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Supporting Information

# Decomposition analysis on the excitation behaviors of thiazolothiazole (TTz)-based dyes via the time-dependent dielectric density functional theory approach

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**Table S1. Absorption spectra changes according to basis sets. Here, the results of Eq. (2) are obtained by using the same dielectric constants described in the manuscript.**

| | 3-21G | 6-31G | 6-31G* |
|---|---|---|---|
| **B3LYP** | | | |
| $Bu_2N$-TTz-Py in toluene | 2.62 | 2.56 | 2.67 |
| $Bu_2N$-TTz-Py in chloroform | 2.58 | 2.53 | 2.64 |
| $Bu_2N$-TTz-Py in DCM | 2.57 | 2.51 | 2.62 |
| $Bu_2N$-TTz-Py in methanol | 2.56 | 2.50 | 2.62 |
| $Ph_2N$-TTz-Py in toluene | 2.52 | 2.43 | 2.55 |
| $Ph_2N$-TTz-Py in chloroform | 2.50 | 2.41 | 2.53 |
| $Ph_2N$-TTz-Py in DCM | 2.49 | 2.40 | 2.52 |
| $Ph_2N$-TTz-Py in methanol | 2.50 | 2.40 | 2.53 |
| $Ph_2N$-TTz-CHO in toluene | 2.36 | 2.25 | 2.36 |
| $Ph_2N$-TTz-CHO in chloroform | 2.35 | 2.22 | 2.35 |
| $Ph_2N$-TTz-CHO in DCM | 2.35 | 2.22 | 2.34 |
| $Ph_2N$-TTz-CHO in methanol | 2.35 | 2.22 | 2.34 |
| $Ph_2N$-TTz-COOH in toluene | 2.45 | 2.33 | 2.46 |
| $Ph_2N$-TTz-COOH in chloroform | 2.44 | 2.31 | 2.45 |
| $Ph_2N$-TTz-COOH in DCM | 2.43 | 2.30 | 2.44 |
| $Ph_2N$-TTz-COOH in methanol | 2.44 | 2.30 | 2.44 |
| **HandH** | | | |
| $Bu_2N$-TTz-Py in toluene | 3.32 | 3.26 | 3.37 |
| $Bu_2N$-TTz-Py in chloroform | 3.30 | 3.23 | 3.35 |
| $Bu_2N$-TTz-Py in DCM | 3.29 | 3.22 | 3.34 |
| $Bu_2N$-TTz-Py in methanol | 3.29 | 3.22 | 3.35 |
| $Ph_2N$-TTz-Py in toluene | 3.26 | 3.19 | 3.29 |
| $Ph_2N$-TTz-Py in chloroform | 3.25 | 3.18 | 3.29 |
| $Ph_2N$-TTz-Py in DCM | 3.25 | 3.17 | 3.29 |
| $Ph_2N$-TTz-Py in methanol | 3.26 | 3.18 | 3.30 |

