52587900 | -1.88785000|
| C     | 1.43739300 | 0.12744900 | 1.61820300 |
| O     | 1.72673500 | -0.14703300| 2.82644400 |
| C     | 0.07232200 | 0.09988200 | 1.15829400 |
| C     | -2.65361300| -0.04185300| 0.42038000 |
| C     | -3.34349000| 0.10527900 | -0.21388700|
| C     | -0.96315900| -0.02793400| 2.13541100 |
| C     | -2.29850900| -0.08744400| 1.77803400 |
| C     | -1.66532100| 0.03586000 | -0.57404000|
| O     | 0.41115800 | 0.12325600 | -1.00099700|
| H     | -0.67990800| -0.07084100| 3.17953900 |
| H     | -3.07508400| -0.17052300| 2.53467600 |
| H     | -1.95377100| 0.03448100 | -1.62279900|
| N     | -4.04343100| -0.10709200| 0.04344600 |
| C     | -4.81743000| 1.03771200 | 0.04392500 |
| C     | -6.46573500| 3.29822500 | 0.02074300 |
| C     | -4.28904400| 2.29751100 | 0.39385600 |
| C     | -6.17969400| 0.94850700 | -0.31883300|
| C     | -7.00281800| 2.07266700 | -0.33024200|
| C     | -5.10813800| 3.40714000 | 0.38034400 |
| H     | -3.24344300| 2.37032000 | 0.66794600 |
| H     | -8.04204400| 1.95542000 | -0.61533600|
| H     | -4.69880600| 4.37390400 | 0.65002200 |
| H     | -7.09565000| 4.18030500 | 0.01617200 |
| C     | -4.61042800| -1.31598000| -0.31249700|
| C     | -5.84685100| -3.71431300| -1.05163500|
| C     | -5.97478700| -1.35610800| -0.67671200|
| C     | -3.87001800| -2.51625100| -0.31981700|
| C     | -4.48658600| -3.69436600| -0.68611200|
| C     | -6.59246100| -2.54913900| -1.08603000|
| Atom | x     | y     | z     |
|------|-------|-------|-------|
| H1   | 3.81593700 | -0.97807000 | 1.65790100 |
| H2   | 3.75257600 | -0.18331800 | 0.91454300 |
| H3   | 3.56131600 | 1.91206000 | -0.94933400 |
| H4   | 2.55447100 | 0.51249700 | 0.78058400 |
| H5   | 4.84992600 | 0.12617400 | 0.10763000 |
| H6   | 4.74252200 | 1.17710100 | -0.82333500 |
| H7   | 2.47924800 | 1.57030200 | -0.14908000 |
| H8   | 1.56331300 | 2.14841200 | -0.22306400 |
| H9   | 3.49204900 | 2.73856300 | -1.64916000 |
| H10  | 1.42308900 | 0.16680400 | 1.70861100 |
| H11  | 0.17931200 | -0.10309800 | 2.90238600 |
| H12  | 0.07011400 | 0.13727500 | 1.22913900 |
| H13  | -2.64276500 | -0.02399000 | 0.43909300 |
| H14  | -0.30979700 | 0.17657200 | -0.15213100 |
| H15  | -0.98590000 | 0.30461000 | 2.18904400 |
| H16  | -2.30275600 | -0.10230700 | 1.81474300 |
| H17  | -1.62523300 | 0.99844000 | -0.54303100 |
| H18  | 0.45284100 | 0.23278000 | -0.92175000 |
| H19  | -0.71171900 | -0.09283200 | 3.23673900 |
| H20  | -3.09040100 | -0.21798100 | 2.55462400 |
| H21  | -1.89471800 | 0.11661700 | -1.59533800 |
| N2   | -4.00474400 | -0.11052100 | 0.03987600 |
| C3   | -4.79681600 | 1.02571600 | -0.00066000 |
| C4   | -6.46052200 | 3.26749600 | -0.10035700 |
| C5   | -4.28919300 | 2.29361600 | 0.34440000 |
| C6   | -6.14080000 | 0.91363900 | -0.39413100 |
| C7   | -6.97845600 | 2.02797000 | -0.44435300 |
| C8   | -5.11713600 | 3.39785700 | 0.29233200 |
| C9   | -3.25238200 | 2.37704000 | 0.65455100 |
| H18  | -8.00947900 | 1.89438000 | -0.75236900 |
| H19  | -4.72439800 | 4.37211900 | 0.55853000 |
| H20  | -7.10063200 | 4.14161700 | -0.13616000 |
| C21  | -4.55512200 | -1.33370700 | -0.30783200 |
| C22  | -5.73738900 | -3.76013500 | -1.02752000 |
| C23  | -5.91076100 | -1.39651700 | -0.70120900 |
| C24  | -3.79653600 | -2.52046000 | -0.28065700 |
| C25  | -4.38760300 | -3.71668900 | -0.63750700 |
| C26  | -6.50082200 | -2.60294100 | -1.05949700 |
| H27  | -2.75810600 | -2.47103400 | 0.02274300 |
| H28  | -3.80219800 | -4.62825800 | -0.61546800 |
| H29  | -7.54400300 | -2.60727100 | -1.35343600 |
| O    | -6.18980100 | -4.70528300 | -1.30533200 |
| C    | -6.68263600 | -0.28331300 | -0.73914000 |
| S    | 6.21692300 | 1.42290600 | -1.72864700 |
| C    | 7.00923600 | 0.11818200 | -0.87630500 |
| C    | 7.96782600 | -1.98799900 | 0.65039000 |
| C    | 8.32238700 | -0.31547100 | -1.07508800 |
| C    | 6.16920100 | -0.48926000 | 0.07641200 |

**DBT-BZ-PXZ-S Geometry (Solvent: THF)**
### DBT-BZ-PTZ-S<sub>6</sub> Geometry (Solvent: THF)

| Atoms | Coordinates (Angstrom) |
|-------|------------------------|
| H     | 2.31241300 -0.00251800 -0.68025700 |
| C     | 3.12073000 -0.69518500 -0.46436700 |
| C     | -2.10645000 -0.70749600 -0.46407900 |
| C     | -0.63894500 -2.00592300 -1.87060900 |
| C     | 0.13274100 -1.22436000 0.28644000 |
| C     | -1.10453200 -0.63103000 0.51159700 |
| C     | -1.69974900 -1.39317400 -1.65492900 |
| H     | -0.44863200 -2.55654000 -2.78611800 |
| H     | 0.90184600 -1.17071300 1.05038000 |
| H     | -1.30540600 -0.10474800 1.44110600 |
| C     | -2.65965400 -1.44238500 -2.39747700 |
| O     | 1.66211700 -3.66929900 -1.81107900 |
| N     | -3.38010300 -0.90658000 -0.26188400 |
| C     | -3.46369000 1.31270000 -0.44109000 |
| C     | -2.32510900 2.10578800 -0.63606500 |
| C     | -4.72025600 1.94251800 -0.45697400 |
| C     | -4.82505400 3.32336700 -0.60770100 |
| C     | -2.44041900 3.48227700 -0.82747300 |
| H     | -1.34240300 1.65091800 -0.65263500 |
| H     | -5.81061900 3.77930300 -0.59513300 |
| H     | -1.54083900 4.06779400 -0.98732900 |
| H     | -3.77598100 5.17401800 -0.94082900 |
| C     | -4.30338000 -0.76412800 0.57688500 |
| C     | -6.18143500 -2.07242000 2.22588000 |
| C     | -5.63411500 -0.31810500 0.65277500 |
| C     | -3.94124600 -1.89317400 1.32323300 |
| C     | -4.87608300 -2.54421600 2.12741100 |
| C     | -6.55202000 -0.94883400 1.48948200 |
| H     | -2.93073300 -2.27918800 1.27060100 |
| H     | -4.56804700 -3.42288300 2.68468800 |
| H     | -7.56697500 -0.56569300 1.53887900 |
| H     | -6.90598400 -2.57100100 2.86035700 |
| S     | -6.18778900 0.96832100 -0.41644900 |
| S     | 6.85355900 -0.32955100 0.77452600 |
| C     | 6.09821500 1.24265300 0.65489900 |
| C     | 4.61624800 0.56538700 0.35888500 |
| C     | 6.70019900 2.46759300 0.95326700 |
| C     | 4.76500700 1.16568200 0.21078600 |
| C     | 4.02347500 2.34527700 0.06283600 |
| C     | 5.94737800 3.62511200 0.80005700 |
| H     | 7.72890100 2.51322200 1.29538000 |
| H     | 2.99392700 2.30478900 -0.28061700 |
| H     | 6.39612300 4.58693700 1.02588600 |
| H     | 4.04714900 4.48206200 0.24353900 |

### DBT-BZ-PTZ-T<sub>1</sub> Geometry (Solvent: THF)
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| H       | 2.4978700 | 0.3224430 | -0.6901470 |
| C       | 3.2398470 | -0.4577090 | -0.5459420 |
| C       | 5.2209080 | -2.4405840 | -0.2743900 |
| C       | 2.9513100 | -1.7753640 | -0.9147930 |
| C       | 4.4965530 | -0.1237600 | -0.0287390 |
| C       | 5.4781000 | -1.1205900 | 0.1119600  |
| C       | 3.9714560 | -2.7480470 | -0.7883440 |
| C       | 3.7490240 | -3.7595390 | -1.1119990 |
| C       | 1.6585420 | -2.1982890 | -1.5269440 |
| H       | -0.6426820 | 2.5481880 | -2.7647860 |
| H       | 1.0405230 | -0.5998070 | 0.7087330  |
| H       | -1.1650220 | 0.2999960 | 1.2703710  |
| O       | 0.4934460 | 0.3112450 | 0.2130550  |
| N       | -3.4400120 | 0.5038500 | 0.0903830  |
| C       | 1.6585420 | -2.1982890 | -1.5269440 |
| C       | -0.7614040 | -1.9098610 | -1.8966520 |
| C       | 0.2109490 | -0.8005720 | 0.0409250  |
| C       | 1.2874594 | 1.0405230 | -0.5998070 |
| H       | -0.6426820 | 2.5481880 | -2.7647860 |
| H       | 1.0405230 | -0.5998070 | 0.7087330  |
| H       | -1.1650220 | 0.2999960 | 1.2703710  |
| O       | 0.4934460 | 0.3112450 | 0.2130550  |
| N       | -3.4400120 | 0.5038500 | 0.0903830  |
| C       | 1.6585420 | -2.1982890 | -1.5269440 |
| C       | -0.7614040 | -1.9098610 | -1.8966520 |
| C       | 0.2109490 | -0.8005720 | 0.0409250  |
| C       | 1.2874594 | 1.0405230 | -0.5998070 |
| H       | -0.6426820 | 2.5481880 | -2.7647860 |
| H       | 1.0405230 | -0.5998070 | 0.7087330  |
| H       | -1.1650220 | 0.2999960 | 1.2703710  |
| O       | 0.4934460 | 0.3112450 | 0.2130550  |
| N       | -3.4400120 | 0.5038500 | 0.0903830  |
| C       | 1.6585420 | -2.1982890 | -1.5269440 |
| C       | -0.7614040 | -1.9098610 | -1.8966520 |
| C       | 0.2109490 | -0.8005720 | 0.0409250  |
| C       | 1.2874594 | 1.0405230 | -0.5998070 |
| H       | -0.6426820 | 2.5481880 | -2.7647860 |
| H       | 1.0405230 | -0.5998070 | 0.7087330  |
| H       | -1.1650220 | 0.2999960 | 1.2703710  |
| O       | 0.4934460 | 0.3112450 | 0.2130550  |
| N       | -3.4400120 | 0.5038500 | 0.0903830  |
| C       | 1.6585420 | -2.1982890 | -1.5269440 |
| C       | -0.7614040 | -1.9098610 | -1.8966520 |
| C       | 0.2109490 | -0.8005720 | 0.0409250  |
| C       | 1.2874594 | 1.0405230 | -0.5998070 |
| H       | -0.6426820 | 2.5481880 | -2.7647860 |
| H       | 1.0405230 | -0.5998070 | 0.7087330  |
| H       | -1.1650220 | 0.2999960 | 1.2703710  |
| O       | 0.4934460 | 0.3112450 | 0.2130550  |
| N       | -3.4400120 | 0.5038500 | 0.0903830  |
| C       | 1.6585420 | -2.1982890 | -1.5269440 |
| C       | -0.7614040 | -1.9098610 | -1.8966520 |
| C       | 0.2109490 | -0.8005720 | 0.0409250  |
| C       | 1.2874594 | 1.0405230 | -0.5998070 |

**DBT-BZ-PTZ-S, Geometry (Solvent: THF)**

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| H       | 2.5300400 | 0.3674430 | -0.8195530 |
| C       | 3.2415580 | -0.4294130 | -0.6203100 |
| C       | 5.1167580 | -2.4834980 | -0.1724370 |
| C       | 2.9269560 | -1.7433930 | -0.9628650 |
| C       | 4.4830660 | 0.1272510 | 0.0473530  |
| C       | 5.4081030 | -1.1618120 | 0.1795190  |
| C       | 3.8856620 | -2.7560000 | -0.7486650 |
| H       | 3.6376580 | -3.7685650 | -1.0505040 |
| H       | 5.8385780 | -3.2762630 | 0.0031170  |
| C       | 1.6410920 | -2.1204810 | -1.6429920 |
C   0.39495600  -1.55463200  -1.21038700
C  -2.14884700  -0.56386300  -0.45781900
C  -0.77959400  -1.81495700  -1.99697700
C   0.21019500  -0.80788200  -0.00105800
C  -1.02246200  -0.32315100    0.36820000
C  -2.01275700  -1.32950000  -1.64155000
H   -0.66433100  -2.40769100  -2.89810500
H    1.04961300  -0.64275700    0.66609400
H   -1.14617300   0.23000000    1.29523700
H   -2.88806400   1.52292700   -2.25646200
O    1.71304100  -2.94915400  -2.59006700
N   -3.42596100  -0.04265900  -0.08604700
C  -3.78119200    1.21236300  -0.57129200
C  -4.42885900    3.75547900  -1.59898000
C  -5.02053100   -0.26707500
C  -5.32978400  -0.78657300
C   -3.19631700   3.15524400  -1.09530500
H   -1.92516900   1.45422700  -1.64530500
H   -6.28602400   3.54549700  -0.53988000
H   -2.48547700   3.69282000  -2.54200900
H   -4.67639400   4.73326700  -1.99608200
H  -4.23220800  -0.82121100   0.73894600
H   -5.80350000  -2.45470900   2.41360600
H   -5.51308300   -0.40045500  1.17615700
C   -3.76376500   2.08655500  1.16560500
C   -4.53613100  -2.88293100   1.98501200
C   -6.28397100  -1.22410700   2.01021000
H   -2.78891100  -2.42249400  0.83893000
H   -4.15483200   -3.84826200  2.29756200
H   -7.26164900  -0.87945000  2.33192700
H   -6.40636500  -3.08454500  3.05775800
S   -6.22046100   1.10785300   0.73695800
S   -6.89240000  -0.58568800   0.90121800
C    6.30197400    1.05922500  0.90766000
C    5.07384700   3.54152800   0.77514500
C    6.99266200   2.17952000  1.37645700
C    5.00350700   1.16536500   0.37297100
C    4.39180000   2.42446400  0.31128000
C    6.36824100   3.41881300  1.30300200
H    7.99353000   2.08410900  1.78566600
H    3.39061800   2.52393700  -0.09813500
H    6.89826200   4.30082800  1.66328100
H    4.60364300   4.51830000  0.72799800

**DBT-BZ-DMAC-S₆ Geometry (Solvent: THF)**

H    4.42329200  -1.70464800  1.08478600
C    4.28626600  -0.70270900  0.68850600
C    3.87470200   1.91179000  -0.28696300
C    3.03074300  -0.10351200   0.77962400
C    5.34147300  -0.01472200   0.08850300
C    5.12309900  -1.29316500  -0.39406500
C    2.83218900   1.20326600   0.29175200
C    1.86056500   1.67629300   0.39022600
H    3.72229400   2.92351200  -0.64727300
C    1.94163300  -0.86536100  1.46223400
C    0.51167500  -0.61967800  1.08583400
C   -2.17994800  -0.29438600  0.44818100
C    0.13494400  -0.29966900  -0.22336800
C   -0.46920800  -0.78752700   2.07020200
C   -1.81201100  -0.61306100   1.75631800
C   -1.21166800  -0.14660400  -0.54335600
H    0.88744400  -0.19240100  -0.99843200
H   -0.16549700  -1.05036300  3.07829200
H   -2.58357200  -0.72497900  2.51213200
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| N    | -3.62605000 | -0.11874800 | 0.11216000 |
| C    | -4.42776100 | -1.18701800 | -0.31041700 |
| C    | -5.98894800 | -3.36493600 | -1.15888500 |
| C    | -3.85105300 | -2.45527100 | -0.51306300 |
| C    | -5.80496800 | -1.00605400 | -0.53444300 |
| C    | -6.55352400 | -2.10978100 | -0.95611500 |
| C    | -4.62402300 | -3.52980600 | -0.93225000 |
| H    | -2.79115100 | -2.59798300 | -0.33959300 |
| H    | -7.61808600 | -1.98277500 | -1.13203800 |
| H    | -4.15252600 | -4.49641100 | -1.07997600 |
| H    | -6.60403800 | -4.19618900 | -1.48655100 |
| C    | -4.15614900 | 1.15930800  | 0.32838200  |
| C    | -5.16600500 | 3.74402300  | 0.77767200  |
| C    | -5.52507600 | 1.41297100  | 0.12480200  |
| C    | -3.31180500 | 2.02246000  | 0.75429800  |
| H    | -2.25761300 | 2.09027100  | 0.91324800  |
| H    | -3.13858000 | 4.26323000  | 1.30493000  |
| H    | -7.05069900 | 2.91798500  | 0.20299700  |
| H    | -5.57013700 | 4.73630600  | 0.94722400  |
| S    | 6.61240300  | 1.88130300  | -1.23419500 |
| C    | 7.61928000  | 0.59487900  | -0.60035800 |
| C    | 8.90396400  | -1.57184200 | 0.52099900  |
| C    | 9.00390400  | 0.51203800  | -0.71974100 |
| H    | 6.86165300  | -0.38381000 | 0.06742900  |
| C    | 7.51691100  | -1.47677600 | 0.63188300  |
| C    | 9.64073700  | -0.58811100 | -0.14805300 |
| H    | 9.56840500  | 1.27905600  | -1.23914000 |
| H    | 10.71844000 | -0.67973100 | -0.22421700 |
| C    | 9.41822700  | -2.42055200 | 0.95914500  |
| C    | -6.50623800 | 0.33622700  | -0.33487300 |
| C    | 7.14676700  | 0.77439200  | -1.66987000 |
| C    | 7.86944300  | 0.03049800  | -0.01720500 |
| H    | 6.37966900  | 0.89687200  | -2.44019000 |
| H    | 7.67521800  | 1.72501200  | -1.55411700 |
| C    | 7.61158600  | 0.17373000  | 0.73113900  |
| H    | 7.17861800  | -0.13673300 | 1.68658100  |
| H    | -8.34238400 | -0.57910600 | 0.42207800  |
| H    | -8.14602000 | 1.11577700  | 0.88365300  |

**DBT-BZ-DMAC-S**

Geometry (Solvent: THF)

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 4.29137500 | -0.99419600 | 1.64783900 |
| C    | 4.21736200 | -0.20110700 | 0.90906200 |
| C    | 4.00011300 | 1.90734800 | -0.94289500 |
| C    | 3.01855200 | 0.50258100 | 0.79761100 |
| C    | 5.30189900 | 0.11424500 | 0.08526200 |
| C    | 5.18139400 | 1.16898700 | -0.83976000 |
| C    | 2.93085600 | 1.56466000 | -0.12591900 |
| H    | 2.01543100 | 2.14582100 | -0.18197200 |
| H    | 3.92110400 | 2.73687200 | -1.63837000 |
| C    | 1.90085800 | 0.15426700 | 1.74123800 |
| C    | 0.54104100 | 0.13297500 | 1.28313200 |
| C    | -2.18667300 | -0.00775600 | 0.53463200 |
| C    | 0.13848300 | 0.18368800 | -0.09120400 |
| C    | -0.50135300 | -0.03582800 | 2.25771400 |
| C    | -1.82433700 | -0.99688000 | 1.90357200 |
| C    | -1.18345300 | 0.11651900 | -0.46151800 |
| H    | 0.88847500 | 0.24017800 | -0.87324500 |
| H    | -0.21149900 | -0.10771500 | 3.30071200 |
| H    | -2.60131400 | -2.21221700 | 2.65480100 |
| O    | -1.46964200 | 0.14162600 | -1.50928600 |
| N    | 2.21537300 | -0.12424000 | 2.92878300 |
| C    | -3.55700000 | -0.07702700 | 0.15558800 |
| C    | -4.10514200 | -1.31106000 | -0.17882400 |
CP-BP-PXZ-S_8 Geometry (Solvent: THF)