| | | | |
|---|---|---|---|
| $Ph_2N$-TTz-CHO in toluene | 3.18 | 3.08 | 3.19 |
| $Ph_2N$-TTz-CHO in chloroform | 3.17 | 3.08 | 3.19 |
| $Ph_2N$-TTz-CHO in DCM | 3.17 | 3.07 | 3.18 |
| $Ph_2N$-TTz-CHO in methanol | 3.18 | 3.08 | 3.20 |
| $Ph_2N$-TTz-COOH in toluene | 3.22 | 3.12 | 3.23 |
| $Ph_2N$-TTz-COOH in chloroform | 3.21 | 3.12 | 3.23 |
| $Ph_2N$-TTz-COOH in DCM | 3.21 | 3.11 | 3.23 |
| $Ph_2N$-TTz-COOH in methanol | 3.22 | 3.12 | 3.24 |
| **Eq. (2)** | | | |
| $Bu_2N$-TTz-Py in toluene | 3.02 | 2.94 | 3.06 |
| $Bu_2N$-TTz-Py in chloroform | 3.00 | 2.92 | 3.04 |
| $Bu_2N$-TTz-Py in DCM | 2.98 | 2.90 | 3.03 |
| $Bu_2N$-TTz-Py in methanol | 2.98 | 2.90 | 3.04 |
| $Ph_2N$-TTz-Py in toluene | 2.94 | 2.84 | 2.96 |
| $Ph_2N$-TTz-Py in chloroform | 2.93 | 2.83 | 2.95 |
| $Ph_2N$-TTz-Py in DCM | 2.93 | 2.82 | 2.96 |
| $Ph_2N$-TTz-Py in methanol | 2.94 | 2.83 | 2.97 |
| $Ph_2N$-TTz-CHO in toluene | 2.82 | 2.70 | 2.84 |
| $Ph_2N$-TTz-CHO in chloroform | 2.82 | 2.69 | 2.83 |
| $Ph_2N$-TTz-CHO in DCM | 2.82 | 2.69 | 2.83 |
| $Ph_2N$-TTz-CHO in methanol | 2.83 | 2.70 | 2.85 |
| $Ph_2N$-TTz-COOH in toluene | 2.88 | 2.76 | 2.91 |
| $Ph_2N$-TTz-COOH in chloroform | 2.87 | 2.75 | 2.90 |
| $Ph_2N$-TTz-COOH in DCM | 2.87 | 2.74 | 2.90 |
| $Ph_2N$-TTz-COOH in methanol | 2.88 | 2.75 | 2.91 |

**Table S2. Emission spectra changes according to basis sets. Here, the results of Eq. (2) are obtained by using the same dielectric constants described in the manuscript.**

| | 3-21G | 6-31G | 6-31G* |
|---|---|---|---|
| **B3LYP** | | | |
| $Bu_2N$-TTz-Py in toluene | 2.43 | 2.38 | 2.46 |
| $Bu_2N$-TTz-Py in chloroform | 2.32 | 2.28 | 2.35 |
| $Bu_2N$-TTz-Py in DCM | 2.26 | 2.22 | 2.29 |
| $Bu_2N$-TTz-Py in methanol | 2.21 | 2.16 | 2.24 |
| $Ph_2N$-TTz-Py in toluene | 1.87 | 1.84 | 2.07 |
| $Ph_2N$-TTz-Py in chloroform | 1.93 | 1.92 | 2.13 |
| $Ph_2N$-TTz-Py in DCM | 1.99 | 1.95 | 2.11 |
| $Ph_2N$-TTz-Py in methanol | 2.00 | 1.95 | 2.09 |
| $Ph_2N$-TTz-CHO in toluene | 1.82 | 1.78 | 2.02 |
| $Ph_2N$-TTz-CHO in chloroform | 1.93 | 1.85 | 2.01 |
| $Ph_2N$-TTz-CHO in DCM | 1.94 | 1.84 | 1.98 |
| $Ph_2N$-TTz-CHO in methanol | 1.92 | 1.82 | 1.95 |
| $Ph_2N$-TTz-COOH in toluene | 1.88 | 1.83 | 2.09 |
| $Ph_2N$-TTz-COOH in chloroform | 1.99 | 1.90 | 2.08 |
| $Ph_2N$-TTz-COOH in DCM | 2.00 | 1.90 | 2.05 |
| $Ph_2N$-TTz-COOH in methanol | 1.98 | 1.88 | 2.02 |
| **HandH** | | | |
| $Bu_2N$-TTz-Py in toluene | 2.80 | 2.77 | 2.82 |
| $Bu_2N$-TTz-Py in chloroform | 2.68 | 2.65 | 2.71 |
| $Bu_2N$-TTz-Py in DCM | 2.61 | 2.58 | 2.64 |
| $Bu_2N$-TTz-Py in methanol | 2.55 | 2.52 | 2.59 |
| $Ph_2N$-TTz-Py in toluene | 2.74 | 2.70 | 2.75 |
| $Ph_2N$-TTz-Py in chloroform | 2.64 | 2.60 | 2.66 |
| $Ph_2N$-TTz-Py in DCM | 2.58 | 2.54 | 2.60 |
| $Ph_2N$-TTz-Py in methanol | 2.53 | 2.49 | 2.55 |