H  0.96549700  0.43647200  -0.60476900
C  1.83361600  -0.21338000  -0.54827600
C  4.11536500  -1.90939800  -0.44076400
C  1.72173700  -1.58120100  -0.80997200
C  3.08521600  0.31661000  -0.24126500
C  4.21626200  -0.53394900  -0.19076600
C  2.86574700  2.40972300  -0.75978100
H  2.74232600  -3.46641500  -0.97291400
H  4.98275400  2.55836600  -0.38656600
C  0.43201000  2.20317000  1.21152100
O  0.40871700  2.32182500  -1.87418300
C  0.86513800  -1.56680000  -0.80240600
C  -3.34194600  -0.51873200  -0.07958000
C  -1.95154000  -1.65379900  -1.68163100
C  -1.03238500  -0.95913500  0.44530500
C  -2.27493100  -0.44217500  0.81014400
C  -3.18444300  1.12629600  -1.32849200
H  -1.81415900  -2.14921600  -2.64028800
H  -0.20262500  -0.90768800  1.14327100
H  -2.42596600  0.02072800  1.78002000
H  -4.03111500  2.17824400  -2.02724400
N  -4.60972500  0.02689800  0.29955300
C  -5.62585700  -0.85704100  0.71563300
C  -7.72007400  -2.50962600  1.60050600
| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| C     | 6.94710100 | -2.51178500 | -2.67017200 |
| C     | 4.92617500  | -2.17315800  | -1.37416300  |
| C     | 6.73155500  | -0.54769900  | -1.32345100  |
| C     | 7.47933200  | -1.32117400  | -2.20868800  |
| C     | 5.67102800  | -2.93524200  | -2.24971100  |
| H     | 3.94454900  | -2.48959900  | -1.04223800  |
| H     | 8.45891700  | -0.96838900  | -2.51022900  |
| H     | 5.26695500  | -3.87180900  | -2.61645800  |
| C     | 5.30771200  | 1.02886500   | 0.42970000   |
| C     | 6.52793000  | 3.39832000   | 1.27968800   |
| C     | 6.59553200  | 1.39348600   | -0.02171100  |
| C     | 4.63323600  | 1.88636900   | 1.32326600   |
| H     | 3.64403200  | 1.60086000   | 1.66819600   |
| H     | 8.19512900  | 2.81072500   | 0.02768300   |
| C     | 6.99205400  | 4.31853300   | 1.61630600   |
| O     | 7.28229500  | 0.60940300   | -0.86805100  |
| C     | -5.01326000 | 1.54939900   | -0.50632900  |
| C     | -3.88501400 | 4.05707000   | -0.86283300  |
| C     | -5.81895700 | 2.57540100   | -1.09922200  |
| C     | -3.65775400 | 1.76854100   | -0.16623600  |
| C     | -3.09374100 | 3.03459800   | -0.35154200  |
| C     | -5.23444000 | 3.82540200   | -1.18265100  |
| H     | -6.86298300 | 2.40675600   | -1.25151000  |
| H     | -2.05389400 | 3.21536700   | -0.09447800  |
| H     | -5.83720100 | 4.63994700   | -1.57206900  |
| N     | -3.46198700 | 5.04497200   | -1.01283500  |
| C     | -5.34309700 | 0.22826400   | -0.22176300  |
| C     | -6.61852100 | -0.36431300  | -0.40322700  |
| C     | -7.22964100 | -0.32980100  | -1.65886800  |
| C     | -7.25854200 | -0.98023800  | 0.67496100   |
| C     | -8.48741400 | -0.90410400  | -1.83008600  |
| C     | -6.71289300 | 0.13795100   | -2.49153100  |
| C     | -8.50736100 | -1.56963600  | 0.49046600   |
| C     | -6.77800300 | -0.98680300  | 1.64863200   |
| C     | -9.12661400 | -1.52904800  | -0.75907700  |
| H     | -8.96189500 | -0.87372300  | -2.80566400  |
| C     | -9.00141700 | -2.05064900  | 1.32850200   |
| C     | -10.10255600| -1.98265500  | -0.89764800  |

**CP-BP-PXZ-S** Geometry (Solvent: THF)

| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| H     | -1.0871300 | 0.87538000 | 0.98612100 |
| C     | -1.89228500| 0.15044800| 0.90310300|
| C     | -4.01617000| -1.72385900| 0.73874100|
| C     | -1.69860700| -1.16632100| 1.32020100|
| C     | -3.13752200| 0.53923100| 0.40105200|
| C     | -4.18955500| -0.39863000| 0.32327200|
| C     | -2.77384700| -2.07940000| 1.24301800|
| H     | -2.60554500| -3.09197100| 1.59605200|
| H     | -4.82167100| -2.44711100| 0.67235400|
| C     | -0.41386600| -1.64074900| 1.93863600|
| O     | -0.49868000| -2.40577700| 2.93503800|
| C     | 0.85199900 | -1.22757400| 1.39890300|
| C     | 3.42478700 | -0.53361300| 0.44170600|
| C     | 2.04251300 | -1.53804400| 2.14232500|
| C     | 1.03034300 | -0.59129100| 0.12710900|
| C     | 2.27541000 | -0.25171900| -0.34494100|
| C     | 3.29084900 | -1.19664900| 1.69047500|
| H     | 1.92636600 | -2.04854500| 3.09246400|
| C     | 0.16965700 | -0.39899400| -0.50493000|
| C     | 2.39317300 | 0.21808100 | -1.31741600|
| H     | 4.17982700 | -1.42422400| 2.27290100|
| N     | 4.71243100 | -0.15782700| -0.02740200|
CP-BP-DMAC-S\textsubscript{6} Geometry (Solvent: THF)

\begin{verbatim}
C 1.36710300 0.32342400 -0.76686000
C 2.25136500 -0.29420900 -0.64078500
C 4.57643400 -1.90792900 -0.34991700
C 2.19340100 -1.67572500 -0.84036200
C 3.47118800 0.29025400 -0.30569100
C 4.62402600 -0.51956600 -0.16389900
C 3.58391900 -2.46323100 -0.69898100
C 3.27701500 -3.53233700 -0.86532700
C 5.45969400 -2.52500700 -0.22532700
C 0.94295200 -2.35672000 -1.27055400
C -0.39008300 -1.74655000 -0.94738300
C -2.93062200 -0.75222100 -0.38082200
C -1.43153900 -1.91099600 -1.86767200
C -0.63304700 -1.09158500 0.26506100
C -1.90554700 -0.60316500 0.55155000
C -2.69645700 -1.40386300 -1.59234500
H -1.23620400 -2.43518200 -2.79766600
H 0.16246100 -0.98278600 0.99569100
H -2.11325700 -0.10606200 1.49427200
H -3.51012900 -1.51049000 -2.30350200
\end{verbatim}
O  0.98305400 -3.41242300 -1.88849000
N  -4.23075000 -0.23783300 -0.09140600
C  -5.16186300 -1.06224200  0.55815900
C  -6.98520300 -2.75624500  1.86129400
C  -4.80244800 -2.37682900  0.91023100
C  -6.45060300 -0.58763400  0.86146000
C  -7.33431300 -3.39874300  2.36409100
C  -5.70523000 -3.21247900  1.55415600
H  -3.81083400 -2.74614600  0.67738700
H  -8.33281800 -1.10191200  1.75114800
H  -5.40153200 -4.22180300  1.81370600
H  -7.70003400 -3.39874300  2.36409100
C  -4.54524600  1.07535700 -0.46672600
C  -5.11916300  3.71500000 -1.23973100
C  -5.81554100  1.64885000 -0.19430700
C  -3.58017600  1.86269100 -1.12257200
C  -3.86579800  3.16697000 -1.50386700
C  -6.06489800  2.93166000 -0.59181200
H  -2.60128900  1.44979300 -1.33551000
H  -3.10295400  3.75121900 -2.00879500
H  -7.04570900  3.36061700 -1.53197500
C  -5.26095400  1.60046900  0.27487500
C  -3.88235700  1.65148400 -0.02655000
C  -3.21493800  2.88044300 -0.01627600
C  -5.30999900  3.96155700  0.57464900
H  7.05638300  2.70601800  0.78799700
H  2.15475700  2.93408500 -0.24552100
H  5.85091800  4.87403300  0.80217400
H  3.43304400  4.99198800  0.30169600
C  -6.91542600  0.73686600 -0.41230000
H  -8.96156000  0.19198600  0.07496600
H  -7.89251600  0.21870100 -1.34121300
H  -8.51823400  1.73485400 -0.66368900
C  -7.30641400  1.56129500  1.81355400
C  -6.44595700  1.63497200  2.48509900
C  -8.10730900  1.02947200  2.33511900
C  -7.66266000  2.57228800  1.59604500
N  5.69608300  0.27831300  0.18806900
C  7.02581500 -0.17130600  0.41530900
C  7.63851400  0.07775500  1.64442400
C  7.70665800 -0.85666000 -0.59212600
C  8.94451400 -0.35682500  1.86076600
C  7.08856400  0.60155900  2.42053300
C  9.00571800 -1.30432900 -0.36046200
C  7.21929890 -1.02803600 -1.54727100
C  9.62770000 -1.05176700  0.86236900
C  9.42336700 -0.16160200  2.81471600
C  9.53498400 -1.84076300 -1.14121000
C 10.64198100 -1.39546200  1.03678100

CP-BP-DMAC-T1 Geometry (Solvent: THF)

H  1.54186000  0.78964800 -1.00392400
C  2.35210700  0.07595100 -0.88224100
C  4.50524400 -1.75309200 -0.63425600
C  2.17219900 -1.26333200 -1.23840700
C  3.59082800  0.50576900 -0.39732300
C  4.65901600 -0.40871700 -0.27828800
C  3.26778700 -2.15153900 -1.11765400
H  3.11627200 -3.18234100 -1.42163200
H  5.32165000 -2.46145600 -0.53736300
C  0.90321600 -1.79187990 -1.82704700
C -0.37995700 -1.34059300  1.35835400
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -2.98522100 | -0.60814100 | -0.52767800 |
| C    | -1.54769800  | -1.73197000 | -2.09473800 |
| C    | -0.60376100  | -0.59021000 | -0.15858200 |
| C    | -1.87368400  | -0.23267600 | 0.24648000  |
| H    | -1.40529300  | -2.32452700 | -2.99134000 |
| H    | 0.23348700   | -0.32254900 | 0.47659500  |
| H    | -2.02325100  | -0.23245700 | -2.99134000 |
| H    | -3.68792900  | -1.66436000 | -2.75304000 |
| O    | 0.99418300   | -2.66322200 | -2.75002300 |
| N    | -4.31334800  | -0.23118100 | -0.10247100 |
| C    | -5.01980500  | -1.08801600 | 0.72932100  |
| C    | -6.38343500  | -2.85273200 | 2.39569600  |
| C    | -4.41072700  | -3.02093000 | 1.13398800  |
| C    | -3.24854000  | -0.75396800 | 1.16514700  |
| C    | -6.97985500  | -1.66032600 | 1.99853500  |
| C    | -5.09105700  | -3.17202700 | 1.95920100  |
| H    | -3.41860000  | -2.53679700 | 0.78922100  |
| H    | -7.98152800  | -1.43452600 | 2.34883800  |
| H    | -4.62160600  | -4.09733000 | 2.26503500  |
| H    | -6.92242800  | -3.53367500 | 3.04471500  |
| C    | -4.80581000  | 0.97594000  | -0.53890100 |
| C    | -5.83771200  | 3.41061700  | -1.44940100 |
| C    | -6.13848300  | 1.37932300  | -0.14286000 |
| C    | -4.05619000  | 1.79531700  | -1.38810800 |
| C    | -4.55517200  | 3.00014300  | -1.83558100 |
| C    | -6.60734200  | 2.60459900  | -0.61649900 |
| H    | -3.06747700  | 1.46498400  | -1.67976300 |
| H    | -3.95188000  | 3.62378900  | -2.48542400 |
| H    | -7.59853300  | 2.94205800  | -0.33209900 |
| H    | -6.23574300  | 4.35726000  | -1.79823800 |
| C    | 5.43544200   | 1.58616900  | 0.44782100  |
| C    | 4.30099700   | 1.01803100  | 0.64834100  |
| C    | 6.22922300   | 2.63666900  | 0.91806900  |
| C    | 4.08909000   | 1.78727900  | 0.06318900  |
| C    | 3.52188500   | 3.06921200  | 0.16974200  |
| C    | 5.64179600   | 3.89361800  | 1.01324400  |
| H    | 7.26671500   | 2.48094300  | 1.19461000  |
| H    | 2.48901100   | 3.22803700  | -0.12226700 |
| H    | 6.23538900   | 4.72701200  | 1.37593100  |
| H    | 3.87522900   | 5.10283300  | 0.73715500  |
| C    | -7.01461600  | 0.53176600  | 0.75686300  |
| C    | -8.31736300  | 0.17994200  | -0.00392200 |
| H    | -8.98000500  | -0.41266700 | 0.63089000  |
| H    | -8.90344000  | -0.39303300 | -0.90571900 |
| H    | -8.84775700  | 1.09095500  | -0.28973100 |
| C    | -7.36065900  | 1.34298100  | 2.03008300  |
| H    | -6.45293100  | 1.60116700  | 2.58167700  |
| H    | -8.01494400  | 0.76297000  | 2.68485700  |
| H    | -7.88207900  | 2.26508500  | 1.76309000  |
| N    | 5.77146200   | 0.25262500  | 0.23824000  |
| C    | 7.03831900   | -0.33130000 | 0.49261900  |
| C    | 7.60945700   | 0.22697500  | 1.76309600  |
| C    | 7.71015300   | -1.00819100 | -0.52813500 |
| C    | 8.85953900   | -0.79220100 | 2.00639200  |
| H    | 7.06832700   | 0.28785300  | 2.55127000  |
| C    | 8.95079100   | -1.58785900 | -0.27100100 |
| H    | 7.26082500   | -1.06888500 | -1.51472300 |
| C    | 9.53046700   | -1.47738600 | 0.99314400  |
| H    | 9.30295100   | -0.70738400 | 2.99330200  |
| H    | 9.46959800   | -2.11615600 | -1.06442800 |
| H    | 10.50026400  | -1.92353600 | 1.18780900  |

**CP-BP-DMAC-S₁ Geometry (Solvent: THF)**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 1.54226000 | 0.85819700 | -1.07344700 |
| XYZ Coordinates | Label |
|-----------------|-------|
| H 7.26092900 -1.05591700 -1.49480000 | H |
| C 9.45146400 -1.55507800 1.06644300 | C |
| H 9.17743100 -0.82834700 3.07696800 | H |
| H 9.44142400 -2.14535700 -1.00645000 | H |
| H 10.40900500 -2.01954700 1.27812400 | H |

### a1-S0 Geometry (Solvent: Toluene)

| XYZ Coordinates | Label |
|-----------------|-------|
| H -2.81501900 1.24883300 1.66773600 | H |
| C -1.86949000 0.82296700 1.98770400 | C |
| C 0.57822000 -0.25179200 2.77289800 | C |
| C -0.95245500 0.41946400 -1.02203000 | C |
| C -1.57508300 0.70054300 3.33496300 | C |
| C -0.34256800 0.15683000 3.75105500 | C |
| C 0.27858400 -0.11691500 1.42364300 | C |
| H -2.92233300 1.03065000 4.07855900 | H |
| H 1.53396600 -0.68253500 3.05149800 | H |
| C -1.29602300 0.56817700 -0.42074200 | C |
| O -2.36653600 1.03424300 -0.77942000 | O |
| C 1.29602300 -0.56817700 0.42074200 | C |
| O 2.36653600 -1.03424300 0.77942000 | O |
| C -0.95245500 -0.41946400 -1.02203000 | C |
| C 0.34256800 -1.56830000 -3.75105500 | C |
| C -0.27858400 0.11691500 -1.42364300 | C |
| C 1.86949000 -0.82296700 -1.98770400 | C |
| C 1.57508300 -0.70054300 -3.33496300 | C |
| C -0.57822000 0.25179200 -2.77289800 | C |
| C 2.81501900 -1.24883300 -1.66773600 | C |
| H 2.92233300 -1.03065000 -4.07855900 | H |
| H -1.53396600 0.68253500 -3.05149800 | H |
| N 0.04150100 -0.03063200 -5.10959000 | N |
| C 1.07468200 0.13143800 -6.07494800 | C |
| C 3.08035300 0.46301600 -7.99558700 | C |
| C 2.09991900 1.05958300 -5.86624000 | C |
| C 1.05250800 -0.62459100 -7.25064400 | C |
| C 2.04891300 -0.45147600 -8.20782400 | C |
| C 3.10205500 2.14363600 -6.82027600 | C |
| H 2.10572700 1.65385400 4.95723100 | H |
| H -0.25013900 -1.33895900 -7.40890100 | H |
| H 2.02278200 -1.04187500 -9.11824700 | H |
| H 3.89469800 1.93588400 -6.64914100 | H |
| H 3.85873300 0.59165100 -8.74042300 | H |
| C -1.30696000 -0.67498000 -5.56556900 | C |
| C -3.94148800 -0.15064500 -6.49845100 | C |
| C -1.75091600 0.87436500 -6.49818700 | C |
| C -2.18326800 -1.05531800 -5.10557800 | C |
| C -3.49698000 -1.08722200 -5.56083000 | C |
| C -3.06162200 0.82530600 -6.96566600 | C |
| H -1.06374000 1.63609800 -6.85415700 | H |
| H -1.83147400 -1.79097700 -4.38838100 | H |
| H -4.17136000 -1.85499400 -5.19938600 | H |
| H -3.39779300 1.56068500 -7.68977100 | H |
| H -4.96439900 -0.18186600 -6.88575100 | H |
| N -0.04150100 0.03063200 5.10959000 | N |
| C 1.30696000 0.67498000 5.56556900 | C |
| C 3.94148800 1.50645000 6.49845100 | C |
| C 2.18326800 1.05531800 5.10557800 | C |
| C 1.75091600 -0.87436500 6.49818700 | C |
| C 3.06162200 -0.82530600 6.96566600 | C |
| C 3.49698000 1.08722200 5.56083000 | C |
| H 1.83147400 1.79097700 4.38838100 | H |
| H 1.06374000 -1.63609800 6.85415700 | H |
| H 3.39779300 -1.56068500 7.68977100 | H |
| H 4.17136000 1.85499400 5.19938600 | H |
| H 4.96439900 0.18186600 6.88575100 | H |
| C -1.07468200 -0.13143800 6.07494800 | C |
| C -3.08035300 -0.46301600 7.99558700 | C |
| Atom  | X     | Y     | Z     |
|-------|-------|-------|-------|
| C     | -2.0991900 | -1.0595830 | 5.8662400 |
| C     | -1.0525080 | 0.6245910 | 7.2506440 |
| C     | -2.0489130 | 0.4514760 | 8.2078240 |
| C     | -3.1020550 | -1.2143630 | 6.8202760 |
| H     | -2.1057270 | -1.6538540 | 4.9572310 |
| H     | -0.2501390 | 1.3389590 | 7.4089010 |
| H     | -2.0227820 | 1.0418750 | 9.1182470 |
| H     | -3.8946980 | -1.9358840 | 6.6491410 |
| H     | -3.8587330 | -0.5916510 | 8.7404230 |

**a1-T₁ Geometry (Solvent: Toluene)**

| Atom  | X     | Y     | Z     |
|-------|-------|-------|-------|
| H     | -2.7215280 | 1.4329640 | 1.6468040 |
| C     | -1.8091960 | 0.9483270 | 1.9781740 |
| C     | 0.5945880 | -0.2661660 | 2.7540690 |
| C     | -0.9119620 | 0.4819060 | 0.9802580 |
| H     | -2.2006970 | 1.0237950 | 4.0627300 |
| H     | 1.5227550 | -0.7534970 | 3.0346940 |
| C     | -1.2689580 | 0.6515160 | -0.9802580 |
| C     | -0.2981770 | 0.1948550 | 3.7171570 |
| H     | -2.3383830 | 1.2020900 | -0.7715650 |
| C     | 1.2689580 | -0.6515160 | 0.4203660 |
| O     | -2.3383830 | -1.2020900 | 0.7715650 |
| C     | 0.9119620 | -0.4819060 | -0.9802580 |
| C     | -0.2981770 | -0.1948550 | -3.7171570 |
| C     | -3.0817700 | 0.1334710 | -1.3970200 |
| C     | 1.8091960 | -0.9483270 | -1.9781740 |
| C     | 1.5240870 | -0.8156990 | -3.0884600 |
| H     | -2.0227820 | 1.0418750 | 9.1182470 |
| N     | 0.0104130 | -0.0820100 | -5.0796790 |
| C     | 1.0518650 | 0.1323960 | -6.0163760 |
| C     | 3.1011040 | 0.5554000 | -7.8644420 |
| C     | 2.1009550 | 1.0087700 | -5.7104800 |
| C     | 1.0270090 | -0.5268920 | -7.2526060 |
| C     | 2.0487410 | -0.3103980 | -8.1696060 |
| C     | 3.1221730 | 1.2110400 | -6.6334690 |
| H     | 2.1012330 | 1.5312700 | -4.7589840 |
| H     | 0.2126630 | -1.2079110 | -7.4794580 |
| H     | 0.3285630 | -0.8283220 | -11.229350 |
| H     | 3.9309000 | 1.8938170 | -7.3926920 |
| C     | -1.3310710 | -0.1220330 | -5.5410570 |
| C     | -3.9631270 | -0.2140510 | -6.4634110 |
| C     | -1.7601460 | 0.7795790 | -6.5222810 |
| C     | -2.2207650 | -1.0723310 | -5.0240140 |
| C     | -3.5315090 | -1.1109780 | -5.4848610 |
| C     | -3.0726270 | 0.7277310 | -6.9797340 |
| H     | -1.0689880 | 1.5189180 | -6.9110300 |
| H     | -1.8773380 | -1.7725190 | -4.2693010 |
| H     | -4.2163010 | -1.6491710 | -5.0818240 |
| H     | -3.4029570 | 1.4345990 | -7.7338260 |
| N     | -0.0104130 | 0.0820100 | 5.0796790 |
| C     | 1.3310710 | 0.1220330 | 5.5410570 |
| C     | 3.9631270 | 0.2140510 | 6.4634110 |
| C     | 2.2207650 | 1.0723310 | 5.0240140 |
| C     | 1.7601460 | -0.7795790 | 6.5222810 |
| C     | 3.0726270 | -0.7277310 | 6.9797340 |
| C     | 3.5315090 | 1.1109780 | 5.4848610 |
| H     | 1.8773380 | 1.7725190 | 4.2693010 |
| H     | 1.0689880 | -1.5189180 | 6.9110300 |
| H     | 3.4029570 | -1.4345990 | 7.7338260 |
S95

|          | x          | y          | z          |
|----------|------------|------------|------------|
| H        | 4.21630100 | 1.84971300 | 5.08182400 |
| H        | 4.98727800 | 0.24804800 | 6.81962300 |
| C        | -1.05186500| -0.13239600| 6.01637600 |
| C        | -3.10110400| 0.52689200 | 7.25260600 |
| H        | -2.04874100| 0.31039800 | 8.16960600 |
|         | -3.12217300| -1.21104000| 6.63346900 |
| H        | -2.10123300| -1.53127000| 4.75898400 |
| C        | -0.21256300| 0.82832200 | 9.12293500 |
| C        | -3.93039000| -1.93817000| 6.39292000 |
| H        | -3.89509000| -0.71902700| 8.58272000 |

*a1-S, Geometry (Solvent: Toluene)*

|          | x          | y          | z          |
|----------|------------|------------|------------|
| H        | -2.57497900| 1.66536900 | 1.64836400 |
| C        | -1.70677400| 1.10509700 | 1.97941100 |
| C        | 0.57903800 | -0.31552700| 2.76129300 |
| C        | -0.85719200| 0.56416600 | 0.99096600 |
| H        | -2.05992400| 1.40331200 | 4.07380700 |
|         | -1.20542300| 0.76693400 | -0.42045400|
| O        | -2.21626300| 1.41101400 | -0.76369800|
| C        | 1.20542300 | 0.76693400 | 0.42045400 |
| C        | 2.21626300 | -1.41101400| 0.76369800 |
| C        | 0.85719200 | -0.56416600| -0.99096600|
| C        | 0.26450100 | -0.22948400| -3.71669300|
| C        | -0.30635000| 0.15957800 | -1.39549500|
| C        | 1.70677400 | -1.10509700| -1.97941100|
| C        | 1.42644300 | -0.95292400| -3.31617300|
| C        | -0.57903800| 0.31552700 | -1.39549500|
| H        | 2.57497900 | -1.66536900| -1.64836400|
| H        | -2.05992400| -1.40331200| -4.07380700|
| H        | -1.46343200| 0.87648500 | -3.04659300|
| N        | -0.01672300| -0.10587800| -5.09096600|
| C        | 1.03352400 | 0.15202300 | -5.99541800|
| C        | 3.13548100 | 0.64293900 | -7.77410100|
| C        | 2.10586200 | 0.97189600 | -5.61080900|
| C        | 1.01930900 | -0.41942900| -7.27840300|
| C        | 2.06410900 | -0.16878300| -8.15763400|
| C        | 3.15006000 | 1.20775200 | -6.49920200|
| H        | 2.10336600 | 1.42902100 | -4.62660060|
| H        | 0.19576100 | -1.06451600| -7.56728100|
| H        | 2.04990100 | -0.62057800| -9.14418200|
| H        | 3.97259100 | 1.84684500 | -6.19527100|
| H        | 3.95044300 | 0.83223000 | -8.46462500|
| C        | -1.35243900| -0.16876900| -5.55122200|
| C        | -3.99290200| -0.30015000| -6.45679200|
| C        | -1.79647700| 0.70669300 | -6.55195900|
| C        | -2.23779600| -1.10841200| -5.60309400|
| C        | -3.54954900| -1.16740200| -5.45605100|
| C        | -3.11057000| 0.63363100 | -7.00100200|
| H        | -1.11352700| 1.44496300 | -6.95978600|
| H        | -1.88831200| -1.78481000| -4.22983100|
| H        | -4.22765200| -1.89895400| -5.02915300|
| H        | -3.44970400| 1.32081200 | -7.76931700|
| H        | -5.01882400| -0.34942500| -6.80590000|
| N        | 0.01672300 | 0.10587800 | 5.09966600 |
| C        | 1.35243900 | 0.16876900 | 5.55122200 |
| C        | 3.99290200 | 0.30015000 | 6.45679200 |
| C        | 2.23779600 | 1.10841200 | 5.00309400 |
| C        | 1.79647700 | -0.16876900| 6.55195900 |
| C        | 3.11057000 | -0.63363100| 7.00100200 |
|   |      |      |      |      |
|---|------|------|------|------|
| C | 3.54954900 | 1.16740200 | 5.45605100 |
| H | 1.88831200 | 1.78481000 | 4.22983100 |
| H | 1.11352700 | -1.44496300 | 6.95978600 |
| H | 3.44970400 | -1.32081200 | 7.76343000 |
| H | 4.22765200 | 1.89895400 | 5.02915300 |
| H | 5.01882400 | 0.34942500 | 6.80590000 |
| C | -1.03352400 | -0.15202300 | 5.99541800 |
| C | -3.13548100 | -0.64293900 | 7.77410100 |
| C | -2.10586200 | -0.97189600 | 5.61080900 |
| C | -1.01930900 | 0.41942900 | 7.27840300 |
| C | -2.06410900 | 0.16878300 | 8.15763400 |
| H | -2.10336600 | -1.42902100 | 4.62660600 |
| H | -0.19576100 | 1.06451600 | 7.56728100 |
| H | -2.04990100 | 0.62057800 | 9.14418200 |
| H | -3.97259100 | -1.84684500 | 6.19527100 |
| H | -3.95044300 | -0.83223000 | 8.46425200 |

**a2-S$_0$ Geometry (Solvent: Toluene)**

|   |      |      |      |      |
|---|------|------|------|------|
| H | 1.65521900 | -2.65263600 | 1.57642000 |
| C | 1.97926600 | -1.74629000 | 1.07463100 |
| C | 2.77306800 | 0.60149700 | -0.19945000 |
| C | 1.00859300 | -0.88885000 | 0.54790100 |
| C | 3.32606900 | -1.44207000 | 0.97477400 |
| C | 1.42330700 | 0.29256000 | -0.08789300 |
| H | 4.06680500 | -2.11148800 | 1.39884000 |
| H | 3.05676400 | 1.51613600 | -0.70929100 |
| C | -0.42450600 | -1.24324300 | 0.67315200 |
| O | -0.78520500 | -2.27057400 | 1.22608900 |
| O | 0.42452500 | 1.24318300 | -0.67345500 |
| O | 0.78522600 | 2.27049900 | -0.70949300 |
| C | -1.00857400 | 0.88879900 | -0.54818700 |
| C | -3.74547000 | -0.26037100 | 0.33096900 |
| C | -1.42328900 | -0.29260700 | 0.08761400 |
| C | -1.97924900 | 1.74658500 | -1.07490300 |
| C | -3.32605300 | 1.44204100 | -0.97501900 |
| C | -2.77305100 | -0.60153100 | 0.19919700 |
| H | -1.65520400 | 2.65258600 | -1.57670100 |
| H | -4.06678800 | 2.11146500 | -1.39907500 |
| H | -3.05674100 | 1.51616700 | 0.70904400 |
| N | -5.10587700 | -0.04672500 | -0.22523200 |
| C | -6.07979600 | 0.98676200 | -0.15306600 |
| C | -8.03068100 | 3.01405900 | 0.00702200 |
| C | -5.89015900 | 2.08512000 | 0.69128900 |
| C | -7.25115900 | 0.90139800 | -0.91095900 |
| C | -8.21412500 | 1.90038500 | -0.82318200 |
| C | -6.85049400 | 3.08783800 | 0.75905700 |
| H | -4.98377200 | 2.15435300 | 1.28546300 |
| H | -7.40838900 | 0.04193700 | -1.55578300 |
| H | -9.12965500 | 1.80642000 | -1.39989000 |
| H | -6.67578500 | 3.94656100 | 1.40070600 |
| C | -5.54570100 | -1.39791500 | -0.16445000 |
| C | -6.44944200 | -0.06457900 | -0.05771100 |
| C | -6.51231100 | -1.77923900 | 0.77033700 |
| C | -5.03653100 | -2.35232000 | -1.05006400 |
| C | -5.47790200 | -3.66900100 | -0.98686400 |
| C | -6.96051000 | -3.09448700 | 0.81421900 |
| H | -6.91928700 | -1.03781000 | 1.45131800 |
| H | -4.28575100 | 2.06181100 | -1.77882200 |
| H | -5.05145400 | 4.40375900 | -1.66344400 |
| N | 5.10589100 | 0.04672400 | 0.22511800 |
| C | 5.54570500 | 1.39792300 | 0.16442900 |
| C | 6.44943200 | 4.06461000 | 0.05804800 |
### a2-T¹ Geometry (Solvent: Toluene)

|    |       |       |       |
|----|-------|-------|-------|
| C  | 5.03641700 | 2.35245500 | 1.05006900 |
| C  | 6.51242300 | 1.77934900 | -0.77020600 |
| C  | 6.96061400 | 3.09460500 | -0.81391000 |
| C  | 5.47778200 | 3.66893500 | 0.98704400  |
| H  | 4.28555200 | 2.06166300 | 1.77871100  |
| H  | 6.91948900 | 1.03799000 | -1.45120900 |
| H  | 7.72924300 | 3.36924400 | -1.53042000 |
| H  | 5.05124100 | 4.40362300 | 1.66364000  |
| C  | 6.07981500 | -0.98675500 | 0.15278900 |
| C  | 8.03068800 | -3.01406500 | -0.00726100 |
| C  | 5.89019400 | -2.08508000 | -0.69155400 |
| C  | 7.25115600 | -0.90143200 | 0.91078000  |
| H  | 4.98382400 | -2.15428200 | -1.28575600 |
| H  | 7.40837600 | -0.04200000 | 1.39973100 |
| C  | 9.12963000 | -1.80649000 | 1.39973100 |
| H  | 6.67582300 | -3.94650000 | -1.40101900 |
| C  | 6.92386400 | 5.46972200 | -0.00038200 |
| C  | 7.82309000 | 8.13051100 | -0.11343100 |
| C  | 7.12391800 | 6.20848300 | 1.17343800  |
| C  | 7.56875000 | 7.52720500 | 1.11781700 |
| H  | 7.00701200 | 5.53696600 | -2.15235800 |
| H  | 6.91948900 | 7.40837600 | 2.13748900 |
| H  | 7.72480600 | 8.08133600 | 2.03823700 |
| H  | 7.81402600 | 7.68707000 | -2.25192100 |
| C  | 8.16998900 | 9.15799700 | -0.15711500 |
| C  | -9.05722600 | 4.08292100 | 0.08937900 |
| C  | -11.00074100 | 6.10778200 | 0.24426500 |
| C  | -9.36144000 | 4.91280000 | 1.31453300 |
| C  | -9.74335300 | 4.50618400 | -1.05684000 |
| C  | -10.70698800 | 5.50895200 | -0.98037000 |
| C  | -10.32376500 | 5.69523500 | 1.39152400 |
| H  | -8.85629500 | 4.35893300 | 2.21710200 |
| H  | -9.50291400 | 4.06221500 | -2.01881000 |
| H  | -11.22254700 | 5.82897500 | -1.88055300 |
| H  | -10.55126300 | 6.14951100 | 2.35090700 |
| H  | -11.75105900 | 6.88970200 | 0.30409800 |
| C  | -6.92388200 | 5.46968000 | 0.00091200 |
| C  | -7.82313000 | 8.13044400 | 0.11433100 |
| C  | -7.18122600 | 6.08668300 | 1.23243400 |
| C  | -7.12410300 | 6.20854800 | -1.17281100 |
| C  | -7.56894700 | 7.52725800 | -1.11700700 |
| C  | -7.62769600 | 7.40474300 | 1.28899800 |
| C  | -7.00673800 | 5.53672100 | 2.15290500 |
| C  | -6.95133800 | 5.73851200 | -2.13693000 |
| C  | -7.72513600 | 8.08147300 | -2.03735400 |
| C  | -7.81377200 | 7.86844300 | 2.25279600 |
| C  | -8.17003800 | 9.15792200 | 0.15815800 |
| C  | 9.05722700 | -0.08293200 | -0.08963100 |
| C  | 11.00073000 | -6.10780300 | -0.24454000 |
| C  | 9.36146400 | -4.69125100 | -1.31479800 |
| C  | 9.74332500 | -4.50623800 | 1.05659000 |
| C  | 10.70695400 | -5.50901100 | 0.98010900 |
| C  | 10.32378300 | -5.69521200 | -1.39180000 |
| H  | 8.85634300 | -4.35887100 | -2.21736700 |
| H  | 9.50286600 | -4.06230000 | 2.01856900 |
| H  | 11.22249000 | -5.82906700 | 1.88029200 |
| H  | 10.55129900 | -6.14945800 | -2.35119300 |
| H  | 11.75104300 | -6.88972600 | -0.30438200 |
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| C       | 7.68132800 | 1.37562700 | 7.30686600 |
| C       | 7.57296500 | -0.10180270 | 7.57090400 |
| H       | 5.00134000 | -1.93953700 | 7.05923900 |
| H       | 5.87825500 | 2.33298100 | 6.63861600 |
| H       | 8.23328300 | 2.30785500 | 7.37499600 |
| H       | 8.04573300 | -1.96068000 | 7.82817100 |
| H       | 9.32873600 | 0.16187100 | 7.98379900 |
| C       | 3.98968200 | 0.18739700 | -8.95570000 |
| C       | 6.04460300 | 0.40262600 | -10.859408 |
| C       | 4.65756200 | 1.40380600 | -9.15314700 |
| C       | 4.36831200 | -0.91924800 | -9.72813900 |
| C       | 5.38714000 | -0.81276000 | -10.67132500 |
| C       | 5.67575700 | 1.51053600 | -10.09701300 |
| H       | 4.36066500 | 2.27804100 | -8.58080800 |
| H       | 3.87911900 | -1.87624100 | -9.57030200 |
| H       | 5.67383300 | -1.68287500 | -11.25355200 |
| H       | 6.17625500 | 2.46271300 | -10.2437400 |
| H       | 6.83878500 | 0.48566700 | -11.59442200 |
| C       | -5.61975600 | -0.19860100 | -6.79604700 |
| C       | -8.29502700 | -1.72230000 | -7.65335200 |
| C       | -6.24684100 | 1.00497300 | -7.14653600 |
| C       | -6.35509000 | -1.38856600 | -8.81517000 |
| C       | -7.68132800 | -1.37562700 | -7.30686600 |
| C       | -7.57296500 | 1.01802700 | -7.57090400 |
| H       | -5.70013400 | 1.93953700 | -7.05923900 |
| H       | -5.87825500 | -2.33298100 | -6.63861600 |
| H       | -8.23328300 | -2.30785500 | -7.37499600 |
| H       | -8.04573300 | 1.96068000 | -7.82817100 |
| H       | -9.32873600 | -0.16187100 | -7.98379900 |
| C       | -3.98968200 | -0.18739700 | 8.95570000 |
| C       | -6.04460300 | -0.40262600 | 10.859408 |
| C       | -4.65756200 | -1.40380600 | 9.15314700 |
| C       | -4.36831200 | 0.91924800 | 9.72813900 |
| C       | -5.38714000 | 0.81276000 | 10.67132500 |
| C       | -5.67575700 | -1.51053600 | 10.09701300 |
| H       | -4.36066500 | -2.27804100 | 8.58080800 |
| H       | -3.87911900 | 1.87624100 | 9.57030200 |
| H       | -5.67383300 | 1.68278500 | 11.25355200 |
| H       | -6.17625500 | -2.46271300 | 10.2437400 |
| H       | -6.83878500 | -0.48566700 | 11.59442200 |

**a3-S Geometry (Solvent: Toluene)**

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| H       | 1.48268400 | 2.18302200 | -2.30111200 |
| C       | 1.86668200 | 1.48234800 | -1.56736200 |
| C       | 2.80807500 | -0.34923100 | 0.32054400 |
| C       | 0.95913000 | 0.75295800 | -0.79515300 |
| C       | 3.23173300 | 1.29167400 | -1.41109800 |
| C       | 3.70905200 | 0.37797900 | -0.45936800 |
| C       | 1.43848800 | -1.07043000 | 0.14565700 |
| H       | 3.93895700 | 1.83038100 | -2.03330500 |
| H       | 3.15992200 | -1.04220100 | 1.07801100 |
| C       | -0.49989300 | 0.97398500 | -0.98802500 |
| C       | 0.49984400 | -0.97404900 | 0.98846300 |
| O       | -0.91867200 | 1.28403600 | -1.79651300 |
| C       | 0.91863300 | -1.78405500 | 1.79699700 |
| C       | -0.95918000 | -0.75300900 | 0.79560500 |
| O       | -3.70909600 | -0.37806600 | 0.45983500 |
| C       | -1.43853700 | 0.17036800 | -0.14521600 |
| C       | -1.86673300 | -1.48219100 | 1.56782100 |
| C       | -3.23178000 | -1.29166900 | 1.41159600 |
| C       | -2.80811900 | 0.34917200 | -0.32010600 |
| H       | -1.48274700 | -2.18305800 | 2.30158000 |
| H       | -3.93898400 | -1.83036300 | 2.03381100 |
| H       | -3.15996100 | 1.04219400 | -1.07752500 |
| N       | 5.09309900 | 0.19221800 | -0.29610900 |
| N       | -5.09314500 | -0.19224100 | 0.29659700 |
|   |   |   |   |
|---|---|---|---|
| H | -11.03886400 | -2.39890400 | 0.47907200 |
| C | -9.33984300 | -4.60788800 | -1.57677600 |
| H | -10.19363300 | -5.28264500 | -1.70344600 |
| H | -9.43325200 | -5.21877100 | -1.53374400 |
| H | -9.93102900 | -3.96504700 | -2.46047500 |
| C | -9.60325500 | -4.69676000 | 0.91874300 |
| H | -10.45850800 | -5.37378600 | 0.81634600 |
| H | -9.72962600 | -4.11823200 | 1.83965100 |
| H | -9.27382700 | -3.96504700 | -2.46047500 |
| H | -8.43325200 | -5.21877100 | -1.53374400 |
| H | -9.27382700 | -3.96504700 | -2.46047500 |
| C | -9.60325500 | -4.69676000 | 0.91874300 |
| H | -10.45850800 | -5.37378600 | 0.81634600 |
| H | -9.72962600 | -4.11823200 | 1.83965100 |
| H | -9.27382700 | -3.96504700 | -2.46047500 |
| H | -8.43325200 | -5.21877100 | -1.53374400 |
| C | -8.04763100 | 5.30806500 | -1.12840600 |
| H | -8.13175000 | 4.75392600 | -2.06884600 |
| H | -8.04763100 | 5.30806500 | -1.12840600 |
| H | -8.13175000 | 4.75392600 | -2.06884600 |

**a3-T<sub>1</sub> Geometry (Solvent: Toluene)**

|   |   |   |   |
|---|---|---|---|
| H | 1.47310100 | 2.22212800 | -2.24998700 |
| C | 1.86243800 | 1.51584600 | -1.52431100 |
| C | 2.78618700 | -0.37181400 | 0.32926600 |
| C | 0.92574200 | 0.76411500 | -0.77159000 |
| C | 3.21173600 | 1.33606800 | -1.36163400 |
| C | 3.68037200 | 0.37798800 | -0.41625000 |
| C | 1.40318500 | -0.19475600 | 0.16668400 |
| H | 3.92678300 | 1.87662600 | -1.97310600 |
| H | 3.12858200 | -1.07983300 | 1.07719200 |
| C | -0.92574300 | -0.76415500 | 0.77154900 |
| C | 0.92574300 | -0.76415500 | 0.77154900 |
| C | 3.92678300 | 1.87662600 | -1.97310600 |
| H | 3.12858200 | -1.07983300 | 1.07719200 |
| O | -0.91720900 | 1.84430900 | -1.80519900 |
| O | 0.91720900 | -1.84431000 | 1.80516600 |
| C | -0.92574300 | -0.76415500 | 0.77154900 |
| C | 0.92574300 | -0.76415500 | 0.77154900 |
| C | 3.92678300 | 1.87662600 | -1.97310600 |
| H | 3.12858200 | -1.07983300 | 1.07719200 |
| N | 5.06456200 | 0.18764100 | -0.26562200 |
| N | -5.06456200 | -0.18765000 | 0.26561200 |
| C | 5.72164800 | -1.04295100 | -0.21281800 |
| C | 7.49958300 | -3.20484600 | -0.12845400 |
| C | 5.20630500 | -2.33679700 | -0.33066000 |
| C | 7.10698900 | -0.81973700 | -0.08389800 |
| C | 7.98926500 | -1.89605050 | -0.04050000 |
| C | 6.10822700 | -3.90353600 | -0.27936900 |
| C | 4.14635800 | -5.20933400 | -0.46219200 |
| H | 9.05255000 | -1.70566300 | 0.05628900 |
| H | 5.71393400 | -4.39827300 | -0.36298200 |
| C | 6.01703400 | 1.20151700 | -0.16059800 |
| C | 8.27786400 | 2.82535100 | 0.13841600 |
| C | 7.29688300 | 0.62351700 | -0.04904300 |
| C | 5.83997600 | 2.58585400 | -0.08337000 |
| C | 6.97759600 | 3.69018000 | 0.05537600 |
| C | 8.42034100 | 1.43328000 | 0.09505400 |
| H | 8.85502500 | 3.03806600 | -0.11231900 |
| H | 6.84847800 | 4.44541600 | 0.11207600 |
| H | 9.39794400 | 0.97199400 | 0.18169600 |

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| C    | -6.01704100 | -1.20151900 | 0.16057800 |
| C    | -8.27788300 | -2.82533400 | -0.13844700 |
| C    | -8.42035100 | -1.43326300 | -0.09506400 |
| C    | -6.97761800 | -3.36901000 | -0.05542200 |
| H    | -4.85504500 | -3.03807500 | 0.11226200 |
| H    | -9.37959000 | -0.97196900 | -0.18169300 |
| C    | -5.72164100 | 1.04294600 | 0.21219300 |
| C    | -7.10698400 | 3.23378800 | 0.33039100 |
| C    | -6.10820500 | 3.39035300 | 0.27942200 |
| H    | -4.14634200 | 2.52091500 | 0.46225000 |
| C    | -5.71390700 | 4.39826600 | 0.36305000 |
| H    | -6.84850800 | -4.44540900 | -0.11214000 |
| C    | -7.49956300 | 3.20449200 | 0.12850900 |
| C    | -7.10698400 | 0.81974300 | 0.08391400 |
| C    | -5.20629000 | 2.33678800 | 0.33039100 |
| C    | -6.10820500 | 3.39035300 | 0.27942200 |
| H    | -4.14634200 | 2.52091500 | 0.46225000 |
| H    | -5.71390700 | 4.39826600 | 0.36305000 |
| H    | -9.37959000 | -0.97196900 | -0.18169300 |
| C    | -8.42035100 | -1.43326300 | -0.09506400 |
| C    | -6.97761800 | -3.36901000 | -0.05542200 |
| H    | -4.85504500 | -3.03807500 | 0.11226200 |
| H    | -9.37959000 | -0.97196900 | -0.18169300 |
| C    | -5.72164100 | 1.04294600 | 0.21219300 |
| C    | -7.10698400 | 3.23378800 | 0.33039100 |
| C    | -6.10820500 | 3.39035300 | 0.27942200 |
| H    | -4.14634200 | 2.52091500 | 0.46225000 |
| C    | -5.71390700 | 4.39826600 | 0.36305000 |
| H    | -6.84850800 | -4.44540900 | -0.11214000 |
| C    | -7.49956300 | 3.20449200 | 0.12850900 |
| C    | -7.10698400 | 0.81974300 | 0.08391400 |
| C    | -5.20629000 | 2.33678800 | 0.33039100 |
| C    | -6.10820500 | 3.39035300 | 0.27942200 |
| H    | -4.14634200 | 2.52091500 | 0.46225000 |
| H    | -5.71390700 | 4.39826600 | 0.36305000 |
| H    | -9.37959000 | -0.97196900 | -0.18169300 |
| C    | -8.42035100 | -1.43326300 | -0.09506400 |
| C    | -6.97761800 | -3.36901000 | -0.05542200 |
| H    | -4.85504500 | -3.03807500 | 0.11226200 |
| H    | -9.37959000 | -0.97196900 | -0.18169300 |
| C    | -5.72164100 | 1.04294600 | 0.21219300 |
| C    | -7.10698400 | 3.23378800 | 0.33039100 |
| C    | -6.10820500 | 3.39035300 | 0.27942200 |
S103

H  -8.53381100  4.63098500  2.24596000
H  -8.91582600  6.11610300  1.35031300
H  -7.23475900  5.59075200  1.51797400

a3-S, Geometry (Solvent: Toluene)