| | | | |
|---|---|---|---|
| $Ph_2N$-TTz-CHO in toluene | 2.62 | 2.57 | 2.63 |
| $Ph_2N$-TTz-CHO in chloroform | 2.52 | 2.47 | 2.53 |
| $Ph_2N$-TTz-CHO in DCM | 2.47 | 2.42 | 2.47 |
| $Ph_2N$-TTz-CHO in methanol | 2.42 | 2.36 | 2.42 |
| $Ph_2N$-TTz-COOH in toluene | 2.66 | 2.61 | 2.67 |
| $Ph_2N$-TTz-COOH in chloroform | 2.56 | 2.51 | 2.57 |
| $Ph_2N$-TTz-COOH in DCM | 2.51 | 2.45 | 2.52 |
| $Ph_2N$-TTz-COOH in methanol | 2.46 | 2.40 | 2.47 |
| **Eq. (2)** | | | |
| $Bu_2N$-TTz-Py in toluene | 2.49 | 2.47 | 2.53 |
| $Bu_2N$-TTz-Py in chloroform | 2.37 | 2.36 | 2.42 |
| $Bu_2N$-TTz-Py in DCM | 2.31 | 2.29 | 2.35 |
| $Bu_2N$-TTz-Py in methanol | 2.24 | 2.23 | 2.29 |
| $Ph_2N$-TTz-Py in toluene | 2.41 | 2.38 | 2.44 |
| $Ph_2N$-TTz-Py in chloroform | 2.31 | 2.28 | 2.34 |
| $Ph_2N$-TTz-Py in DCM | 2.25 | 2.22 | 2.29 |
| $Ph_2N$-TTz-Py in methanol | 2.20 | 2.17 | 2.23 |
| $Ph_2N$-TTz-CHO in toluene | 2.30 | 2.25 | 2.32 |
| $Ph_2N$-TTz-CHO in chloroform | 2.20 | 2.15 | 2.21 |
| $Ph_2N$-TTz-CHO in DCM | 2.14 | 2.09 | 2.16 |
| $Ph_2N$-TTz-CHO in methanol | 2.08 | 2.04 | 2.10 |
| $Ph_2N$-TTz-COOH in toluene | 2.33 | 2.29 | 2.35 |
| $Ph_2N$-TTz-COOH in chloroform | 2.23 | 2.19 | 2.26 |
| $Ph_2N$-TTz-COOH in DCM | 2.17 | 2.13 | 2.20 |
| $Ph_2N$-TTz-COOH in methanol | 2.12 | 2.08 | 2.15 |

**Table S3. Dipole moment [debye] of asymmetric TTz dyes in the ground and excited states calculated by the dielectric-dependent density functional theory (DFT) method using Eq. (2).**

| | toluene | chloroform | dichloromethane | methanol |
|---|---|---|---|---|
| **Ground-state** | | | | |
| Bu2N-TTz-Py | 8.78 | 9.58 | 9.85 | 10.1 |
| Ph2N-TTz-Py | 6.23 | 6.62 | 6.78 | 6.93 |
| Ph2N-TTz-CHO | 6.88 | 7.18 | 7.34 | 7.51 |
| Ph2N-TTz-COOH | 4.86 | 5.13 | 5.28 | 5.44 |
| **Excited-state** | | | | |
| Bu2N-TTz-Py | 18.70 | 21.12 | 22.68 | 24.10 |
| Ph2N-TTz-Py | 17.14 | 18.86 | 19.91 | 20.91 |
| Ph2N-TTz-CHO | 20.77 | 22.81 | 24.04 | 25.24 |
| Ph2N-TTz-COOH | 16.89 | 18.62 | 19.66 | 20.64 |