H  1.47221700  -2.01863600  -2.42743600
C  1.86228000  -1.37720100  1.64383200
C  2.79110300   0.32811400  -0.37465000
C  0.93298100   0.69118000   0.83484100
C  3.21713400  -1.21484200  1.46372600
C  3.67948300  -0.35035500  0.43699500
C  1.40757800   0.17079100  -0.19109000
H  3.93475600  -1.70484400  -2.11414100
H  3.13867200   0.97332600  -1.17565100
C  -0.49770700  -0.90066600  1.07602900
C  0.49771600   0.90011200  -1.07648200
O  -0.91359900  -1.66185400  -1.97208800
C  -0.93297200   0.69071500   0.83521800
C  -3.67947400   0.35004500  -0.43724600
C  -1.40757100  -0.17125700  0.19071300
C  -1.86226900  1.37679400  -1.64416200
C  -3.21712400  1.21449600  -1.46400700
C  -2.79109700  -0.32849300  0.37434400
H  -1.47220600   2.01821500   2.42777700
H  -3.93475000  -1.70455100  -2.11482000
H  -3.13866800  -0.97369100  -1.07656000
N  5.07198200  -0.16959800   0.27320500
C  5.73816900   1.05018900  -0.22474600
C  5.22933400  -2.34783300  0.33068800
C  7.12220000   0.81491600  -0.08602200
C  8.09974900  -1.88621000  -0.03560800
C  6.13820600   3.39523600  -0.27844000
H  4.16842500   2.35487600   0.45534000
H  9.07129700   1.69065500  -0.06932400
H  5.75148300   4.40652500   0.35621900
C  6.00542500  -1.19068700  0.15645100
C  8.23729200  -2.85071800  -0.13767800
C  7.29504200  -0.63014700  0.04275200
C  5.80466400  -2.57335900  -0.09427800
C  6.92946000  -3.37470500  -0.04410900
C  8.04350800  -1.45951000  -0.10011200
H  4.81092800  -3.00556900   0.13724500
H  6.78501500  -4.44959800  -0.09123100
H  9.38940500  -1.01645300  -0.18759800
C  -6.00529800  1.19062600  -0.15651600
C  -8.23694400   2.85091500  0.13781400
C  -5.80437000  2.57327500  -0.09436800
C  -7.29496700  0.63023300  -0.04269300
C  -8.40332400  1.45972400  -0.10027200
C  -6.92906000  3.37475100  0.04412100
C  -4.81058800  3.00536800  -0.13743200
H  -9.38926400  1.01678200  0.18785600
H  -6.78448700  4.44962800   0.09122200
C  -5.73829800  -1.05027800  -0.22482200
C  -7.52836700  -3.19878900  -0.12526500
C  -7.12229000  -0.81485000  -0.08596700
C  -5.22961400  -2.34802800  -0.33317400
C  -6.13859600  -3.39528100  -0.27826000
H  -8.00995100  -1.88604600  -0.03545700
H  -4.16873500  -2.53512700  -0.45554100
H  -5.75199200  -4.40661300  -0.35626000
H  -9.07146800  -1.09037400  0.06957400
C  8.45036300  4.41840300  0.06653000
| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| C     | 8.30598900 | 5.23170400 | 1.36603300 |
| H     | 8.96648500  | 6.10487000  | -1.13330200 |
| H     | 8.57771400  | 4.62488100  | 2.23566200 |
| H     | 7.28261100  | 5.59039600  | 1.50833500 |
| C     | 9.92277000  | 4.02365400  | -0.09269100 |
| H     | 10.53723400 | 4.92818900  | -0.13066700 |
| H     | 10.09422100 | 3.46557700  | 0.92643700 |
| H     | 10.27304900 | 3.41845400  | 0.75005400 |
| C     | 8.05313200  | 5.29819600  | -1.13330200 |
| H     | 8.70976100  | 6.17320900  | -1.18724200 |
| H     | 7.02277400  | 5.65544100  | -0.49829000 |
| H     | 8.14400500  | 4.73994900  | -2.07049000 |
| C     | 9.41627500  | -3.81437100 | -0.28960000 |
| H     | 10.27304900 | -3.41845400 | -0.74969400 |
| H     | 10.09422100 | -3.46557700 | 1.01943800 |
| H     | 10.53723400 | -4.92818900 | 0.13106300 |
| C     | 8.05313200  | -5.29819600 | 1.13330200 |
| H     | 8.70976100  | -6.17320900 | 1.18724200 |
| H     | 7.02277400  | -5.65544100 | -0.49829000 |
| H     | 8.14400500  | -4.73994900 | -2.07049000 |
| C     | 9.41627500  | -4.02365400 | 0.09302600 |
| H     | 10.27304900 | -3.41845400 | -0.74969400 |
| H     | 10.09422100 | -3.46557700 | 1.01943800 |
| H     | 10.53723400 | -4.92818900 | 0.13106300 |
| C     | 8.05313200  | -5.29819600 | 1.13330200 |
| H     | 8.70976100  | -6.17320900 | 1.18724200 |
| H     | 7.02277400  | -5.65544100 | -0.49829000 |
| H     | 8.14400500  | -4.73994900 | -2.07049000 |

**a4-S0 Geometry (Solvent: Toluene)**

| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| C     | 3.14912100  | 1.53005900 | 0.00000000 |
| C     | 2.12979100  | 1.90132400 | 0.00000000 |
| C     | -0.51749500 | 2.80457400 | 0.00000000 |
| O     | 1.07850700  | 0.98191500 | 0.00000000 |
| C     | 1.85902700  | 3.26430300 | 0.00000000 |
| C     | 0.53499700  | 3.71360700 | 0.00000000 |
| C     | -0.24876300 | 1.43547800 | 0.00000000 |
| H     | 2.66233700  | 3.99496000 | 0.00000000 |
| H     | -1.54583000 | 3.15303900 | 0.00000000 |
| O     | 1.39528400  | -0.47746500 | 0.00000000 |
O    -2.54654100   0.87313200   0.00000000
C    -1.07850700  -0.98191500   0.00000000
C    -0.53499700  -3.71360700   0.00000000
C     0.24876300  -1.43547800   0.00000000
C    -2.12979100  -1.90132400   0.00000000
C    -1.85902700  -3.26430300   0.00000000
C     0.51749500  -2.80457400   0.00000000
H    -3.14912100  -1.53005900   0.00000000
H    -2.66233700  -3.99496000   0.00000000
H     1.54583000  -3.15303900   0.00000000
N    -0.26414200  -5.11442100   0.00000000
N     0.26414200   5.11442100   0.00000000
C     0.15503400   5.78615700   1.22686500
C    -0.06009200   7.08476000   -3.70673300
C     0.28495400   5.06971900   2.43053500
C    -0.08554800   7.17072800   1.26191000
C    -0.18794500   7.78662100   2.51302600
C     0.17856500   5.71386800   3.65577900
H     0.46633200   4.00213700   2.40855100
H    -0.37602900   8.85568500   2.55486500
H     0.28222200   5.13688400   4.56927200
H    -0.14654200   7.60052000   4.65719900
C     0.15503400   5.78615700  -1.22686500
C    -0.06009200   7.08476000  -3.70673300
C     0.08554800   7.17072800  -1.26191000
C     0.17856500   5.71386800  -3.65577900
H     0.46633200   4.00213700  -2.40855100
H    -0.37602900   8.85568500  -2.55486500
H     0.28222200   5.13688400  -4.56927200
H    -0.14654200   7.60052000  -4.65719900
C     0.18794500   7.78662100  -2.51302600
H     0.46633200   4.00213700  -2.40855100
H    -0.37602900   8.85568500  -2.55486500
H     0.28222200   5.13688400  -4.56927200
H    -0.14654200   7.60052000  -4.65719900
C     0.24466300  -8.01651000   0.00000000
C     1.64910100  -8.01651000   0.00000000
H     1.78887900  -9.28697700   0.88423500
H     2.42305400  -7.85676000   0.00000000
H     1.78887900  -9.28697700  -0.88423500
C    -0.82587200  -9.12917700   0.00000000
a4-T, Geometry (Solvent: Toluene)

H    -0.72548600   -9.76612500   0.88328700
H    -0.72548600   -9.76612500  -0.88328700
H    -1.82968200   -8.69474600   0.00000000

H    3.15178900    1.49686800   0.00000000
C    2.13567000    1.87818000   0.00000000
C   -0.51054400    2.78977100   0.00000000
C    1.08088400    0.93830300   0.00000000
C    1.88159300    3.23174700   0.00000000
C    0.54041300    3.67521400   0.00000000
C    -0.26220000   -1.40076000   0.00000000
H    2.68604100    3.96140900   0.00000000
H   -0.53951900   -3.13748100   0.00000000
C    1.40273600   -0.48652400   0.00000000
O    2.58439400    0.90112900   0.00000000
C   -3.15178900   -1.49686800   0.00000000
O   -2.68604100   -3.96140900   0.00000000
C    1.53951900   -3.13748100   0.00000000
N    -0.27634400   -5.09225100   0.00000000
N     0.27634400    5.09225100   0.00000000
C     0.16719400    5.75547900    1.21875700
C    -0.04823600    7.03721700    3.69585200
C     0.31052800    5.02608300    2.42030000
C    -0.08525400    7.14413400    1.25830200
C    -0.18866700    7.75189700    2.51036300
C     0.20405000    5.66440000    3.64248700
H     0.50112100    3.96103600    2.38161300
C    -0.38749300    8.81786300    2.56392900
H     0.31537400    5.08921500    4.55536800
H    -0.13619200    7.54528500    4.65008800
C     0.16719400    5.75547900   -1.21875700
C    -0.04823600    7.03721700   -3.69585200
C    -0.08525400    7.14413400   -1.25830200
C     0.31052800    5.02608300   -2.42030000
C     0.20405000    5.66440000   -3.64248700
C    -0.18866700    7.75189700   -2.51036300
C     0.50112100    3.96103600   -2.38161300
C     0.31537400    5.08921500   -4.55536800
C    -0.38749300    8.81786300   -2.56392900
H    -0.13619200    7.54528500   -4.65008800
C    -0.25714000    7.98220300   0.00000000
C     0.79533700    9.11501700   0.00000000
H     0.68024400    9.74849700    0.88321400
H     0.68024400    9.74849700   -0.88321400
H     1.80687600    8.69987500   0.00000000
C    -1.67583600    8.59873500   0.00000000
H    -1.82281800    9.22402400    0.88469200
H    -2.43616400    7.81303400   0.00000000
H    -1.82281800    9.22402400   -0.88469200
C    -0.16719400   -5.75547900   -1.21875700
C     0.04823600   -7.03721700   -3.69585200
C     0.08525400   -7.14413400   -1.25830200
C    -0.31052800   -5.02608300   -2.42030000
C    -0.20405000   -5.66440000   -3.64248700
C     0.18866700   -7.75189700   -2.51036300
H    -0.50112100   -3.96103600   -2.38161300
H  -0.31537400  -5.08921500  -4.55368000
H  0.38749300  -8.81786300  -2.56392900
H  0.13619200  -7.54528500  -4.65008800
C  -0.16719400  -5.75547900  1.21875700
C  0.04823600  -7.03721700  3.69585200
C  -0.31052800  -5.02608300  2.42030000
C  0.08525400  -7.14413400  1.25830200
C  0.18866700  -7.75189700  2.51036300
H  -0.50112100  -3.96103600  2.38161300
H  0.38749300  -8.81786300  2.56392900
H  -0.31537400  -5.08921500  4.55536800
H  0.13619200  -7.54528500  4.65008800
C  0.25714000  -7.98220300  0.00000000
C  1.67583600  -8.59783500  0.00000000
H  1.82281800  -9.22402400  0.88469200
H  2.43616400  -7.81303400  0.00000000
H  1.82281800  -9.22402400  -0.88469200
C  -0.79533700  -9.11501700  0.00000000
H  -0.68024400  -9.74849700  0.88321400
H  -0.68024400  -9.74849700  -0.88321400
H  -1.80687600  -8.69987500  0.00000000
a4-S1 Geometry (Solvent: Toluene)

H  3.15553200  1.48716100  0.00000000
C  2.14034000  1.87123700  0.00000000
C  -0.50279700  2.78772200  0.00000000
C  1.08515900  0.93694300  0.00000000
C  1.89133800  0.93694300  0.00000000
C  0.55090000  3.67426500  0.00000000
C  -0.25769500  1.40348300  0.00000000
H  -1.50746000  3.13835400  0.00000000
C  1.40603700  -0.49136300  0.00000000
O  2.58150500  -0.90891700  0.00000000
C  -1.40603700  0.49136300  0.00000000
O  -2.58150500  0.90891700  0.00000000
C  -1.08515900  -0.93694300  0.00000000
C  -0.55090000  -3.67426500  0.00000000
C  0.25769500  -1.40348300  0.00000000
C  -2.14034000  -1.87123700  0.00000000
C  -1.89133800  -3.22798700  0.00000000
C  0.50279700  -2.78772200  0.00000000
H  -3.15553200  -1.48716100  0.00000000
H  -2.69793100  -3.95458900  0.00000000
H  1.50746000  -3.13835400  0.00000000
N  -0.28553200  -5.08711000  0.00000000
N  0.28553200  5.08711000  0.00000000
C  0.17376800  5.75036700  1.21862400
C  -0.04819300  7.03066500  3.69633500
C  0.32235000  5.02233400  2.42015100
C  -0.08672300  7.13767400  1.25851000
C  -0.19325400  7.74444700  2.51007700
C  0.21256900  5.66025400  3.64291500
H  0.52022300  3.95891800  2.38211300
H  -0.39855300  8.80920200  2.56371200
H  0.32817400  5.08564600  4.55557300
H  -0.13908900  7.53859900  4.65032000
C  0.17376800  5.75036700  -1.21862400
C  -0.04819300  7.03066500  -3.69633500
C  -0.08672300  7.13767400  -1.25851000
C  0.32235000  5.02233400  -2.42015100
C  0.21256900  5.66025400  -3.64291500
C  -0.19325400  7.74444700  -2.51007700
H  0.52022300  3.95891800  -2.38211300
H  0.32817400  5.08564600  -4.55557300
b1-S\textsubscript{6} Geometry (Solvent: Toluene)

| Atom | Coordinates |
|------|-------------|
| C    | 3.69989400  | 0.69634500 -0.28437400 |
| H    | 3.20939900  | -1.27518000 0.46941900 |
| C    | 2.82790800  | -0.33080600 0.09366100 |
| C    | 1.77292400  | 2.08853700 -0.79788900 |
| C    | 1.44760500  | -0.15896800 0.02561000 |
| C    | 3.14769000  | 1.90821100 -0.73433700 |
| C    | 1.90044700  | 1.05826400 -0.41919700 |
| C    | 0.56014900  | -1.28669700 0.44349900 |
| C    | 3.80675200  | 2.70789700 -1.05850300 |
| C    | 1.34701600  | 3.02209700 -1.15048900 |
| C    | -0.91105900 | -1.06933500 0.36923000 |
| C    | -1.77386800 | -2.09779100 0.75295400 |
| C    | -1.44870400 | 1.14637800 -0.07961400 |
| H    | -3.21005600 | 1.28701700 -0.45718200 |
| C    | -0.56124800 | 1.27429800 -0.49702800 |
| C    | -3.14858700 | -1.91761200 0.68936700 |
| C    | -1.34791500 | -3.03764000 1.08836600 |
| H    | -3.80762700 | -2.73599400 0.96269600 |
| C    | -3.70111900 | -0.70206000 0.24815400 |
| C    | -2.82896400 | 0.32351500 -0.13322000 |
| O    | 1.02357070  | -2.34508000 0.83026300 |
| O    | -1.02680400 | 2.33183100 -0.88728700 |
| C    | -5.16787500 | -0.51250300 0.18882100 |
| Atom | Coordinates                  |
|------|-----------------------------|
| C    | -7.96915200, -0.15164900, 0.07517900 |
| C    | -5.75728100, 0.25900900, -0.82209000 |
| C    | -6.01203100, -1.09776200, 1.14253800 |
| C    | -7.38771700, -0.91641300, 1.09655700 |
| C    | -7.13327100, 0.43203000, -0.88760700 |
| H    | -5.13486500, 0.70106900, -1.59474100 |
| H    | -5.58575800, -1.67204500, 1.96011100 |
| H    | -8.02052600, -1.36024900, 1.85844300 |
| H    | -9.56957200, 0.25900900, -0.82209000 |
| C    | 5.16735600, 0.51097900, -0.21065600 |
| C    | 7.96856400, 0.15745300, -0.06727300 |
| C    | 5.75509800, -0.72921900, -0.49405700 |
| C    | 6.01263500, 1.56990800, 0.14675300 |
| C    | 7.38963700, 1.40338200, 0.21313400 |
| C    | 7.12995800, -0.90577000, -0.42010200 |
| H    | -9.36590800, 0.02655900, 0.01823700 |
| H    | 9.36527900, -0.01834900, 0.00549300 |
| C    | -9.91194900, 1.26040300, -0.42022600 |
| C    | -10.99862200, 3.69594700, -1.28085700 |
| C    | -11.01435000, 1.27606000, -1.28259600 |
| C    | -11.55620100, 2.48839800, -1.70088000 |
| C    | -8.50766000, 2.45966600, 0.68501900 |
| H    | -9.45618900, 4.61853000, -0.08637100 |
| H    | -11.41900400, 4.63892200, -1.64306000 |
| C    | -10.23711300, -1.02994600, 0.38817100 |
| C    | -11.96828400, -3.11255600, 1.11028100 |
| C    | -11.38194100, -0.76495300, 1.14878600 |
| C    | -9.96602500, -2.34422200, -0.01071400 |
| C    | -8.80231600, -2.54883100, -0.60753700 |
| H    | -10.60151300, -4.39154800, 0.04236500 |
| H    | -13.12841900, -1.58185700, 2.08741000 |
| H    | -12.63849700, -3.91970400, 1.38652000 |
| C    | 10.02726000, -0.88232300, -0.90440400 |
| C    | 11.34674600, -2.58278800, -2.69950300 |
| C    | 9.68256900, -0.88145600, -2.26124300 |
| C    | 11.38694000, -1.73802600, -0.45282300 |
| C    | 11.69732600, -2.57496400, -1.34949000 |
| C    | 10.33406500, -1.73450900, -3.14773900 |
| H    | 8.90263100, -0.21283800, -2.61295100 |
| H    | 11.30535700, -1.73847100, 0.59970000 |
| C    | 12.48060500, -3.23303400, -0.98629600 |
| H    | 10.05603200, -1.72504000, -4.19707700 |
| H    | 11.85708600, -3.24145500, -3.39435100 |
| C    | 10.12158800, 0.66463000, 0.99265200 |
| C    | 11.62438900, 2.00593500, 2.94120700 |
| C    | 9.64878200, 0.76074500, 2.30678400 |
| C    | 11.35290000, 1.24174200, 0.66120300 |
| C    | 12.10016300, 1.89984300, 1.63429600 |
| C    | 10.39410900, 1.43603700, 3.26931800 |
| H    | 8.69707400, 0.30656700, 2.56566600 |
| H    | 11.71898900, 1.16634900, -0.35825300 |
| H    | 13.05412100, 2.34209300, 1.36433600 |
| H    | 10.01547600, 1.50423000, 4.28449900 |
| H    | 12.20597700, 2.52540800, 3.69556800 |

b1-T1 Geometry (Solvent: Toluene)
C 3.68406300  0.72269000  0.12280600
H 3.15758000 -1.33164100 -0.37859500
C 2.79991700 -0.33844100 -0.12844200
C 1.75820200  2.19413000  0.43416600
C 1.41761700 -0.17432300 -0.11591000
C 3.11221800  2.01808700  0.40344300
C 0.86659700  1.11636400  0.17754000
C 0.56719700 -1.32989800 -0.40268700
H 3.75429600  2.85958100  0.63576700
H 1.32318400  3.16071900  0.66477300
C -0.88146000 -1.09202200 -0.35078700
C -1.76123500 -2.16278000 -0.60075300
C -1.42104100  0.18156200 -0.05622600
H -3.19767100  1.32924400  0.24446800
C -0.56391000  1.34492500  0.21952700
C -3.12784900 -1.98175300 -0.55906000
H -1.33043500 -3.13058000 -0.83631000
H -3.78938900 -2.81432000 -0.78072700
C -3.68079300 -0.71263500 -0.26068200
C -2.81655500  0.34602300 -0.01434100
O  1.04609700 -2.49706000 -0.66870800
O -1.04127900  2.47542700  0.47610100
C -5.11570000  0.52696600  0.09707400
C -7.94848400 -0.15084400 -0.07609300
C -5.74280200  0.67067200 -0.64076600
C -5.99245400 -1.52843700  0.28796900
C -7.36851700 -1.34673500  0.36302100
C -7.11857100  0.85504500 -0.58644300
H -5.11585000  1.45646600 -1.05758400
H -5.56274200 -2.45430100  0.65954600
H -8.00114300 -2.12933900  0.77081000
H -7.55955000  1.78144900 -0.94175000
C  5.11157000  0.52696600  0.09707400
C  7.93591900  0.14429100  0.05035600
C  5.69409800 -0.77645200  0.14066800
C  6.01800500  1.62710200  0.02989300
C  7.37669000  1.45058500 -0.00430900
C  7.04914600 -0.96763500  0.12720800
H  5.05441600 -1.64846400  0.19754600
H  5.63808000  2.63862800 -0.00925700
H  8.03775000  2.31196700 -0.04374500
H  7.45384500 -1.97307500  0.14931600
N -9.34912300  0.04301300 -0.00205700
N  9.29493000 -0.04144000  0.03287200
C -9.86635500  1.29111200  0.42214100
C -10.8899500  3.76642900  1.25940000
C -9.23984100  2.00504800  1.45159500
C -11.00936600  1.82744100 -0.18478100
C -11.51816000  3.05145800  0.24001300
C -9.74566800  3.23674600  1.85751700
H -8.35493600  1.59160900  1.92550400
H -11.49413900  1.27837600 -0.98623700
H -12.40498100  3.45373000 -0.20431800
H -9.24692300  3.77879500  2.65506300
H -11.28384000  4.72402400  1.58233800
C -10.22809300 -1.02317000 -0.30929900
C -11.96520500 -3.14112800 -0.91897600
C -11.37593600 -1.24298800  0.46291100
C -9.95748400 -1.87325700 -1.38940000
C -10.81754100 -2.92763000 -1.68281300
C -12.23918200 -2.28970000  0.15144000
H -11.58606500 -0.58888400  1.30355500
H -9.07004300 -1.70291800 -1.99126000
H -10.59341700 -3.57815400 -2.52267300
H -13.12490200 -2.44679200  0.75940500
H -12.63673100 -3.96009700 -1.15460400
C  9.88944300 -1.21154600  0.59576800
**b4-S₆ Geometry (Solvent: Toluene)**