**Table S4. Charge distributions in the asymmetric TTz dyes in the ground and excited states.**

| | ground-state | | | excited-state | | |
|---|---|---|---|---|---|---|
| | Acceptor | TTz-core | Donor | Acceptor | TTz-core | Donor |
| **$Bu_2N$-TTz-Py** | | | | | | |
| toluene | 0.009 | -0.106 | 0.096 | -0.246 | 0.032 | 0.214 |
| chloroform | -0.002 | -0.120 | 0.122 | -0.277 | 0.039 | 0.239 |
| dichloromethane | 0.024 | -0.126 | 0.102 | -0.299 | 0.044 | 0.255 |
| methanol | 0.016 | -0.128 | 0.113 | -0.317 | 0.041 | 0.276 |
| **$Ph_2N$-TTz-Py** | | | | | | |
| toluene | 0.007 | -0.102 | 0.095 | -0.230 | 0.046 | 0.185 |
| chloroform | 0.008 | -0.112 | 0.105 | -0.254 | 0.038 | 0.216 |
| dichloromethane | 0.044 | -0.157 | 0.114 | -0.269 | 0.034 | 0.235 |
| methanol | 0.042 | -0.168 | 0.126 | -0.284 | 0.031 | 0.252 |
| **$Ph_2N$-TTz-CHO** | | | | | | |
| toluene | -0.005 | -0.087 | 0.092 | -0.330 | 0.143 | 0.186 |
| chloroform | 0.031 | -0.134 | 0.102 | -0.357 | 0.139 | 0.218 |
| dichloromethane | 0.037 | -0.144 | 0.107 | -0.375 | 0.138 | 0.237 |
| methanol | 0.046 | -0.161 | 0.116 | -0.393 | 0.137 | 0.255 |
| **$Ph_2N$-TTz-COOH** | | | | | | |
| toluene | 0.003 | -0.086 | 0.083 | -0.301 | 0.133 | 0.168 |
| chloroform | 0.038 | -0.137 | 0.099 | -0.323 | 0.124 | 0.199 |
| dichloromethane | 0.046 | -0.153 | 0.107 | -0.337 | 0.119 | 0.218 |
| methanol | 0.052 | -0.173 | 0.121 | -0.351 | 0.116 | 0.236 |

**Table S5. Major contributions (configurational interaction (CI) coefficients) of electronic transition for photon absorption.**

| | toluene | chloroform | dichloromethane | methanol |
|---|---|---|---|---|
| **$Bu_2N$-TTz-Py** | | | | |
| H → L | 0.67 | 0.67 | 0.66 | 0.67 |
| H-1 → L | -0.13 | -0.12 | -0.12 | -0.12 |
| **$Ph_2N$-TTz-Py** | | | | |
| H → L | 0.66 | 0.66 | 0.66 | 0.66 |
| H-1 → L | 0.15 | 0.15 | 0.15 | 0.14 |
| **$Ph_2N$-TTz-CHO** | | | | |
| H → L | 0.65 | 0.65 | 0.65 | 0.65 |
| H-1 → L | -0.17 | -0.17 | -0.16 | -0.16 |
| **$Ph_2N$-TTz-COOH** | | | | |
| H → L | 0.65 | 0.65 | 0.65 | 0.65 |
| H-1 → L | 0.16 | -0.16 | -0.16 | -0.16 |

* HOMO=H, HOMO-1=H-1, LUMO=L

**Table S6. Major contributions (CI coefficients) of electronic transition for photon emission.**

| | toluene | chloroform | dichloromethane | methanol |
|---|---|---|---|---|
| **$Bu_2N$-TTz-Py** | | | | |
| H → L | 0.69 | 0.69 | 0.69 | 0.69 |
| **$Ph_2N$-TTz-Py** | | | | |
| H → L | 0.69 | 0.69 | 0.69 | 0.69 |
| **$Ph_2N$-TTz-CHO** | | | | |
| H → L | 0.69 | 0.69 | 0.69 | 0.69 |
| **$Ph_2N$-TTz-COOH** | | | | |
| H → L | 0.69 | 0.69 | 0.69 | 0.69 |

* HOMO=H, LUMO=L

**Table S7. Contributions [eV] of geometrical changes and solvent reorientation effect to the Stokes shift [eV] of asymmetric TTz dyes.**

| | geometrical change | solvent reorientation | Stokes shift |
|---|---|---|---|
| **$Bu_2N$-TTz-Py** | | | |
| toluene | 0.56 | 0.01 | 0.57 |
| chloroform | 0.57 | 0.09 | 0.65 |
| dichloromethane | 0.59 | 0.13 | 0.72 |
| methanol | 0.60 | 0.19 | 0.79 |
| **$Ph_2N$-TTz-Py** | | | |
| toluene | 0.54 | 0.01 | 0.54 |
| chloroform | 0.56 | 0.07 | 0.64 |
| dichloromethane | 0.60 | 0.11 | 0.71 |
| methanol | 0.64 | 0.16 | 0.80 |
| **$Ph_2N$-TTz-CHO** | | | |
| toluene | 0.55 | 0.01 | 0.56 |
| chloroform | 0.60 | 0.08 | 0.67 |
| dichloromethane | 0.62 | 0.12 | 0.74 |
| methanol | 0.64 | 0.17 | 0.81 |
| **$Ph_2N$-TTz-COOH** | | | |
| toluene | 0.59 | 0.01 | 0.60 |
| chloroform | 0.63 | 0.07 | 0.70 |
| dichloromethane | 0.65 | 0.11 | 0.76 |
| methanol | 0.67 | 0.16 | 0.84 |