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | -3.68959600 | 0.57721000 | 0.52965500|
| H       | -3.22484100 | -1.00710300 | -0.87281200|
| C       | -2.83195300 | -0.24031900 | -0.21214700|
| C       | -1.75227100 | 1.66740400  | 1.51025300 |
| C       | -1.44953900 | -0.10953200 | -0.09975800|
| C       | -3.12915000 | 1.53371800  | 1.39204700 |
| C       | -0.90163000 | 0.84818500  | 0.76600700 |
| C       | -0.57325100 | -1.00981700 | -0.90879900|
| H       | -3.78196600 | 2.19247500  | 1.95680000 |
| H       | -1.31628200 | 2.41026700  | 2.16994000 |
| C       | 3.22482800  | 1.00718900  | 0.87288700 |
| C       | 0.57323700  | 1.00992800  | 0.90902800 |
| H       | 3.12913600  | 0.53364800  | 1.39195400 |
| C       | -3.16267000 | -2.41018600 | -2.16985900|
| C       | 3.78195100  | -2.19245100 | -1.95669600|
| C       | 3.68958200  | -0.57713800 | -0.52956400|
| H       | 2.83194000  | 0.24040300  | 0.21222400 |
| O       | -1.04838800 | -1.84391000 | -1.65992600|
| O       | 1.04837400  | 1.84397200  | 1.66000800 |
| C       | 5.16182100  | -0.43635300 | -0.40791900|
| C       | 7.94053700  | -0.17249400 | -0.17808100|
| C       | 5.75281900  | -0.17622700 | 0.83579400 |
| C       | 5.98557200  | -0.56065300 | -1.53471000|
| C       | 7.36608800  | -0.42799900 | -1.42204300|
| C       | 7.13340100  | -0.04686400 | 0.95128200 |
| H       | 5.13097200  | -0.09815800 | 1.72262200 |
| H       | 5.54233800  | -0.73636800 | -2.51042800|
| H       | 8.00773500  | -0.51382800 | -2.29398500|
| H       | 7.59664700  | 0.14512500  | 1.91453000 |
| C       | -5.16183500 | 0.43641200  | 0.40802000 |
| C       | -7.94054800 | 0.17251900  | 0.17819700 |
| C       | -5.98557900 | 0.56096200  | 1.53481700 |
| C       | -5.75283800 | 0.17629100  | -0.83569300|
| C       | -7.13341800 | 0.04691100  | -0.95117300|
| C       | -7.36609500 | 0.42802000  | 1.42215700 |
| H       | -5.54234100 | 0.73640300  | 2.51053300 |
| H       | -5.13099600 | 0.09823800  | -1.72252500|
| H       | -7.59666800 | -0.14507500 | -1.91441900|
| H       | -8.00773800 | 0.51358700  | 2.29410500 |
| N       | 9.35867600  | -0.09377700 | -0.06083800 |
b4-T1 Geometry (Solvent: Toluene)

C  3.66203500  -0.55075100  0.57950200
H  3.21043800  0.90427000  -0.95037700
C  2.81825200  0.19736200  -0.85586300
C  1.24997380  2.26316700  -0.54179700
C  -1.30502000  -0.50090300  -1.49181000
H  -1.61537500  -1.43531300  -1.43014800
H  -1.35376300  -0.57365600  -2.33207000
H  -1.75873400  0.30598000  -1.69982100
C  -1.29154900  -0.13421200  0.98860400
H  -1.40025570  0.67960100  0.81989700
H  -1.76838000  0.05428800  1.93047200
H  -1.86236600  -1.06162400  1.09069200

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ACRXTN-S$_0$ Geometry (Solvent: DCM)

H  -3.15573400  1.96366600  0.00000000
C  -2.12835500  1.61453800  0.00000000
C   0.54593000  0.78688100  0.00000000
C  -1.10549900  2.57674000  0.00000000
C  -1.82730400  0.26586600  0.00000000
C  -0.48243300 -0.14012100  0.00000000
C   0.22606700  2.14818400  0.00000000
H  -2.60758600 -0.48823200  0.00000000
H   1.58369100  0.47049500  0.00000000
C  -1.41810600  4.01659000  0.00000000
C  -0.23855400  4.90131800  0.00000000
C   2.01653500  6.54753100  0.00000000
C  -0.38076000  6.29872100  0.00000000
C   1.04902700  4.35440900  0.00000000
C   2.18251700  5.17283000  0.00000000
C   0.73274100  7.11876500  0.00000000
H  -1.38648400  6.70645600  0.00000000
H   3.16490500  4.71313200  0.00000000
H   0.61885500  8.19705300  0.00000000
H   2.89250600  7.18783600  0.00000000
O   1.27592300  3.01043600  0.00000000
O  -2.56716000  4.44411000  0.00000000
N  -0.16813600 -1.53354600  0.00000000
C  -0.06477100 -2.20641900  1.22607800
C   0.14977100 -3.50500700  3.70699300
C  -0.20931700 -1.49194300  2.42979600
C   0.18785600 -3.85930400  1.26176200
C   0.29079600 -4.20533900  2.51331000
C  -0.10353800 -2.13608300  3.65548600
H  -0.40496100 -0.42645200  2.40653600
H   0.48946500 -5.27245500  2.55607800
H  -0.21955100 -1.56904400  4.56871700
H   0.23645400 -4.02071000  4.65764800
C  -0.06477100 -2.20641900 -1.22607800
C  0.14977100  -3.50500700  -3.70699300
C  0.18785600  -3.58930400  -1.26176200
C  -0.20931700 -1.49194300  -2.42979600
C  -0.10353800 -2.13608300  -3.65548600
C  0.29079600  -4.20533900  -2.51331000
H  -0.40496100  -0.42645200  -2.40653600
H  -0.21955100 -1.56094400  -4.56871700
H   0.48946500  -5.27245500  -2.55607800
H   0.23645400  -4.02007100  -4.65764800
C   0.36007600  -4.43294700   0.00000000
C  -0.69333400  -5.56195800   0.00000000
H  -0.58277900  -6.19751100   0.88292800
H  -0.58277900  -6.19751100  -0.88292800
H  -1.70374400  -5.14268400  0.00000000
C   1.77371900  -5.05437500  0.00000000
H   1.92191600  -5.68096500   0.88423500
H   2.53666200  -4.27031400  0.00000000
H   1.92191600  -5.68096500  -0.88423500

ACRXTN-T1 Geometry (Solvent: DCM)

H   -3.18753400  1.98078900  0.00000000
C   -2.16321200  1.62590900  0.00000000
C    0.51374500  0.77245800  0.00000000
C   -1.12389700  2.60158300  0.00000000
C   -1.88083600  0.26871100  0.00000000
C   -0.55227800 -0.15115700  0.00000000
C    0.21445700  2.11926400  0.00000000
H   -2.67931400 -0.46819500  0.00000000
H    1.54779600  0.44298700  0.00000000
C   -1.40444300  4.06068700  0.00000000
C   -0.22444900  4.88047500  0.00000000
C    2.06203600  6.52701000  0.00000000
C   -0.34080100  6.27955000  0.00000000
C    1.07088900  4.33520000  0.00000000
C    2.20491700  5.13651200  0.00000000
C    0.78721000  7.09657600  0.00000000
H   -1.34191200  6.69890900  0.00000000
H    3.18255700  4.66533600  0.00000000
H    0.67447400  8.17626900  0.00000000
H    2.94598400  7.15647200  0.00000000
O    1.28292700  2.97695300  0.00000000
O   -2.58135100  4.47829500  0.00000000
N   -0.24464500 -1.56355700  0.00000000
N   -0.09798400 -2.21574000  1.21541100
C    0.17772500 -3.46994700  3.68457700
C   -0.25382000 -1.47405800  2.41295400
C    0.20109500 -3.59906200  1.25468300
C    0.33129900 -4.19625600  2.50827800
C   -0.11562700 -2.10070200  3.63290300
H   -0.48156400 -0.41718400  2.36035300
H    0.55832000 -5.25503400  2.57315100
H   -0.23510600 -1.53010200  4.54681000
H    0.28618000 -3.96833100  4.64180100
C   -0.09798400 -2.21574000  1.21541100
C    0.17772500 -3.46994700 -3.68457700
C    0.20109500 -3.59906200 -1.25468300
C   -0.25382000 -1.47405800 -2.41295400
C   -0.11562700 -2.10070200 -3.63290300
C    0.33129900 -4.19625600 -2.50827800
H   -0.48156400 -0.41718400 -2.36035300
H   -0.23510600 -1.53010200 -4.54681000
H    0.55832000 -5.25503400 -2.57315100
H    0.28618000 -3.96833100 -4.64180100
C    0.37981900 -4.28904000  0.00000000
C   -0.66740600 -5.57043800  0.00000000
H   -0.54262500 -6.20031600  0.88362400
H  -0.54262500  -6.20031600  -0.88362400
H  -1.68181100  -5.16329600  0.00000000
C   1.80593600  -5.03437000  0.00000000
H   1.95303900  -5.65909100  0.88385300
H   1.95303900  -5.65909100 -0.88385300

ACRXTN-S₁ Geometry (Solvent: DCM)

H   -3.19312100   1.97047000  0.00000000
C   -2.16917400   1.61379300  0.00000000
C    0.52554400   0.77302900  0.00000000
C   -1.12155700   2.59775200  0.00000000
C   -1.89004400   0.26979700  0.00000000
C   -0.54748800  -0.16279600  0.00000000
C    0.21743100   2.11614500  0.00000000
H   -2.68756000  -0.46825600  0.00000000
H    1.55980800   0.44738700  0.00000000
C   -1.40848300   3.99318400  0.00000000
C   -0.22106100   4.87659800  0.00000000
C    2.05337800   6.52201100  0.00000000
C   -0.34652600   6.72719700  0.00000000
C    1.06857400   5.29504000  0.00000000
C    2.20365600   5.13694400  0.00000000
O    0.77652600   7.09250900  0.00000000
H   -1.35021100   6.68546200  0.00000000
H    3.18293300   4.66986600  0.00000000
H    0.66317200   8.17168400  0.00000000
H    2.93502800   7.15408900  0.00000000
O    1.28273800   2.97813300  0.00000000
O   -2.56999600   4.47510900  0.00000000
N   -0.24379900  -1.55471900  0.00000000
C   -0.09419500  -2.21315000  1.21571200
C    0.18042500  -3.46233700  3.68649300
C   -0.24548600  -4.46943600  2.41072000
C    0.20133400  -3.59674700  1.25557500
C    0.33019000  -4.19126200  2.50815100
C   -0.10730400  -2.09531200  3.63407800
H   -0.46863000  -0.41222600  2.35480800
H    0.55286400  -5.25093300  2.57472800
H   -0.22311400  -1.52235600  4.54680600
H    0.28843100  -3.96151200  4.64320200
C   -0.09419500  -2.21315000 -1.21571200
C    0.18042500  -3.46233700 -3.68649300
C    0.20133400  -3.59674700 -1.25557500
C   -0.24548600  -4.46943600 -2.41072000
C   -0.10730400  -2.09531200 -3.63407800
C    0.33019000  -4.19126200 -2.50815100
H   -0.46863000  -0.41222600 -2.35480800
H   -0.22311400  -1.52235600 -4.54680600
H    0.55286400  -5.25093300 -2.57472800
H    0.28843100  -3.96151200 -4.64320200
C    0.37498400  -4.42907900  0.00000000
C   -0.68011900  -5.56197400  0.00000000
H   -0.56058300  -6.19278500  0.88384800
H   -0.56058300  -6.19278500 -0.88384800
H   -1.69149500  -5.14717400  0.00000000
C    1.79633200  -5.04260700  0.00000000
H    1.94048400  -5.66814000  0.88385800
H    2.55578900  -4.25636200  0.00000000
H    1.94048400  -5.66814000 -0.88385800

MCz-XT-S₀ Geometry (Solvent: Toluene)
| Atom Type | X-Coordinate | Y-Coordinate | Z-Coordinate |
|-----------|--------------|--------------|--------------|
| H         | -2.34200500  | 0.00043200   | 3.24283300   |
| C         | -1.85287900  | 0.00026100   | 2.27414700   |
| C         | -0.67030000  | -0.00016400  | -0.26128700  |
| C         | -2.66674000  | 0.00010000   | 1.13077600   |
| C         | -0.47576900  | 0.00021500   | 2.15966400   |
| C         | 0.10882700   | 0.00001900   | 0.88495800   |
| H         | -2.06150400  | -0.00013100  | -0.13069300  |
| H         | 0.16676300   | 0.00032600   | 3.03381300   |
| H         | -0.21431300  | -0.00031100  | -1.24442800  |
| C         | -2.04827700  | 0.22612400   | 3.15008400   |
| C         | -1.68327400  | 0.15672500   | 2.13154100   |
| C         | -0.82733200  | -0.02945900  | -0.54466900  |
| C         | -2.65808700  | 0.09162500   | 1.08659400   |
| C         | -0.32999010  | 0.13065500   | 1.85372900   |
| C         | 0.09724000   | 0.03607500   | 0.52582100   |
| C         | -2.17357100  | 0.00078800   | -0.24865300  |
| H         | 0.40655300   | 0.18031800   | 2.65230700   |
| H         | -0.49721900  | -0.09979700  | -1.57640200  |

**MCz-XT-T₁ Geometry (Solvent: Toluene)**

| Atom Type | X-Coordinate | Y-Coordinate | Z-Coordinate |
|-----------|--------------|--------------|--------------|
| H         | -2.04827700  | 0.22612400   | 3.15008400   |
| C         | -1.68327400  | 0.15672500   | 2.13154100   |
| C         | -0.82733200  | -0.02945900  | -0.54466900  |
| C         | -2.65808700  | 0.09162500   | 1.08659400   |
| C         | -0.32999010  | 0.13065500   | 1.85372900   |
| C         | 0.09724000   | 0.03607500   | 0.52582100   |
| C         | -2.17357100  | 0.00078800   | -0.24865300  |
| H         | 0.40655300   | 0.18031800   | 2.65230700   |
| H         | -0.49721900  | -0.09979700  | -1.57640200  |
C     -4.06049600   0.11566300   1.36859700
C     -4.93518200   0.03107900   0.18291000
C     -6.57664200  -0.12674900  -2.09308100
C     -6.33113600   0.03121700   0.30305700
C     -4.38681000  -0.05272500  -1.10493900
C     -5.18849700  -0.13045700  -2.23777500
C     -7.14805500  -0.04667400  -0.82124800
H     -6.74321300   0.09306800   1.30540400
H     -4.71665100  -0.19246100  -3.21299900
H     -8.22778200  -0.04516000  -0.70969700
H     -7.20658000  -0.18683300  -2.97492500
O     -3.02941800  -0.06230200  -1.31616500
O     -4.53513300   0.19923200   2.53055500
N      1.49830600   0.00984400   0.22998200
C      2.25865200  -1.13863300   0.08912500
C      4.21801400  -3.07680700  -0.26759200
C      1.86396200  -2.49056600   0.19891900
C      3.59988800  -0.76008500  -0.18552000
C      4.57572900  -1.71219500  -0.36324800
H      5.64049520  -1.43224600  -0.57089900
H      2.63815900  -4.77721700   0.08325600
H      2.92289300  1.12920400   0.05237600
H      4.30618300  2.99477300  -0.38199200
H      3.62235700   0.70169000  -0.20832800
H      1.93419600  2.49501000   0.09395400
C      2.98846600   3.38971100  -0.12988200
C      4.62473600   1.61759400  -0.42432800
H      2.76343600   4.45244100  -0.10779300
H      5.64433100  1.30021800  -0.62655400
C      0.54821100   3.01522800   0.34766600
C     -0.71360500   2.95102000  -0.35851500
C      0.54354200  4.10248400   0.25657300
H      0.19549300  2.74328900  1.34663100
C      0.46844000  -2.96054200   0.49507600
C      0.45367600  -4.05080900   0.55110600
H      0.23430100  -2.63661200  -0.27791200
H      0.09827000  -2.55033700   1.43884300
C      5.26703700  -4.13377400  -0.46627200
H      4.86016100  -5.13434100  -0.31270900
H      6.09903000  -3.98671100   0.22934900
C      5.67720400  -4.08019200  -1.48040000
H      5.38659200  -4.01287800  -0.61248700
C      5.83974100   3.87539500  -1.59942700
H      6.18361900  3.90158700   0.12955900
H      4.99692800   5.02998600  -0.55031600

MCz-XT-Si Geometry (Solvent: Toluene)

H     -2.04520700   0.00010900   3.15839200
C     -1.67711900   0.00005100   2.13841200
C     -0.82386600  -0.00021100  -0.55308500
C     -2.65305100   0.00002400   1.08596300
C     -0.33149200   0.00000100   1.86515500
C      0.10630500  -0.00013000   0.52520500
C     -2.16903000  -0.00012500  -0.25047700
H      0.40281800   0.00003400   2.66664200
H     -0.49610100  -0.00034500  -1.58678700
C     -4.05364200   0.00013500   1.37276400
C     -4.93108700   0.00038000   0.17951800
C     -6.56905300  -0.00019100  -2.09753300
C     -6.32587400   0.00063000   0.30253700
C     -4.37955000  -0.00013000  -1.10740000
C     -5.18364300  -0.00023100  -2.24438000
C     -7.14286000  -0.00049900  -0.82278400
H     -6.73671100   0.00018000   1.30732600
H     -4.71283000  -0.00035300  -3.22178600

S118
3-PXZ-XO-S₆ Geometry (Solvent: Toluene)

H  -1.37139500  -0.00018800  3.02230900
C  -1.09269900  -0.00019900  1.97349900
C  -0.45858500  0.00005200  -0.75362200
C  -2.12551200  -0.00007800  1.02147000
C  0.23037700  -0.00007400  1.57723500
C  0.53848700  0.00001000  0.20482700
C  -1.79462300  0.00002200  -0.33637500
H  1.08323500  -0.00009700  2.30242700
H  -0.21478800  0.00010700  -1.81031400
C  -3.54214000  -0.00016200  1.43987400
C  -4.50736500  -0.00005100  0.32470500
C  -6.31095300  0.00022100  -1.80542600
C  -5.89020700  -0.00005100  0.56732300
C  -4.05429800  0.00008300  -0.99829910
C  -4.95132000  0.00022000  -2.06989700
C  -6.78814600  0.00008500  -0.48450200
H  -6.22166000  -0.00015600  1.60076300
H  -4.56269500  0.00032400  -3.08224100
H  -7.85548300  0.00008700  -0.29325000
H  -7.01267500  0.00033100  -2.63325200
O  -3.88208500  -0.00036400  2.61436000
O  -2.72963900  0.00007700  -1.32216700
N  1.90279300  0.00023000  -0.22298000
C  2.63087300  1.20556200  -0.13191800
C  4.17701700  3.54831800  -0.04204800
C  2.04103100  2.43289100  0.17303100
3-PXZ-XO-T\textsubscript{1} Geometry (Solvent: Toluene)

H  -1.52366800  -1.35498200  2.88346600
C  -1.18091800  -0.91790000  1.95267400
C  -0.38634800  0.24358600  -0.48772200
C  -2.17835600  -0.50178000  1.01476200
C   0.16510800  -0.76489200  1.68465900
C   0.56393600  -0.18607500  0.47385900
C  -1.72466700  0.07677200  -0.20393300
H   0.91654800  -1.08297500  2.40317800
H  -0.08177300  0.68381800  -1.43177600
C  -3.57417300  -0.66156300  1.28705400
C  -4.47509400  -1.81758000  0.22036000
C  -6.16554870  0.74328300  -1.85222200
C  -5.86768300  -0.26662400  0.34667800
C  -3.95524200  0.37732500  -0.95554500
C  -4.78144200  0.83834000  -1.97405000
C  -6.70099800  0.19053000  -0.66334900
H  -6.25797900  -0.70124200  1.26140900
H  -4.33199100  1.26320400  -2.86527200
H  -7.78582700  0.11723500  -0.54846000
H  -6.81462100  1.10190900  -2.61774300
O  -4.02189600  -1.16712700  2.34759500
O  -2.60333800  0.50173000  -1.16459600
N   1.96193500  -0.03692500  0.17252500
C   2.55179600  1.21336800  -0.21534600
C   3.82680200  3.70243400  0.27907500
C   1.82669000  2.36679000  0.58127100
C   3.92233400  1.34272600  -0.09937400
C   4.55920200  2.58103600  -0.07014300
C   2.46279700  3.59089400  0.60780400
H   0.77921900  2.26636500  0.83879600
H   5.61347900  2.63035600  -0.31720600
H   1.90238700  4.47484100  0.88996200
H   4.31202600  4.67168200  0.30605000
C   2.72264400  -1.13678300  -0.17990100
C   4.34553600  -3.30511100  -0.88581700
C   4.09640300  -0.96392000  -0.46390100
C   2.16885000  -2.43016300  -0.27570500
C   2.97537300  -3.49378900  -0.62340900
C   4.90663000  -2.04224500  -0.81094400
H   1.11222400  -2.56229100  -0.07598200
H   2.54401900  -4.48550100  -0.69725500
H   5.95495500  -1.86024500  -1.01833900
H   4.96630200  -4.15204300  -1.15588000
O   4.67275900  0.26213500  -0.42422300

3-PXZ-XO-S\textsubscript{1} Geometry (Solvent: Toluene)
| At. | X        | Y        | Z        |
|-----|----------|----------|----------|
| H   | -1.52236300 | 0.00140400 | 3.17533700 |
| C   | -1.17692000 | 0.00100100 | 2.14768800 |
| C   | -0.38369000 | -0.00011500 | -0.56316100 |
| C   | -2.17584900 | 0.00049900 | 1.11646400 |
| C   | 0.16267000  | 0.00095100 | 1.84567900  |
| C   | 0.56934300  | 0.00040500 | 0.49568000  |
| C   | -1.72215400 | -0.00002200 | -0.23005500 |
| H   | 0.91309600  | 0.00128300 | 2.63173600  |
| H   | -0.08013700 | -0.00057600 | -1.60391900 |
| C   | -3.57010800 | 0.00053200 | 1.43374800  |
| C   | -4.47341700 | 0.00014800 | 0.25989200  |
| C   | -6.16033100 | -0.00061400 | -1.98116600 |
| C   | -5.86517400 | 0.00024300 | 0.41317000  |
| C   | -3.95021600 | -0.00032400 | -1.03867700 |
| C   | -4.77854300 | -0.00070600 | -2.15806700 |
| C   | -6.70633800 | -0.00014700 | -0.69416300 |
| H   | -6.25385900 | 0.00059900 | 1.42664000  |
| H   | -4.32905000 | -0.00105800 | -3.14545300 |
| C   | -7.78325700 | -0.00078000 | -0.56062700 |
| C   | -6.80999600 | -0.00090600 | -2.85062400 |
| O   | -4.02427600 | 0.00107000 | 2.59036000  |
| O   | -6.60201000 | -0.00042700 | -1.27901800 |
| N   | 1.95772600  | 0.00010500 | 0.16784200  |
| C   | 2.63647300  | 1.19407600 | 0.00163500  |
| C   | 4.08138900  | 3.56192500 | -0.33310100 |
| C   | 1.98930100  | 2.43801000 | 0.14189900  |
| C   | 4.01462800  | 1.17122600 | -0.31144200 |
| C   | 4.73581150  | 2.34822400 | -0.47627700 |
| C   | 2.70972200  | 3.60353400 | -0.02593700 |
| H   | 0.93303900  | 2.45133600 | 0.37993800  |
| H   | 5.79168900  | 2.28438000 | -0.71242800 |
| H   | 2.20947100  | 4.55876600 | 0.08141100  |
| H   | 4.63541900  | 4.85135900 | -0.45968700 |
| C   | 2.63607100  | -1.19416900 | 0.00215000  |
| C   | 4.08015200  | -3.56264400 | -0.33177100 |
| C   | 4.01422900  | -1.17191500 | -0.31097200 |
| C   | 1.98846700  | -2.43783100 | 0.14286900  |
| C   | 2.70847700  | -3.60366600 | -0.02456000 |
| C   | 4.73500100  | -2.34922500 | -0.47539200 |
| H   | 0.93220300  | -2.45070500 | 0.38092800  |
| H   | 2.20789500  | -4.55868600 | 0.08312600  |
| H   | 5.79089000  | -2.28583600 | -0.71159800 |
| H   | 4.63385400  | -4.48690200 | -0.45805500 |
| O   | 4.68041600  | -0.00048800 | -0.45856400 |