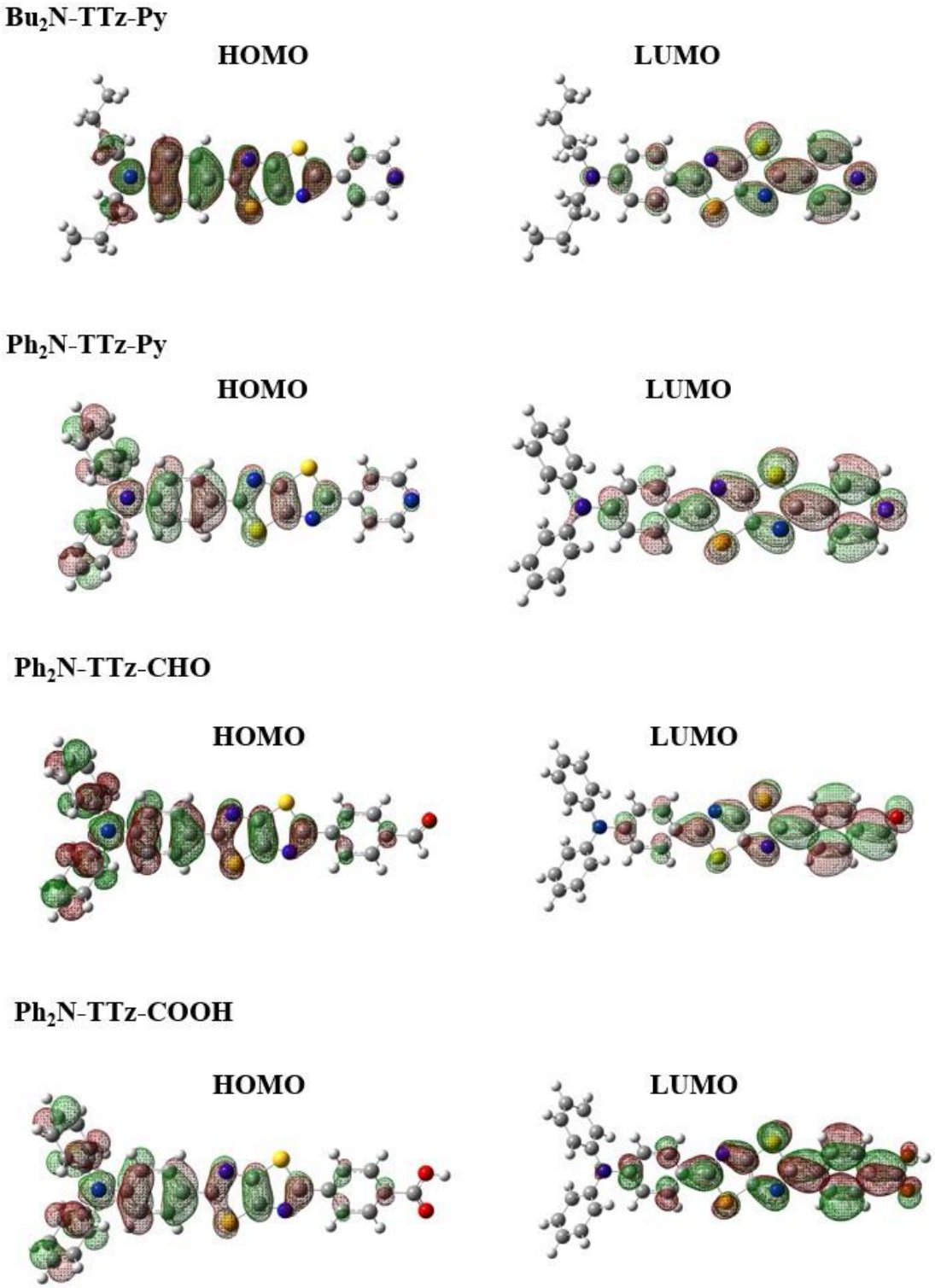


**Figure S1. HOMO and LUMO shapes of TTz-based dyes calculated from the dielectric DFT method of Eq. (2). These are obtained by the ground-state optimized structure in DCM.**

We show XYZ coordinates of asymmetric TTz dyes for absorption cases. These coordinates are obtained based on the dielectric DFT method of Eq. (2) with the 6-31+G* basis set.