**PTZ-XT-S$_0$ Geometry (Solvent: THF)**

| At. | X            | Y            | Z            |
|-----|--------------|--------------|--------------|
| H   | 1.71974800   | -0.00148200  | 3.25948600   |
| C   | 1.35686300   | -0.00098200  | 2.23692500   |
| C   | 0.49269600   | 0.00030100   | -0.42390000  |
| C   | 2.30364100   | -0.00051100  | 1.20256300   |
| C   | 0.00217900   | -0.00081000  | 1.95471100   |
| C   | -0.42294000  | -0.00014700  | 0.61864500   |
| C   | 1.85647900   | 0.00013100   | -0.12390300  |
| H   | -0.74196000  | -0.00155700  | 2.74358400   |
| H   | 0.16663000   | 0.00076800   | -1.45949200  |
| C   | 3.75046900   | -0.00068300  | 1.49512200   |
| C   | 4.61645000   | -0.00014900  | 0.30320900   |
| C   | 6.23166700   | 0.00086500   | -1.97378300  |
| C   | 6.01555800   | -0.00024300  | 0.42640000   |
| C   | 4.05186000   | 0.00046600   | -0.97671200  |
| C   | 4.85422600   | 0.00097300   | -2.12113200  |
| C   | 6.82039000   | 0.00025900   | -0.69813400  |
| H   | 6.43668500   | -0.00071600  | 1.42662700   |
| H   | 4.38178800   | 0.00143900   | -3.09720300  |
| H   | 7.90012700   | 0.00018500   | -0.59895500  |

S121
H      6.85998700  0.00125500  -2.85848600  
O      2.70465100  0.00060800  -1.18569700  
O      4.19119800 -0.00125800   2.63785200  
N     -1.83092200  0.00003400   0.35082200  
C     -2.42652800 -1.23193900  -0.02060000  
C     -3.66436300 -3.66104600  -0.74314100  
C     -3.82651800 -1.34037500  -0.07939500  
C     -1.66221000 -2.37061900  -0.30628800  
C     -2.27887800 -3.57317000  -0.65043400  
H     -1.66017300 -4.44093000  -0.85453400  
H     -5.51782800 -2.57649000  -0.51893200  
H     -4.14445300 -4.92471000  -1.02257300  
C     -2.42651200  1.23201700  -0.02013000  
C     -3.66436800  3.66139300  -0.74175200  
C     -3.82650500  1.34046000  -0.07891400  
C     -1.66220900  2.37083400  -0.30530900  
C     -2.27888600  3.57350800  -0.64900600  
H     -0.58160000  2.33008500  -0.24801900  
H     -1.66018800  4.44136300  -0.85272400  
H     -5.51782000  2.57671800  -0.51802200  
H     -4.14446300  4.59291700  -1.02084400  
S     -4.83321200  0.00000000   0.46330100  

PTZ-XT-T\textsubscript{1} Geometry (Solvent: THF)

H      1.67960600  -0.14920100   3.17073300  
C      1.33897800  -0.10523400   2.14253300  
C      0.52554400   0.00746000  -0.54404700  
C      2.33027100  -0.06572700   1.11845200  
C      -0.01369200  -0.08591500   1.83940300  
C      -0.41536100  -0.02933300   0.50640000  
C      1.86797400  -0.01038800  -0.22587100  
H      -0.76275300  -0.11481900   2.62632900  
H       0.21207600   0.05022100  -1.58235700  
C      3.73048100  -0.07973500   1.41982000  
C      4.62214000  -0.02140200   0.25396100  
C      6.30262600   0.08565800  -2.00489700  
C      6.01910000  -0.01307300   0.39185600  
C      4.09631100   0.02825300  -1.04829500  
C      4.91455900   0.08039300  -2.16896200  
C      6.85295600   0.03975200  -0.72243800  
H      6.42236700  -0.04878500   1.39888100  
H      4.45796700   0.11598400  -3.15286100  
H      7.93080200   0.04509900  -0.59325700  
H      6.94528700   0.12592400  -2.87838600  
O      2.74161000   0.02689700  -1.28081100  
O      4.18554900  -0.13498000   2.60153300  
N     -1.82424100  -0.00602700   0.17981800  
C     -2.46626900  -1.22397500   0.00537500  
C     -3.72074000  -3.73205300  -0.31874400  
C     -3.84869400  -1.32051200  -2.08662000  
C     -1.72830000  -2.42619500   0.12715800  
C     -2.34532000  -3.64754200  -0.03278000  
C     -4.46168100  -2.57725600  -0.44530000  
H     -1.75662500  -4.55281000   0.06495100  
H     -5.52335300   2.61997300  -0.66719900  
H     -4.19721900  -4.69808800  -0.44023300  
C     -2.43599500   1.23325900   0.05253500  
C     -3.62495100   3.78239900  -0.18743700  
C     -3.81393100   1.37538300  -0.24422900  
C     -1.66997100   2.41120800   0.22722300  
C     -2.25511500   3.65275200   0.10812500  
C     -4.39777100   2.65206300  -0.36048100  
H     -0.61591500   2.32587300   0.45613800  

S122
PTZ-XT-S<sub>1</sub> Geometry (Solvent: THF)

| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | -1.64536300 | 4.53867700 | 0.24566300 |
| H    | -5.45235100  | 2.72922300  | -0.58790800 |
| H    | -4.07570100  | 4.76400500  | -0.56351000 |
| H    | -0.67037700  | -2.37541300 | 0.34848300  |
| S    | -4.87743200  | 0.04434800  | -0.47245400 |

PTZ-XT-S<sub>1</sub> Geometry (Solvent: Toluene)

| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | -1.65552200 | -0.00047900 | 3.17542100 |
| C    | 1.31809400  | -0.00022600 | 2.14517100 |
| C    | 0.52875700  | 0.00040300  | -0.56351000 |
| C    | 2.32131900  | -0.00014500 | 1.11702900 |
| C    | -0.02162400 | -0.00002100 | 1.83781600 |
| C    | -0.42611800 | 0.00024300  | 0.48980200 |
| C    | 1.86704800  | 0.00021300  | -0.23039400 |
| H    | -0.77540600 | -0.00014300 | 2.62064000 |
| H    | 0.22366700  | 0.00060000  | -1.60416900 |
| C    | 3.71309600  | -0.00042100 | 1.43078800 |
| C    | 4.61781800  | -0.00074000 | 0.26112500 |
| C    | 6.30649100  | 0.00060000  | -1.98248000 |
| C    | 6.01185500  | 0.00030500  | -1.03918800 |
| C    | 4.92423300  | 0.00064100  | -2.15866300 |
| C    | 6.52318000  | 0.00023400  | -0.69491100 |
| H    | 6.40518500  | -0.00037300 | 1.42393100 |
| H    | 4.47540100  | 0.00092300  | -3.14643400 |
| H    | 7.92918300  | 0.00021500  | -0.56114300 |
| H    | 6.95589900  | 0.00086200  | -2.85195200 |
| O    | 2.74850100  | 0.00033700  | -1.27889200 |
| O    | 4.17034200  | -0.00085900 | 2.60188400 |
| N    | -1.81681800 | 0.00077000  | 0.15928500 |
| C    | -2.44699400 | -1.23061800 | 0.00592000 |
| C    | -3.66907400 | -3.75931100 | -0.25525300 |
| C    | -3.83508900 | -1.35061400 | -0.25525300 |
| C    | -1.68466800 | -2.41693400 | 0.12612100 |
| C    | -2.28343400 | -3.65257200 | -0.00414500 |
| C    | -4.42664400 | -2.61734400 | -0.37841700 |
| H    | -1.67661900 | -4.54650000 | 0.08869300 |
| H    | -5.49254000 | -2.68343100 | -0.57191800 |
| H    | -4.12610400 | -4.73421200 | -0.35263500 |
| C    | -2.44728000 | 1.23063200  | 0.00612500 |
| C    | -3.66179000 | 3.75971400  | -0.25464700 |
| C    | -3.83538800 | 1.35036000  | -0.25464700 |
| C    | -1.68521400 | 2.41693800  | 0.12695100 |
| C    | -2.28323900 | 3.65261200  | -0.00414500 |
| C    | -4.42721200 | 2.61698400  | -0.37804400 |
| H    | -0.62416400 | 2.34247500  | 0.32263900 |
| H    | -1.67762700 | 4.54665500  | 0.08957000 |
| H    | -5.49311600 | 2.68287400  | -0.57157100 |
| H    | -4.12712600 | 4.73391100  | -0.35188200 |
| H    | -0.62362100 | -2.34216000 | 0.32210500 |
| S    | -4.89067700 | -0.00023200 | -0.42286500 |

MC2-S<sub>0</sub> Geometry (Solvent: Toluene)

| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | -5.13939400 | -2.66373900 | -0.49887100 |
| C    | -5.11656900 | -1.59412900 | -0.31621400 |
| C    | -5.02872000 | 1.14911100 | 0.20453900 |
| C    | -3.91492800 | -1.00864600 | 0.11679600 |
| C    | -6.24736500 | -0.82500400 | -0.51083800 |
| C    | -6.20956300 | 0.55458800  | -0.25004500 |
| C    | -3.89012200 | 0.36296600  | 0.37640900 |
| C    | -7.17783300 | -1.26051100 | -0.85891800 |
| H    | -2.98261800 | 0.83124800  | 0.74505300 |
| H    | -4.98374400 | 2.20765000  | 0.42958100 |
| C    | -2.74225300 | -1.89573000 | 0.35544000 |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| O    | -2.90077900 | -3.07848300 | 0.61894000 |
| C    | -1.35324400 | -1.33811500 | 0.27123000 |
| C    | 1.29134300  | -0.45421000 | 0.10238800 |
| C    | -0.36273500 | -1.91223800 | 1.07592900 |
| C    | -1.00389000 | -0.32602600 | -0.62924700 |
| C    | 0.31568900  | 0.10383100  | -0.72721400 |
| C    | 0.94872800  | -1.46138400 | 1.01113000 |
| H    | -0.64056200 | -2.70598400 | 1.76197100 |
| H    | -1.75486600 | 0.10132500  | -1.28645100 |
| H    | 0.59967000  | 0.85806500  | -1.66248800 |
| N    | 2.62862700  | -0.00472600 | 0.01918000 |
| C    | 3.75027600  | -0.81569600 | -0.15223300 |
| C    | 6.24470000  | -1.96447500 | -0.51987800 |
| C    | 3.82394000  | -2.20045400 | -0.32512300 |
| C    | 4.90406500  | -0.00179000 | -0.18165100 |
| H    | 6.16060400  | -0.58657800 | -0.36427200 |
| C    | 5.08478900  | -2.75776800 | -0.50493600 |
| H    | 2.93367400  | -2.82015400 | -0.32797200 |
| H    | 7.05488000  | 0.02916200  | -0.38846000 |
| H    | 5.17165100  | -3.83115300 | -0.64040700 |
| H    | 7.21211900  | -2.43469600 | -0.66118100 |
| C    | 3.04834500  | 1.32255500  | 0.10112100 |
| C    | 4.37448100  | 3.75140300  | 0.24701400 |
| C    | 4.45520900  | 1.36627000  | -0.01755500 |
| C    | 2.29353700  | 2.47923000  | 0.31188700 |
| C    | 2.97696600  | 3.68814700  | 0.37929400 |
| C    | 5.11895500  | 2.59437100  | 0.05338300 |
| H    | 1.21567700  | 2.43928200  | 0.42695000 |
| H    | 2.41541500  | 4.60281600  | 0.54116700 |
| H    | 6.20029800  | 2.64034800  | -0.03593300 |
| H    | 4.87400700  | 4.71278700  | 0.30335700 |
| C    | -7.36467500 | 1.22487200  | -0.46386100 |
| C    | -7.38329500 | 2.62049500  | -0.21275600 |
| H    | -8.39199600 | 2.95349400  | -0.45078800 |
| H    | -7.16554500 | 2.83217400  | 0.83954100 |
| H    | -6.66340300 | 3.14284000  | -0.85192400 |

**MC2-T1 Geometry (Solvent: Toluene)**

| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | -4.99030800 | -2.66506100 | -0.43355100 |
| C    | -5.03454900 | -1.59090600 | -0.28905100 |
| C    | -5.14137100 | 1.16238900  | 0.15049970 |
| C    | -3.90734100 | -0.93605200 | 0.23420200 |
| C    | -6.18240600 | -0.88909300 | -0.61140200 |
| C    | -6.24130700 | 0.49689200  | -0.39536500 |
| C    | -3.98692600 | 0.43915000  | 0.45778800 |
| C    | -7.05314100 | -1.38388500 | -1.02664200 |
| H    | -3.14806700 | 0.96963600  | 0.90754900 |
| H    | -5.17135800 | 2.22655900  | 0.35085300 |
| C    | -2.71905700 | -1.75549700 | 0.61406700 |
| O    | -2.89704200 | -2.91443500 | 1.07320600 |
| C    | -1.37956600 | -1.27144000 | 0.43141900 |
| C    | 1.33083100  | -0.43584600 | 0.17189800 |
| C    | -0.28219900 | -2.04496400 | 1.01419300 |
| C    | -1.02227500 | -1.09123000 | -0.37167900 |
| C    | 0.26631200  | 0.29957000  | -0.47549500 |
| C    | 1.00510500  | -1.63883300 | 0.89281100 |
| H    | -0.54420500 | -2.92630400 | 1.58631800 |
| H    | -1.79423900 | 0.40211400  | -0.93509800 |
| H    | 0.52891100  | 1.13028600  | -1.12380000 |
| H    | 1.80091600  | -2.17750800 | 1.39801800 |
| N    | 2.63965000  | -0.01427600 | 0.04502200 |
| C    | 3.75523400  | -0.82997700 | -0.21522000 |
| C    | 6.20599000  | -1.97639500 | -0.77616100 |
| C    | 3.79588500  | -2.19744200 | -0.48872400 |
| C    | 4.91137200  | -0.62442700 | -0.26920900 |
C 6.14661500 -0.60255800 -0.54728900
C 5.04271600 -2.75780400 -0.75596000
H 2.89707900 -2.80229500 -0.51608900
H 7.04369900 0.00671700 -0.59677000
H 5.10866100 -3.82018700 -0.96540900
H 7.16034900 -2.44473900 -0.99197400
C 3.08679200 1.31342000 0.15366200
C 4.44077400 3.71361300 0.34128700
C 4.48307200 1.34757600 -0.03850200
C 2.35927200 2.45519100 0.49017700
C 3.05842700 3.65757600 0.56551600
C 5.16476400 2.55772600 0.05183100
H 1.29793000 2.41205100 0.70632900
H 2.52088800 4.56548700 0.81794600
H 6.24043400 2.59862400 -0.08870400
H 4.95520000 4.66589700 0.41375000
O -7.40924500 1.10206700 -0.73873400
C -7.51978900 2.49572200 -0.51730700
H -8.51596400 2.77649900 -0.85602600
H -7.41399500 2.73513800 0.54679300
H -6.76831300 3.04738000 -1.09552600

MC2-S1 Geometry (Solvent: Toluene)

H -3.37739200 -1.49013500 -1.42672500
C -4.11789100 -0.90122000 -0.89451900
C -6.04190700 0.58084400 0.51548800
C -3.92496400 -0.61055700 0.47217700
C -5.21926300 -0.40219400 -1.55896700
C -6.18953800 0.34142700 -0.85783800
C -4.91947400 0.90959200 1.71204000
H -5.36876000 -0.57524800 -2.61924900
H -4.79145000 0.26723900 2.23413400
H -6.78453900 1.14011700 1.07040500
C -2.72729200 -1.11566600 1.20109400
O -3.13641200 -1.97066900 2.07725500
C -1.35839100 -0.83069300 0.90023500
C 1.34415400 -0.27259500 0.36851500
C -0.32588600 -1.50693500 1.60393300
C -0.99978600 0.13206900 -0.06406400
C 0.33269600 0.39765500 -0.32348700
C 1.00362500 -1.21909500 1.34117600
H -0.58610800 -2.24462000 2.35622900
H -1.77422200 0.66569800 -0.60676800
H 0.60533200 1.12244600 -1.09134200
H 1.79371400 -1.72325000 1.89043800
N 2.70609500 0.00895900 0.09245900
C 3.65985400 -0.91698600 -0.31499900
C 5.87796200 -2.35000700 -1.15174900
C 3.51023000 -2.28393100 -0.56563100
C 4.89863400 -0.25895800 -0.49093400
C 6.01500900 -0.98826800 -0.91140400
C 4.63517000 -2.98564000 -0.98274300
H 2.55134300 -2.77680700 -0.44319700
H 6.97309300 -0.49575900 -1.05031800
H 4.54960700 -4.04886900 -1.18420500
H 6.73506500 -2.93029900 -1.47704100
C 3.31183100 1.25271100 0.18190100
C 4.95371600 3.48798600 0.23096300
C 4.67473600 1.13708900 -0.17397600
C 2.75924200 2.47869900 0.57724600
C 3.59871500 3.58642800 0.59347100
C 5.49768900 2.26722500 -0.14931900
H 1.71614600 2.55694900 0.86579200
H 3.19753000 4.54862800 0.89618900
H 6.54666800 2.18952000 -0.42023300
H 5.57886000 4.37447200 0.25410900
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| O       | -7.22890600 | 0.77568500 | -1.59331200 |
| C       | -8.25292700 | 1.51857000 | -0.94562100 |
| H       | -8.73201300 | 0.92041900 | -0.16413500 |
| H       | -7.85021000 | 2.44130300 | -0.51585200 |

**OPM-S\textsubscript{0}** Geometry (Solvent: Toluene)

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | 6.10262100 | -1.72721100 | -1.30077400 |
| C       | 6.03757700 | -0.76920800 | -0.79473600 |
| C       | 5.85017400 | 1.65421400 | 0.56345600 |
| C       | 4.84594900 | -0.44677400 | -0.12919000 |
| C       | 7.11048900 | 0.11670600 | -0.80140700 |
| C       | 7.02037800 | 1.33514200 | -0.12578100 |
| C       | 4.77226400 | 0.77157000 | 0.56196200 |
| H       | 8.02176900 | -0.14406700 | -0.33129000 |
| H       | 7.85862400 | 2.02491100 | -0.12707500 |
| H       | 3.87850900 | 1.01846800 | 1.12875400 |
| H       | 5.78021900 | 2.58798400 | 1.11339600 |
| C       | 3.74892300 | -1.45572900 | -0.11613700 |
| C       | 2.36578200 | -1.07527900 | -0.11867900 |
| C       | -0.41395500 | 0.04623200 | 0.09881100 |
| C       | 1.35895600 | -2.11444600 | 0.06732000 |
| C       | 1.86675200 | 0.25784000 | -0.41838000 |
| C       | 0.54691300 | 0.55489200 | -0.29739700 |
| C       | 0.04098100 | -1.80725400 | 0.18983600 |
| H       | 2.55379800 | -3.13926900 | -0.77626700 |
| H       | 0.19719200 | 1.55098500 | -0.54961300 |
| H       | -0.67651400 | -2.60519600 | 0.33874300 |
| O       | 4.04207500 | -2.68788900 | -0.14959300 |
| N       | -1.74036100 | -0.10178200 | 0.27671700 |
| C       | -2.18486000 | 1.25104000 | 0.17238300 |
| C       | -3.09199000 | 3.85743600 | -0.17369400 |
| C       | -1.75242900 | 2.23393500 | 1.07720500 |
| C       | -3.10963800 | 1.54991600 | -0.83655100 |
| C       | -3.55080000 | 2.85961300 | -1.01593600 |
| C       | -2.19900200 | 3.54125600 | 0.86877100 |
| H       | -4.27173700 | 3.08476600 | -1.79495600 |
| H       | -1.87023300 | 4.31973800 | 1.55106800 |
| H       | -3.40365100 | 4.88087000 | -0.30706000 |
| C       | -2.78821200 | -1.06681000 | 0.35521300 |
| C       | -4.85881700 | -2.92702300 | 0.39552400 |
| C       | -3.78879700 | -1.01484200 | -0.62255200 |
| C       | -2.85415200 | -2.00519000 | 1.38495400 |
| C       | -3.88379300 | -2.94145200 | 1.39440800 |
| C       | -4.82539800 | -1.94882800 | -0.60086300 |
| H       | -2.99610900 | -1.99726300 | 2.16230000 |
| H       | -3.92948200 | -3.68052200 | 2.18680800 |
| H       | -5.60357500 | -1.90238700 | -1.35598900 |
| H       | -5.66362800 | -3.64799400 | 0.40676300 |
| S       | -3.71761700 | 0.24347500 | -1.85797900 |
| C       | -0.85218500 | 1.90642100 | 2.23823500 |
| H       | -0.99357600 | 2.62804800 | 3.03973000 |
| H       | 0.20362100 | 1.91804800 | 1.94685800 |
| H       | -1.06630500 | 0.90230000 | 2.62954100 |

**OPM-T\textsubscript{1}** Geometry (Solvent: Toluene)

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | 6.10262100 | -1.72721100 | -1.30077400 |
| C       | 6.03757700 | -0.76920800 | -0.79473600 |
| C       | 5.85017400 | 1.65421400 | 0.56345600 |
| C       | 4.84594900 | -0.44677400 | -0.12919000 |
| C       | 7.11048900 | 0.11670600 | -0.80140700 |
| C       | 7.02037800 | 1.33514200 | -0.12578100 |
O  3.77522500  -0.39559700  -2.51885800
N  -1.67653200  -0.05092600  0.37067200
C  -2.44803300  1.14849400  0.25204900
C  -3.96066400  3.44396300  -0.10780400
C  -2.22751000  2.23881800  1.10463100
C  -3.46005800  1.17546900  -0.71384300
C  -4.22017400  2.32915700  -0.90004800
C  -2.98957600  3.39089900  0.89114700
H  -5.01029000  2.34331500  -1.64368100
H  -2.82597400  4.25339200  1.53060400
H  -4.54316300  4.34869600  -0.24746800
C  -2.46024000  -1.23580000  0.53197400
C  -4.00485300  -3.53730100  0.73632900
C  -3.48064600  -1.47407800  -0.39468100
C  -2.24868600  -2.11632500  1.59059700
C  -3.01211800  -3.27716900  1.68267800
C  -4.25547400  -2.63046200  -0.29037700
H  -1.47556900  -1.89195500  2.31969100
H  -2.83793900  -3.97317900  2.49609100
H  -5.60428100  -4.43842200  0.81164900
S  -3.77461500  -0.28187600  -1.66495600
C  -1.20022200  2.17107500  2.20277600
H  -1.40647200  2.92735800  2.96243600
H  -0.18930600  2.34550900  1.81837900
H  -1.20187300  1.18538900  2.67619600