### $Bu_2N$-TTz-Py in absorption state

| **toluene** | | | | **chloroform** | | | |
|---|---|---|---|---|---|---|---|
| **C** | -3.2479 | -0.7372 | -0.0152 | **C** | -3.2400 | -0.7477 | -0.0094 |
| **C** | -2.8983 | 0.6194 | -0.0760 | **C** | -2.8924 | 0.6047 | -0.1442 |
| **S** | -4.3920 | 1.6034 | -0.0586 | **S** | -4.3833 | 1.5904 | -0.1431 |
| **C** | -5.3332 | 0.0238 | 0.0422 | **C** | -5.3244 | 0.0200 | 0.0432 |
| **N** | -4.5863 | -1.0706 | 0.0462 | **N** | -4.5774 | -1.0749 | 0.0913 |
| **S** | -1.7485 | -1.7222 | -0.0358 | **S** | -1.7399 | -1.7323 | 0.0004 |
| **C** | -0.8057 | -0.1302 | -0.1526 | **C** | -0.7986 | -0.1489 | -0.2061 |
| **N** | -1.5615 | 0.9624 | -0.1547 | **N** | -1.5571 | 0.9426 | -0.2570 |
| **C** | -6.8408 | -0.0003 | 0.0937 | **C** | -6.8314 | 0.0005 | 0.1174 |
| **C** | 0.6909 | -0.1159 | -0.2131 | **C** | 0.6969 | -0.1316 | -0.2809 |
| **C** | -7.5511 | -1.2233 | -0.1589 | **C** | -7.5462 | -1.2352 | -0.0487 |
| **C** | -8.9750 | -1.2123 | -0.1007 | **C** | -8.9692 | -1.2198 | 0.0305 |
| **N** | -9.7228 | -0.1067 | 0.1776 | **N** | -9.7125 | -0.0974 | 0.2515 |
| **C** | -9.0462 | 1.0491 | 0.4163 | **C** | -9.0320 | 1.0711 | 0.4080 |
| **C** | -7.6235 | 1.1635 | 0.3920 | **C** | -7.6098 | 1.1816 | 0.3555 |
| **C** | 1.4120 | 1.1061 | 0.0366 | **C** | 1.4116 | 1.1034 | -0.0788 |
| **C** | 2.8280 | 1.1554 | -0.0125 | **C** | 2.8265 | 1.1583 | -0.1282 |
| **C** | 3.6243 | -0.0208 | -0.3315 | **C** | 3.6335 | -0.0230 | -0.3977 |
| **C** | 2.8876 | -1.2511 | -0.5623 | **C** | 2.9028 | -1.2665 | -0.5888 |
| **C** | 1.4675 | -1.2861 | -0.5087 | **C** | 1.4828 | -1.3070 | -0.5343 |
| **N** | 5.0298 | 0.0365 | -0.3909 | **N** | 5.0354 | 0.0434 | -0.4509 |
| **C** | 5.7350 | 1.3337 | -0.6488 | **C** | 5.7476 | 1.3516 | -0.6270 |
| **C** | 5.8464 | -1.2104 | -0.5243 | **C** | 5.8633 | -1.2005 | -0.5538 |
| **C** | 6.4411 | 1.9455 | 0.6240 | **C** | 6.3543 | 1.9467 | 0.7049 |
| **C** | 7.2553 | 3.2680 | 0.3326 | **C** | 7.1835 | 3.2745 | 0.4893 |
| **C** | 6.3721 | 4.5266 | -0.0237 | **C** | 6.3271 | 4.5318 | 0.0696 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | 5.9484 | -2.0599 | 0.8056 | **C** | 5.9631 | -2.0217 | 0.7949 |
| **C** | 6.6570 | -3.4587 | 0.6151 | **C** | 6.6583 | -3.4307 | 0.6356 |
| **C** | 8.1820 | -3.3825 | 0.2164 | **C** | 8.1838 | -3.3786 | 0.2360 |
| **H** | -7.0025 | -2.1645 | -0.3999 | **H** | -7.0033 | -2.1909 | -0.2411 |
| **H** | -9.5481 | -2.1536 | -0.2952 | **H** | -9.5441 | -2.1714 | -0.0966 |
| **H** | -9.6731 | 1.9466 | 0.6481 | **H** | -9.6540 | 1.9826 | 0.5938 |
| **H** | -7.1525 | 2.1516 | 0.6201 | **H** | -7.1382 | 2.1820 | 0.5180 |
| **H** | 0.8465 | 2.0337 | 0.2960 | **H** | 0.8422 | 2.0386 | 0.1424 |
| **H** | 3.3232 | 2.1228 | 0.2373 | **H** | 3.3170 | 2.1344 | 0.0805 |
| **H** | 3.4180 | -2.2007 | -0.8015 | **H** | 3.4373 | -2.2224 | -0.7907 |
| **H** | 0.9641 | -2.2619 | -0.7276 | **H** | 0.9857 | -2.2938 | -0.7132 |
| **H** | 6.5176 | 1.1495 | -1.4496 | **H** | 6.5898 | 1.1831 | -1.3658 |
| **H** | 5.0040 | 2.0628 | -1.0972 | **H** | 5.0516 | 2.0927 | -1.1137 |
| **H** | 5.4537 | -1.8569 | -1.3741 | **H** | 5.4787 | -1.8658 | -1.3922 |
| **H** | 6.8782 | -0.8869 | -0.8373 | **H** | 6.8937 | -0.8754 | -0.8700 |
| **H** | 5.6639 | 2.1413 | 1.4296 | **H** | 5.5191 | 2.1342 | 1.4525 |
| **H** | 7.1478 | 1.1665 | 1.0499 | **H** | 7.0323 | 1.1664 | 1.1730 |
| **H** | 7.8785 | 3.5092 | 1.2494 | **H** | 7.7269 | 3.5115 | 1.4568 |
| **H** | 7.9972 | 3.0756 | -0.5084 | **H** | 7.9931 | 3.0907 | -0.2889 |
| **H** | 5.6171 | 4.7392 | 0.7974 | **H** | 5.4878 | 4.7186 | 0.8117 |
| **H** | 7.0178 | 5.4508 | -0.1406 | **H** | 6.9717 | 5.4640 | 0.0388 |
| **H** | 5.8001 | 4.3937 | -0.9928 | **H** | 5.8609 | 4.4150 | -0.9567 |
| **H** | 6.5093 | -1.4494 | 1.5824 | **H** | 6.5315 | -1.4004 | 1.5568 |
| **H** | 4.9117 | -2.2301 | 1.2267 | **H** | 4.9262 | -2.1742 | 1.2228 |
| **H** | 6.5621 | -4.0368 | 1.5867 | **H** | 6.5583 | -3.9848 | 1.6211 |
| **H** | 6.0929 | -4.0642 | -0.1659 | **H** | 6.0868 | -4.0473 | -0.1314 |
| **H** | 8.7687 | -2.7646 | 0.9674 | **H** | 8.7761 | -2.7491 | 0.9732 |
| **H** | 8.6436 | -4.4173 | 0.1904 | **H** | 8.6348 | -4.4188 | 0.2342 |
| **H** | 8.3380 | -2.9209 | -0.8070 | **H** | 8.3438 | -2.9412 | -0.7976 |