**p-Cz-S Window (Solvent: THF)**

H  -3.53660500  1.43820300  0.75014900
C  -4.46463900  1.07681800  0.31766400
C  -6.87113100  0.14813000  -0.75410000
C  -4.63040500  -2.08125000  -1.00393700
C  -6.70229200  1.50764400  -0.48250200
C  -5.84334900  -0.74756000  -0.47838700
H  -5.37766600  0.30232560  0.28596000
H  -5.96301500  -1.80927800  -0.66993900
H  -7.80431700  -0.21080500  -1.17583200
C  -3.57135900  -1.29388000  0.36663300
O  -3.88225500  -2.42871800  0.69731200
C  -2.12778300  -0.91126900  0.27882000
C  -0.60110200  -3.45472000  0.10669800
C  -1.66191000  0.04401800  -0.63215500
C  -1.21262700  -1.58830900  1.09318700
C  0.14252000  -1.29591800  1.02598800
C  -0.30116800  0.31474700  -0.73129900
H  -2.35562900  0.55259300  -1.29403000
H  -1.58072100  -2.33225100  1.79224800
H  0.84945400  -1.78872400  1.68575200
H  0.06798500  1.02475200  -1.46433100
N  1.98142300  -0.05440100  0.02380700
C  3.00358500  -0.99153800  -0.12452900
C  5.35386600  -2.42378000  -0.45499600
C  4.24336500  -3.15041000  -0.16360200
C  2.92047700  -2.73931300  -0.26940100
C  4.11080000  -3.07986500  -0.43085800
C  5.42658900  -1.04203000  -0.32731800
H  1.96632200  -2.89508700  -0.26352800
H  4.07541800  -4.15877700  -0.54374700
H  6.38513100  -0.53243000  -0.35868000
H  6.26204900  -3.00381100  -0.58109700
C  2.54983900  1.21787000  0.08222900
C  4.14567400  3.48202500  0.19004400
C  1.93158800  2.45773200  0.26735900
C  3.95304700  1.09857500  -0.02909800
C                  4.75379500    2.24374200    0.02269300
C                  2.74916700    3.58159400    0.31582800
H                  0.85599800    2.54559500    0.37610300
H                  5.83354400    2.16362100   -0.06184600
H                  2.29521400    4.55730900    0.45723400
H                  4.75171600    4.38094100    0.23098000
H                 -7.50673800    2.20585100   -0.69117600

p-Cz-T₁ Geometry (Solvent: THF)

H                 -3.68271300    1.58267000    0.70176900
C                 -4.55816900    1.13509100    0.23892700
C                 -6.84769000    0.00027000   -0.87178000
C                 -4.62548000   -0.25553000    0.07326700
C                 -5.62010400    1.94867800   -0.15202900
C                 -6.76484300    1.38547000   -0.71697400
C                 -5.79139300   -0.81284100   -0.47035800
H                 -5.55705400    3.02277900   -0.00647600
H                 -5.85403900   -1.89195600   -0.57167600
H                 -7.73883800   -0.44586200   -1.30284000
C                 -3.54360000   -1.17643100    0.53486700
O                 -3.86776000   -2.28457100    1.05298100
C                 -2.15478300   -0.84799100    0.37465300
C                 -1.65548000    0.22876700    0.45826100
C                 -1.16737000   -1.69960000    1.02084300
C                  0.16467200   -1.44648600    0.91328700
C                 -0.32299600    0.48744800   -0.55093000
H                 -2.35041600    0.80688200   -1.05592100
H                 -1.53077600    2.51845500    1.62908800
H                  0.88204000   -2.04525100    1.46601500
H                  0.03894500   -1.25788000   -1.22503300
C                  1.98581800   -0.05870000    0.04183600
C                 -3.01029700   -1.00363200   -0.14391900
C                  5.33019500   -2.43790600   -0.56943700
C                  4.24974000   -0.33236000   -0.19789700
C                  2.90409500   -2.37881100   -0.35280100
C                  4.08851200   -3.08592600   -0.55153300
C                  5.41930000   -1.05375400   -0.40751600
C                  1.94484200   -2.88190500   -0.38242900
H                  4.04201900   -4.15813600   -0.70849400
H                  6.38026300   -0.55161700   -0.45644500
H                  6.23247400   -3.01783900   -0.73123700
C                  2.57189300    1.21698000    0.10447300
C                  4.17263500    3.46150100    0.22646400
C                  1.96344300    2.44435500    0.36785100
C                  3.96850200    1.08991700   -0.04460300
C                  4.77567200    2.22060500    0.01240900
C                  2.78803700    3.56725000    0.41000100
C                  0.89900900    2.52749600    0.55395900
C                  5.85261400    2.13918500   -0.09500400
C                  2.34665400    4.53887500    0.60396300
C                  4.78666200    4.35454700    0.27181000
H                 -7.58988000    2.02033000   -1.02515200

p-Cz-S₁ Geometry (Solvent: THF)

H                 -3.57535400    1.58598700    0.36018300
C                 -4.52406000    1.14185000    0.07794500
C                 -7.00595100    0.01987000   -0.54527700
C                 -4.66981300   -0.25855600    0.05085100
C                 -5.60638700    1.95880800   -0.22611900
C                 -6.85801100    1.40611500   -0.54167600
C                 -5.92941600   -0.81143500   -0.25243300
H                 -5.48046400    3.03679100   -0.20220800
H                 -6.05097900   -1.88969100   -0.27327000
H                 -7.96991500   -0.41947900   -0.78224100
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 5.75120900 | -2.72472100| 0.35772500 |
| H    | 9.50240400 | 0.42110900 | 1.42944900 |
| H    | 7.97408700 | -3.58160600| 1.02565600 |
| H    | 9.83547300 | 2.39301500 | -0.32662300|
| C    | 5.55535900 | 1.43847500 | 0.26600300 |
| C    | 6.65488600 | 3.96629200 | 0.56163600 |
| C    | 4.74955000 | 2.54873600 | -0.00239000|
| C    | 6.40582600 | 2.85701600 | 0.81041900 |
| C    | 5.31881400 | 3.80778700 | 0.15435400 |
| H    | 3.72034800 | 2.43901500 | -0.32662300|
| H    | 8.49026900 | 2.97733800 | 1.11308800 |
| H    | 7.47148100 | 4.67815400 | -0.04563100|
| H    | 7.06434500 | 4.96447000 | 0.67556600 |
| C    | -4.78339200| 0.71744300 | -1.15093400|
| C    | -7.26843000| 2.14914000 | -1.11685900|
| C    | -5.05603600| 1.75988800 | -2.04603700 |
| C    | -5.80726500| 0.42666000 | -0.24673600 |
| C    | -7.02796700| 1.11646900 | -0.20840900 |
| H    | -4.30552200| 2.01608400 | -2.78784900 |
| H    | -6.42849900| 3.25263100 | -2.75721100 |
| O    | -5.74391000| -0.53420500| 0.72934500 |
| C    | -6.93475800| -0.47041000| 1.40844100 |
| C    | -9.40521200| -0.08323200| 2.53423700 |
| C    | -7.77471500| 0.51769200 | 0.88536600 |
| C    | -7.28229300| -1.28312000| 2.47950800 |
| C    | -8.54107800| -1.06756300| 3.03652000 |
| C    | -9.03351200| 0.71986800 | 1.45816400 |
| H    | -6.60563300| -2.04210300| 2.85738200 |
| O    | -8.85906700| -1.67564600| 3.87704000 |
| C    | -9.70410500| 1.48142600 | 1.07299000 |
| H    | -10.37758100| 0.05829600| 2.99490300 |

**ODFRCZ-Tj Geometry (Solvent: DCM)**

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | -2.12761000| -2.83609800| -1.42600100|
| C    | -2.20331700| -1.75384400| -1.38926700|
| C    | -2.38943500| 1.01696000 | -1.35730300|
| C    | -1.03652900| -0.99148800| -1.54551500|
| C    | -3.43718300| -1.14518500| -1.19561900|
| C    | -3.55107200| 0.25323700 | -1.78583000|
| C    | -1.15306400| -0.40591600| -1.53717400|
| H    | -4.32516400| -1.75679100| -1.07226700|
| H    | -0.27474100| 1.02512600 | -1.69640300|
| H    | -2.45262700| 2.10135900 | -1.34803100|
| C    | 0.25124900 | -1.69617300| -1.80664700|
| C    | 1.49829500 | -1.20978000| -1.28311500|
| C    | 4.04355300 | -0.38229200| -0.31798700|
| C    | 2.72664300 | -1.82317600| -1.75697800|
| C    | 1.61820000 | -0.20684400| -0.23062600|
| C    | 2.83751600 | 0.20159200 | 0.20250400 |
| C    | 3.94357700 | -1.42332100| -1.29530000|
| H    | 2.64578400 | -2.58291400| -2.52433600|
| H    | 0.72397200 | 0.18979900 | 0.21987500 |
| H    | 2.90890000 | 0.90819100 | 1.02378500 |
| H    | 4.85315100 | -1.83968500| -1.71720200|
| O    | 0.23439200 | -2.76479000| -2.48746200|
| N    | 5.27491900 | 0.03278600 | 0.15446900 |
| C    | 6.35717500 | -0.79900700| 0.49030100 |
| C    | 8.69855400 | -1.99102600| 1.33400300 |
| C    | 6.41392200 | -2.19268900| 0.51264300 |
| C    | 7.43125000 | 0.00157000 | 0.93244600 |
| C    | 8.61253100 | -0.59674600| 1.35340700 |
| C    | 7.61055400 | -2.77401800| 0.92843600 |
| H    | 5.56292600 | -2.80588800| 0.24082500 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | 9.446364  | 0.004528  | 1.701285  |
| H    | 7.691725  | -3.855348 | 0.949746  |
| H    | 9.613810  | -2.475640 | 1.656571  |
| C    | 5.656856  | 1.365189  | 0.383842  |
| C    | 6.876826  | 3.779957  | 0.949746  |
| C    | 4.947279  | 2.534694  | 1.515175  |
| C    | 6.980777  | 1.387358  | 0.212365  |
| C    | 7.595372  | 2.602557  | 1.134038  |
| C    | -4.864086 | 0.918437  | -1.012968 |
| C    | -7.400656 | 2.228076  | -0.691130 |
| C    | -5.205816 | 2.074937  | -1.726540 |
| C    | -5.849505 | 0.452734  | -0.138660 |
| C    | -7.093170 | 1.076963  | 0.037675  |
| C    | -6.441924 | 2.716772  | -1.572870 |
| H    | -4.490054 | 2.472758  | -2.439784 |
| H    | -6.651892 | 3.604798  | -2.159662 |
| H    | -8.357862 | 2.725361  | -0.571955 |
| O    | -5.720972 | -0.644951 | 0.674870  |
| C    | -6.890862 | -0.740084 | 1.383223  |
| C    | -9.393803 | -0.630806 | 2.615885  |
| C    | -7.783194 | 0.285031  | 1.042420  |
| C    | -7.175667 | -1.720960 | 2.322286  |
| C    | -8.424241 | -1.646951 | 2.936517  |
| C    | -9.030890 | 0.342089  | 1.669990  |
| C    | -6.459794 | -2.499487 | 2.560488  |
| C    | -8.693612 | -2.391600 | 3.678420  |
| H    | -9.741229 | 1.125246  | 1.424808  |
| O    | -10.302644| -0.606652 | 3.115304  |

**ODFRCZ-S1 Geometry (Solvent: DCM)**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -2.277305 | -2.867399 | -1.237888 |
| C    | -2.286166 | -1.788033 | -1.124280 |
| C    | -2.316221 | 0.978044  | -0.836875 |
| C    | -1.063968 | -1.086833 | -1.053124 |
| C    | -3.494744 | -1.111668 | -1.044554 |
| C    | -3.535920 | 0.283049  | -0.896070 |
| C    | -1.101200 | 0.315870  | -0.917037 |
| C    | -4.421516 | -1.672239 | -1.076860 |
| H    | -0.180650 | 0.889110  | -0.893344 |
| H    | -2.319021 | 2.057534  | -0.717041 |
| C    | 0.187214  | -1.813842 | -1.160845 |
| C    | 1.531506  | -1.317987 | -0.812396 |
| C    | 4.113809  | -0.445613 | -0.166752 |
| C    | 2.645535  | -1.776395 | -1.543907 |
| C    | 1.739248  | 0.461933  | 0.286242  |
| C    | 3.015314  | -0.016371 | 0.592746  |
| C    | 3.922104  | 1.334262  | -1.230570 |
| H    | 2.492898  | 2.444433  | -2.384120 |
| H    | 0.903246  | -0.162970 | 0.909570  |
| H    | 3.174920  | 0.638133  | 1.439600  |
| H    | 4.772802  | -1.651296 | -1.825714 |
| O    | 0.189407  | -3.048625 | -1.544981 |
| N    | 5.407547  | 0.011799  | 0.153938  |
| C    | 6.536324  | -0.789985 | 0.328954  |
| C    | 9.017168  | -1.924030 | 0.813975  |
| C    | 6.646796  | -2.182976 | 0.294382  |
| C    | 7.644145  | 0.035183  | 0.624824  |
| C    | 8.894211  | -0.540688 | 0.865645  |
| C    | 7.901258  | -2.732733 | 0.536839  |
| H    | 5.789745  | -2.816921 | 0.095056  |
| H    | 9.752917  | 0.083467  | 1.094369  |
| Atoms | X      | Y      | Z      |
|-------|--------|--------|--------|
| H     | 8.01658700 | -3.81163600 | 0.51434000 |
| H     | 9.98076700 | -2.38866600 | 0.99668000 |
| C     | 5.77952600 | 1.34591800 | 0.33059900 |
| C     | 7.01236300 | 3.79643400 | 0.72220000 |
| C     | 5.00800300 | 2.50437100 | 0.20453900 |
| C     | 7.15988600 | 1.40228300 | 0.62480400 |
| C     | 7.77720500 | 2.63974200 | 0.82548000 |
| C     | 5.64447900 | 3.72415200 | 0.40884000 |
| H     | 3.95464800 | 2.46134100 | -0.04997500 |
| H     | 8.83774000 | 2.69561700 | 1.05227500 |
| H     | 5.06893000 | 4.63992700 | 0.31940700 |
| C     | -4.81826600 | 1.01750000 | -0.83466500 |
| C     | -7.29685100 | 2.46505800 | -0.69966500 |
| C     | -4.98549700 | 2.27506800 | -1.43116000 |
| C     | -5.94792000 | 0.52391000 | -0.17595000 |
| C     | -7.16654500 | 1.21322300 | -0.09420600 |
| C     | -6.19213000 | 2.98411100 | -1.36740500 |
| H     | -4.15201400 | 2.70920100 | -1.98015300 |
| H     | -6.26221500 | 3.95054000 | -1.85535500 |
| H     | -8.22082700 | 3.01522500 | -0.69216000 |
| O     | -6.00363000 | -0.67136700 | 0.49621400 |
| C     | -7.26917400 | -0.76433700 | 1.01558100 |
| C     | -9.82962700 | -0.62270300 | 1.89840800 |
| C     | -8.04151200 | 0.35878700 | 0.69149400 |
| C     | -7.74450500 | -1.82826000 | 1.76867800 |
| C     | -9.06389600 | -1.73617300 | 2.20725400 |
| C     | -9.36311300 | 0.43225600 | 1.14072300 |
| H     | -7.11684100 | -2.68138400 | 2.00023200 |
| H     | -9.48150800 | -2.54313800 | 2.80042700 |
| H     | -9.98437400 | 1.29022700 | 0.90367800 |
| H     | -10.88603500 | -0.58739700 | 2.25767400 |

**ODBTCZ-S Geometry (Solvent: DCM)**

| Atoms | X      | Y      | Z      |
|-------|--------|--------|--------|
| H     | -1.55017800 | -3.50214400 | -2.38184200 |
| C     | -1.78582000 | -2.68158000 | -1.71166700 |
| C     | -2.37588100 | -0.53820300 | -0.03304200 |
| C     | -0.81704000 | -1.70012700 | -1.47285800 |
| C     | -3.02983100 | -2.60259000 | -1.09989000 |
| C     | -3.34301400 | -1.52618500 | -0.25654100 |
| C     | -1.12055400 | -0.62781700 | -0.62713000 |
| H     | -3.77696500 | -3.36762200 | -1.28914600 |
| H     | -0.38566300 | 0.14975900 | -0.44324700 |
| O     | -2.59684400 | 0.29474900 | 0.62734500 |
| C     | 0.48943700 | -1.80131600 | -2.19364900 |
| C     | 1.72887500 | -1.24018000 | -1.56790500 |
| C     | 4.12083000 | -0.28840300 | -0.49232300 |
| C     | 2.74601200 | -0.77927900 | -2.40982300 |
| C     | 1.92525500 | -1.23721200 | -0.18250300 |
| C     | 3.11703600 | -0.76275900 | 0.35574500 |
| C     | 3.93539400 | -0.29873700 | -1.87919900 |
| H     | 2.59562700 | -0.80778700 | -3.48415400 |
| H     | 1.15258700 | -1.61144700 | 0.48165400 |
| H     | 3.26837100 | -0.74529100 | 1.43024600 |
| H     | 4.73020000 | 0.05331300 | -2.52908600 |
| O     | 0.54539400 | -2.33604600 | -3.29120800 |
| N     | 5.33065100 | 0.20050300 | 0.05156600 |
| C     | 5.90465500 | 1.44028400 | -0.22725500 |
| C     | 7.40313400 | 3.76494400 | -0.41032800 |
| C     | 5.42922100 | 2.47399900 | -1.03921700 |
| C     | 7.10611800 | 1.56456100 | 0.50536000 |
| C     | 7.86047400 | 2.73800000 | 0.40729400 |
| C     | 6.19690300 | 3.63058300 | -1.11970000 |
| H     | 4.49535500 | 2.38487400 | -1.58384200 |
| H     | 8.78595100 | 2.84470800 | 0.96546200 |
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**ODBTCZ-T$_1$ Geometry (Solvent: DCM)**

| Atoms | X       | Y       | Z      |
|-------|---------|---------|--------|
| H     | 1.61980200 | -4.40397000 | 1.29551000 |
| C     | 1.86957900  | -3.41555400 | 0.92651200  |
| C     | 2.43962100  | -0.81156700 | 0.04457000  |
| C     | 0.80707700  | -2.45275700 | 0.81153700  |
| C     | 3.14723500  | -3.11013700 | 0.58128000  |
| C     | 3.52886300  | -1.77149500 | 0.14952500  |
| C     | 1.15425200  | -1.13581310 | 0.35403900  |
| H     | 3.91095600  | -3.68404000 | 0.70692700  |
| C     | 0.38288400  | -0.38145000 | 0.24849700  |
| C     | 2.63372200  | -0.17170500 | -0.36601900 |
| C     | -0.53141500 | -2.85286400 | 1.20975300  |
| C     | -1.72053000 | -2.00778900 | 0.86610600  |
| C     | -4.03773400 | -0.55703200 | 0.26975800  |
| C     | -2.74478100 | -1.88350900 | 1.81222900  |
| C     | -1.88277500 | -1.41552900 | -0.39171200 |
| C     | -3.03166600 | -0.68908700 | -0.68994400 |
| C     | -3.89618500 | -1.16173600 | 1.52209800  |
| H     | -2.63252300 | -2.37010100 | 2.77584500  |
| H     | -1.14857000 | -1.53040700 | -1.15120100 |
| H     | -3.15096500 | -0.21931800 | -1.66131100 |
| H     | -4.69398800 | -1.07328300 | 2.25312700  |
| O     | -0.71118700 | -3.90024600 | 1.85908900  |
| N     | -5.20707400 | 0.18492200  | -0.02820800 |
| C     | -5.71309300 | 1.23963200  | 0.72739600  |
| C     | -7.07740600 | 3.37889400  | 1.84268300  |
| C     | -5.19963100 | 1.82043100  | 1.89079000  |
| C     | -6.88728600 | 1.72675800  | 0.10980200  |
| C     | -7.57346000 | 2.80489400  | 0.67826600  |
| C     | -5.89973500 | 2.89072900  | 2.43603000  |
| H     | -4.28788100 | 1.45547800  | 2.35154400  |
| H     | -8.47733000 | 3.18779100  | 0.21350900  |
| H     | -5.52492700 | 3.35984500  | 3.34026900  |
H  -7.59838400  4.21478600  2.29764300
C  -6.04075000  -0.01479100  -1.12574000
C  -7.99828600  -0.03455800  -3.08780200
C  -5.95750500  -0.97695500  -2.13659000
C  -7.09787800   0.92209600  -1.07726000
C  -8.08168600   0.90946700  -2.07134400
C  -6.94751800  -0.96871700  -3.11262200
H  -5.15577000  -1.70735500  -2.15898300
H  -8.89886800   1.62444100  -2.04511800
H  -6.90725200  -1.70384800  -3.91022000
H  -8.75231300  -0.05740400  -3.86756600
C  4.86127200   -1.46252000  -0.15521700
C  7.55839100  -0.93103200  -1.04412300
C  5.80406600  -2.51479900  -0.49863000
C  5.42158200  -0.12159500  -0.19450400
C  6.72644400  0.12743600  -0.64131000
C  7.07405300  -2.25266300  -0.94506500
H  5.46342300  -3.54173900  -0.48159600
H  7.71524500  -3.07764900  -1.23641100
H  8.56870800  -0.73698900  -1.38787400
C  6.05882300  2.28829200  0.12442700
C  8.41423300  3.53049600  -0.69598600
C  7.09016400  1.52768400  -0.53525900
C  6.18413900  3.64996000  0.26001100
C  7.37083500  4.27592100  -0.11639900
C  8.28334000  2.16627800  -0.90524800
H  5.37681600  4.23478800  0.70780200
H  7.49544200  5.34249700  0.03831400
H  9.09339700  1.59916900  -1.35329800
H  9.33253500  4.03207300  -0.98263200
S  4.68085300  1.31049700  0.43915600

ODBTCZ-S Geometry (Solvent: DCM)

H  1.60843800  -3.54773000  2.34732300
C  1.84353900  -2.72329000  1.68217100
C  2.45365500  -0.62172800  -0.03927700
C  0.84481000  -1.78781000  1.34731600
C  3.12165900  -2.60436800  1.15256100
C  3.45031300  -1.55769300  0.28117600
C  1.17477700  -0.72162100  0.48866300
C  3.88211000  -3.32971700  1.42765400
C  0.43649100  0.03543000  0.24720900
H  2.67791700  0.19310500  -0.72149400
C  -0.48773500  -1.90409000  1.93621900
C  -1.74012800  -1.35375000  1.40980200
C  -4.17063300  -0.34846600  0.43922100
C  -2.80102800  -1.06925600  2.29128200
C  -1.92973200  -1.15884400  0.02760700
C  -3.12368000  -0.63729800  -0.44588300
C  -4.00686800  -0.57906600  1.80676900
H  -2.67240900  -1.22396100  3.35701800
H  -1.14355100  -1.41821600  -0.67293100
H  -3.25346500  -0.45351400  -1.50792500
H  -4.82734800  -0.37560500  2.48787700
O  -0.59452400  -2.58876900  3.03222400
N  -5.39051300  0.17202900  -0.05201000
C  -6.02450800  1.23711400  0.40267800
C  -7.63048000  3.52896900  0.91135500
C  -5.61937200  2.23083700  1.38945200
C  -7.20971900  1.52386000  -0.34116300
C  -8.01833500  2.63412300  -0.07838000
C  -6.43972200  3.32740600  1.63108700
H  -4.69826700  2.08979400  1.94475500
H  -8.93218900  2.79453100  -0.64320800
H  -6.14977600  4.04418700  2.39286500
| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| H     | -8.24677300 | 4.39488700 | 1.12923500 |
| C     | -6.15376200 | -0.37734900 | -1.08023900 |
| C     | -8.01341600 | -1.07805300 | -3.01285000 |
| C     | -5.94122700 | -1.54941700 | -1.81225800 |
| C     | -7.29234300 | 0.43268700  | -1.29119900 |
| C     | -8.22602200 | 0.07672700  | -2.26929900 |
| C     | -6.88399300 | -1.88195100 | -2.77665800 |
| H     | -5.07948300 | -2.18305800 | -1.63173100 |
| H     | -9.10429800 | 0.69206400  | -2.44112200 |
| H     | -6.74332700 | -2.78595700 | -3.36289100 |
| C     | 5.81394300  | -1.46500900 | -0.29511300 |
| C     | 7.43687400  | -1.35372500 | -1.38077500 |
| C     | 5.43325700  | -2.59624300 | -3.83179300 |
| C     | 6.85037300  | -0.20137000 | -0.84363200 |
| C     | 6.72495900  | -2.54468400 | -1.37055500 |
| H     | 4.88466000  | -3.53363900 | -0.84440400 |
| H     | 7.16712900  | -3.44706000 | -1.78463700 |
| H     | 8.44074600  | -3.15367000 | -1.79263800 |
| C     | 6.54818500  | 2.02044600  | -0.84440200 |
| C     | 7.16712900  | -3.44706000 | -1.78463700 |
| C     | 8.44074600  | -3.15367000 | -1.79263800 |
| C     | 6.54818500  | 2.02044600  | -0.84440200 |
| H     | 4.88466000  | -3.53363900 | -0.84440400 |
| H     | 7.16712900  | -3.44706000 | -1.78463700 |
| H     | 8.44074600  | -3.15367000 | -1.79263800 |
| C     | 6.54818500  | 2.02044600  | -0.84440200 |
| C     | 7.16712900  | -3.44706000 | -1.78463700 |
| C     | 8.44074600  | -3.15367000 | -1.79263800 |
| C     | 6.54818500  | 2.02044600  | -0.84440200 |
| H     | 4.88466000  | -3.53363900 | -0.84440400 |

**C1-S6 Geometry (Solvent: THF)**

| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| H     | 2.50949000 | 0.86604400 | -0.28802000 |
| C     | 2.46896400 | -0.17767500 | 0.00901600 |
| C     | 2.34562300 | -2.88300600 | 0.68325400 |
| C     | 1.23047600 | -0.79084800 | 0.22159800 |
| C     | 3.64152600 | -9.10575000 | 0.17210700 |
| C     | 3.58138300 | -2.62657500 | 0.51425500 |
| C     | 1.16686600 | -2.14764300 | 0.55265800 |
| C     | 4.50305400 | -2.82362500 | 0.64890200 |
| C     | 0.20481500 | -2.63550400 | 0.68568000 |
| C     | 2.30032600 | -3.93788200 | 0.93156600 |
| C     | -0.01809000 | 0.03607100 | -0.00632000 |
| C     | -1.25611900 | -0.28296400 | 0.75038800 |
| C     | -3.64722400 | -0.70987400 | 2.12473700 |
| C     | -2.47602100 | 0.00419000  | 0.13226400 |
| C     | -1.23305600 | -0.79064100 | 2.05328200 |
| C     | -2.43062700 | -0.99817900 | 2.73598500 |
| C     | -3.66904400 | -0.21435500 | 0.81650600 |
| H     | -2.48696700 | 0.38809900  | -0.88343300 |
| H     | -0.28736300 | -0.99814600 | 2.54340900 |
| H     | -2.41576600 | -1.37220300 | 3.75400700 |
| O     | 0.01432100  | 0.95307700  | -0.80513200 |
| H     | -4.58269900 | -0.85269800 | 2.65697600 |
| N     | -4.90552800 | 0.07429900  | 0.19105800 |
| C     | -5.25476800 | 1.28875900  | -0.39677100 |
| C     | -6.42415400 | 3.47319900  | -1.63748900 |
| C     | -4.51900700 | 2.47403700  | -0.48430600 |
| C     | -6.56841800 | 1.19005700  | -0.90745100 |
| C     | -7.15329900 | 2.29463600  | -1.53504000 |
| C     | -5.12267700 | 3.55772000  | -1.11245500 |
| H     | -3.51599700 | 2.55203200  | -0.07815600 |
| H     | -8.16224300 | 2.23179900  | -1.93201100 |
| H     | -4.57346400 | 4.49066200  | -1.19705100 |
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| H    | -6.86189400 | 4.33909900 | -2.12296300 |
| C    | -5.97718900 | -0.80647800 | 0.06302700 |
| C    | -8.33290200 | -2.16491700 | -0.47190700 |
| C    | -7.03052900 | -0.15214000 | -0.61450500 |
| C    | -6.07888700 | -2.14178100 | 0.46373300 |
| C    | -7.26962000 | -2.80506100 | 0.18845800 |
| C    | -8.21809800 | -0.84126200 | -0.87962900 |
| H    | -5.26074900 | -2.64780800 | 0.96533100 |
| H    | -7.37662300 | -3.84247600 | 0.48923800 |
| H    | -9.03462400 | -0.34916800 | -1.39984900 |
| H    | -9.24780800 | -2.71378700 | -0.66871000 |
| N    | 4.89828900 | -0.28482200 | -0.01272300 |
| C    | 5.90474000 | -0.72307400 | -0.87017100 |
| C    | 8.16029300 | -1.15536200 | -2.42046300 |
| C    | 5.90531200 | -1.80730300 | -1.75234900 |
| C    | 7.00883700 | 0.15268600 | -0.76783400 |
| C    | 8.14584400 | -0.07143800 | -1.55073300 |
| C    | 7.04730600 | -2.00873400 | -2.51950900 |
| H    | 2.38928000 | 0.63419900 | -0.35335600 |
| C    | 2.44127500 | -0.41249500 | -0.06896000 |
| C    | 2.57734900 | -3.12131300 | 0.55651000 |
| C    | 1.25104600 | -1.14221400 | 0.06782400 |
| C    | 3.67478200 | -1.02149800 | 0.14465100 |
| C    | 3.75354500 | -2.37878100 | 0.46878800 |
| C    | 1.33947700 | -2.51215600 | 0.36346300 |
| C    | 4.72203800 | -2.83769900 | 0.64180200 |
| C    | 0.43762400 | -3.11526200 | 0.40910000 |
| C    | 2.62772000 | -4.18277900 | 0.77727100 |
| C    | -0.03497400 | -0.44120300 | -0.21981400 |
| C    | -1.24474900 | -0.79037800 | 0.47702200 |
| C    | -3.75285300 | -1.41404500 | 1.75144100 |
| C    | -2.45714000 | -0.23541800 | 0.00650100 |
| C    | -1.33317500 | -1.60315700 | 1.67111500 |
| C    | -2.54932800 | -1.89494900 | 2.26868900 |
| C    | -3.67325700 | -0.54993400 | 0.61088500 |
| C    | -2.43033100 | 0.36753800 | -0.89558800 |
| C    | -0.42452100 | -1.96529600 | 2.13839300 |
| C    | -2.56352900 | -2.48512300 | 3.17940800 |
| O    | -0.03037600 | 0.48783000 | -1.08518200 |
| H    | -4.69443500 | -1.55777900 | 2.26575300 |
| N    | -4.84642200 | 0.00726900 | 0.12050800 |
| C    | -5.01346300 | 1.33782700 | -0.30983700 |
| C    | -5.87343600 | 3.82160700 | -1.14339000 |
| C    | -4.09977700 | 2.39179900 | -0.28409200 |
| C    | -6.35714200 | 1.52090400 | -0.69847700 |
| C    | -6.79301700 | 2.76644200 | -1.12177000 |
| C    | -4.55296200 | 3.63572200 | -0.72273800 |
| C    | -3.08424500 | 2.26451900 | 0.06994600 |
| C    | -7.82447800 | 2.92446600 | -1.41893000 |
| C    | -3.86535000 | 4.47400100 | -0.72685900 |
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| H    | -6.194713 | 4.802979 | -1.475348 |
| C    | -6.075723 | -0.662646 | -0.008532 |
| C    | -8.640437 | -1.534284 | -0.515475 |
| C    | -7.035725 | 0.241001 | -0.509007 |
| C    | -6.359421 | -2.015172 | 0.184199 |
| C    | -7.668059 | -2.430461 | -0.060632 |
| H    | -5.597028 | -2.721854 | 0.488596 |
| H    | -7.927078 | -3.472708 | 0.088498 |
| H    | -9.077879 | 0.486672 | -1.150516 |
| H    | -9.647076 | -1.809974 | -0.705098 |
| N    | 4.867462 | -0.256923 | 0.029314 |
| C    | 5.942944 | -0.553405 | -0.800376 |
| C    | 8.288447 | -0.937610 | -2.271854 |
| C    | 6.090501 | -1.599336 | -1.716801 |
| C    | 6.946672 | 0.426893 | -0.624568 |
| C    | 8.129036 | 0.349819 | -1.368140 |
| C    | 7.274398 | -1.653449 | -2.443254 |
| H    | 5.309068 | -2.338260 | -1.859612 |
| H    | 8.907225 | 1.097143 | -1.242370 |
| H    | 7.416053 | -2.458010 | -3.161900 |
| H    | 9.199760 | -0.768822 | -2.855930 |
| C    | 5.161715 | 0.990612 | 0.739519 |
| C    | 6.216909 | 3.181454 | 1.912753 |
| C    | 6.445784 | 1.359390 | 0.364104 |
| C    | 4.400137 | 1.563645 | 1.707652 |
| C    | 4.964080 | 2.705411 | 2.282860 |
| C    | 6.972032 | 2.512112 | 0.957374 |
| H    | 3.420010 | 1.201119 | 1.998937 |
| H    | 4.375760 | 3.240636 | 3.035645 |
| H    | 7.956700 | 2.874383 | 0.676323 |
| H    | 6.609386 | 4.077873 | 2.381446 |

C1-S1 Geometry (Solvent: THF)

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| H    | 2.485233 | 0.781082 | -0.175411 |
| C    | 2.472205 | -0.250156 | 0.162386 |
| C    | 2.472646 | -2.909451 | 1.000114 |
| C    | 1.254991 | -0.889340 | 0.459702 |
| C    | 3.673476 | -0.941063 | 0.310257 |
| C    | 3.685187 | -2.269702 | 0.739011 |
| C    | 1.264012 | -2.238735 | 0.861783 |
| H    | 4.630111 | -2.787680 | 0.866099 |
| H    | 0.331677 | -2.761979 | 1.041393 |
| H    | 2.471341 | -3.947026 | 1.317738 |
| C    | -0.000089 | -0.158062 | 0.268118 |
| C    | -1.291719 | -0.453370 | 0.903095 |
| C    | -3.781635 | -0.951236 | 2.097672 |
| C    | -2.478202 | -0.081611 | 0.248084 |
| C    | -1.361793 | -1.065047 | 2.169140 |
| C    | -2.600762 | -1.323470 | 2.741885 |
| C    | -3.710372 | -0.327577 | 0.850772 |
| H    | -2.444409 | 0.368570 | -0.738800 |
| H    | -0.453301 | -1.312248 | 2.706815 |
| H    | -2.648126 | -1.794853 | 3.718075 |
| O    | 0.020184 | 0.844759 | -0.547661 |
| H    | -4.748242 | -1.124176 | 2.559536 |
| N    | -4.899603 | 0.055614 | 0.182345 |
| C    | -5.193477 | 1.334611 | -0.284010 |
| C    | -6.248003 | 3.668534 | -1.341728 |
| C    | -4.441018 | 2.508203 | -0.181630 |
| C    | -6.467991 | 1.319304 | -0.894272 |
| C    | -6.994632 | 2.499642 | -1.428612 |
| C    | -4.986802 | 3.668130 | -0.720109 |
| H    | -3.469545 | 2.518089 | 0.301322 |
| H    | -7.972966 | 2.501271 | -1.900182 |
| H    | -4.424039 | 4.594069 | -0.656452 |
H  -6.64097500  4.59261600  -1.75250500
C  -5.96684600  -0.78526300  -0.12214000
C  -8.29114300  -2.03204800  -0.97214400
C  -6.96284800  -0.03920000  -0.79211800
C  -6.10978000  -2.15530300   0.11578200
C  -7.28402000  -2.76177800  -0.31622900
C  -8.13514000  -0.67284800  -1.21655800
H  -5.33426000  -2.72740200   0.61403600
H  -7.42273400  -3.82445200  -0.14399400
H  -8.90808100  -0.11085700  -1.73259400
H  -9.19489600  -2.53881900  -1.29388000
N   4.89277600  -0.28152800   0.01776900
C   5.85902500  -0.72748100  -0.88055900
C   8.02467700  -1.15809100  -2.55294000
C   5.85044600  -1.86173800  -1.69737300
C   6.92687100   0.19766400  -0.90384200
C   8.01889200  -0.02566700  -1.74816000
C   6.94720700  -2.06937000  -2.52855500
H   5.01930100  -2.55891300  -1.68916000
H   8.84605300  -0.77627000  -1.77529600
H   6.96187700  -2.93371900  -3.17349000
H   8.86455100  -1.34698800  -3.21453600
C   5.32310700   0.92065300  -0.57385300
C   6.62358900   3.22490700   1.39996000
C   6.58413800   1.25290200   0.02902200
C   4.70710900   1.71932900   1.54171200
C   5.37479100   2.87193300   1.94115900
C   7.23509600   2.41742500   0.44742400
H   3.74680200   1.45162500   1.96959100
H   4.91915300   3.51214600   2.68988100
H   8.20429400   2.68362000   0.03598900
H   7.11405700   4.13221800   1.73435300

C2-S$_6$ Geometry (Solvent: THF)

H   -2.32107100  -0.43566400  -1.07671300
C   -2.33301700   0.01066000  -0.07775500
C   -2.37140300   1.11718000   2.47811500
C   -1.13278200   0.20156500   0.61158500
C   -3.54005200   0.31996800   0.52214600
C   -3.56488500   0.88638400   1.80503000
C   -1.15550400   0.76865500  -1.88982100
H   -4.52030500   1.14316000   2.24900300
H   -0.22687300   0.95565000   2.41900300
H   -2.38576600  -1.56853500   3.46415700
C   -0.14781300  -0.12659300  -0.09233200
C   -1.34543000  -0.55242100   0.70077600
C   -3.63817000  -1.40742200   2.04791000
C   -2.61013600  -0.26509100   1.80784000
C   -1.23185700  -1.27789200   1.89311100
C   -2.37662100  -1.71013500   2.55871300
C   -3.74988800  -0.68462600   0.86077400
H   -2.70034900   0.28515300  -0.75200200
H   -0.25202600  -1.52570600   2.28898500
H   -2.28659100  -2.28403100   3.47463700
O   -0.22687300   0.95565000   2.41900300
H   -0.21592900  -0.04828000  -1.30795800
H   -4.54213500  -1.72733600   2.55678900
N   -5.04945800  -0.37958800   0.34610600
N   -4.76338600   0.08140900  -0.18108500
C   -5.57273500   0.91130600   0.55776600
C   -6.74101700   3.43086100   0.94693500
C   -4.95317700   1.86279600   1.36997000
C   -6.78909400   1.24954100  -0.05496800
C   -7.36467500   2.49528800   0.12555000
C   -5.53921500   3.11579400   1.56698100
H   -4.01524900   1.62096000   1.85742900
| Atoms | Coordinates |
|-------|-------------|
| H     | 8.30480900  2.70663000 -0.37326500 |
| H     | 5.04304700  3.83594400  2.20891500 |
| H     | 7.19731100  4.41052300  1.09546900 |
| C     | 5.52634800  -1.10339300 -0.76530600 |
| C     | 6.60632900  -2.49994100 -2.95259700 |
| C     | 7.19731100  -1.10339300 -0.76530600 |
| C     | 4.86231200  -2.90458300 -2.38356300 |
| H     | 8.21822200  -1.04645200 -2.84013400 |
| H     | 7.02795300  -3.05975000 -3.79571000 |
| O     | 7.47659100  0.32936100 -0.81809500 |
| C     | -5.55416300 -1.02100300 0.20051700 |
| C     | -7.20048600 -3.20654900 0.84655400 |
| C     | -6.82670900 -1.16479400 -0.37329200 |
| C     | -5.12118800 -1.99511700 1.10213800 |
| C     | -5.93888300 -3.08306000 1.41727200 |
| C     | -7.64528300 -2.23396300 -0.05238300 |
| H     | -4.13826800 -1.90889300 1.55183900 |
| H     | -5.57697200 -3.83137900 2.11462200 |
| H     | -8.62093200 -2.96030300 -0.52312400 |
| C     | -7.83864600 -4.04878300 1.09015200 |
| C     | -5.41734600 1.17583800 -0.78283200 |
| C     | -6.79725200 3.27087400 -2.05096400 |
| C     | -4.84403400 2.44452100 -0.88518900 |
| C     | -6.69347800 0.97610300 -1.33100400 |
| C     | -7.38168900 2.00610000 -1.94868300 |
| C     | -5.52945900 3.48266600 -1.52104900 |
| H     | -3.85476100 2.61922100 -0.47706500 |
| H     | -8.36658600 1.79842300 -2.35392500 |
| H     | -5.05948800 4.48754300 -1.59567000 |
| H     | -7.32839300 4.07488600 -2.54355200 |
| O     | -7.28351800 -0.27030100 -1.31787900 |

**C2-T1 Geometry (Solvent: THF)**

| Atoms | Coordinates |
|-------|-------------|
| H     | 2.28318100  -0.23438800 0.92621700 |
| C     | 2.37561900  0.22039100 -0.05485500 |
| C     | 2.63636400  1.43685100 -2.54447500 |
| C     | 1.20938500  0.56441500 -0.76738600 |
| C     | 3.63218300  0.45449800 -0.59252600 |
| C     | 3.78115200  1.06053800 -1.84353100 |
| C     | 1.36967000  1.19397800 -2.01601000 |
| H     | 4.77568100  1.23977600 -2.24212900 |
| H     | 0.49686300  1.53427000 -2.56400600 |
| H     | 2.73103300  1.93540000 -3.50451100 |
| C     | -0.09976400 0.32759900 -0.11067400 |
| C     | -1.29523300 0.05475900 -0.87888600 |
| C     | -3.76355200 -0.56740100 -2.20927100 |
| C     | -2.54023500 0.07315100 -0.18520000 |
| C     | -1.34241400 -0.32624900 -2.25387600 |
| C     | -2.53497700 -0.62319200 -2.89056200 |
| C     | -3.70794100 -0.22182100 -0.85714700 |
| H     | -2.55273300 0.32592500 0.86980500 |
| H     | -0.41946000 -0.42970600 -2.81331300 |
| H     | -2.52048400 -0.92129600 -3.93461900 |
| O     | -0.14880400 0.35173200 1.16330900 |
| H     | -4.70811600 -0.79598500 -2.68996100 |
| N     | -4.95345000 -0.17367500 -0.11418400 |
| N     | 4.79668700  0.06381700 0.15167900 |
| C     | -5.72203300 0.97149400 -0.13727600 |
| C     | -7.35605600 3.24040400 -0.11152000 |
| C     | -5.33278000 2.12520900 -0.84904900 |
| C     | -6.93666600 0.99145000 0.58256400 |
| C     | -7.75322500 2.12066200 0.59628100 |
C   -6.14491100  3.23956300  -0.83156200
H   -4.39792500  2.11815300  -1.39644000
H   -8.67628700  2.08990400  1.16364200
H   -5.84336700  4.12594000  -1.37766200
H   -7.98151000  4.12584600  -0.10838600
C   -5.36786200  -1.27552600  0.60478900
C   -6.30441500  -3.44782700  2.09510600
C   -6.58441000  -1.20703500  1.31217100
C   -4.61786500  -2.46903500  0.65331200
C   -5.08687400  -3.53533300  1.39109200
C   -7.05658800  -2.28804400  2.05657600
H   -3.68087100  -2.52733300  0.11271400
H   -4.50784400  -4.45073700  1.42919800
H   -7.99763100  -2.18900800  2.58524400
H   -6.65643400  -4.29565200  2.67175200
O   -7.34900600  -0.08740100  1.28866400
C   5.47646700  -1.10701600  -0.22672500
C   6.89900700  -3.44608000  -0.87716000
C   6.69924400  -1.41024000  0.39341100
C   4.97955900  -2.00197400  -1.17709000
C   5.68489700  -3.16554200  -1.49396000
C   7.40806900  -2.55459900  0.07112300
H   4.03340000  -1.78931900  -1.66208600
H   5.27327600  -3.84835500  -2.22986100
H   8.34899500  -2.73865700  0.57944700
H   7.45045300  -4.34715700  -1.12234100
C   5.52939200  1.05315200  0.83070100
C   7.05477600  2.94255400  2.25138600
C   5.08601100  2.37083100  0.96421400
C   6.75067800  0.70079500  1.42674000
C   7.51013500  1.62792000  2.11922100
C   5.84257000  3.05656500  1.67515800
H   4.14075500  2.65989700  0.51855200
H   8.44740300  1.30216400  2.55859500
H   5.47190300  4.32075300  1.77188200
H   7.64550100  3.66619600  2.80233600
O   7.21050900  -0.59964500  1.38588300