## $Bu_2N$-TTz-Py in absorption state

| DCM | | | | methanol | | | |
|---|---|---|---|---|---|---|---|
| **C** | -3.2334 | -0.7415 | 0.0137 | **C** | -3.2327 | -0.7405 | -0.0036 |
| **C** | -2.8923 | 0.6101 | -0.1352 | **C** | -2.8950 | 0.6143 | -0.1300 |
| **S** | -4.3909 | 1.5861 | -0.1654 | **S** | -4.3957 | 1.5871 | -0.1465 |
| **C** | -5.3225 | 0.0130 | 0.0430 | **C** | -5.3248 | 0.0075 | 0.0130 |
| **N** | -4.5700 | -1.0764 | 0.1082 | **N** | -4.5694 | -1.0805 | 0.0742 |
| **S** | -1.7287 | -1.7192 | 0.0427 | **S** | -1.7259 | -1.7154 | 0.0047 |
| **C** | -0.7940 | -0.1329 | -0.1806 | **C** | -0.7947 | -0.1238 | -0.1901 |
| **N** | -1.5573 | 0.9541 | -0.2464 | **N** | -1.5605 | 0.9630 | -0.2367 |
| **C** | -6.8297 | -0.0133 | 0.1089 | **C** | -6.8313 | -0.0214 | 0.0922 |
| **C** | 0.7009 | -0.1168 | -0.2501 | **C** | 0.7000 | -0.1038 | -0.2561 |
| **C** | -7.5403 | -1.2413 | -0.1182 | **C** | -7.5056 | -1.1861 | 0.5955 |
| **C** | -8.9635 | -1.2325 | -0.0453 | **C** | -8.9296 | -1.1822 | 0.6523 |
| **N** | -9.7095 | -0.1223 | 0.2240 | **N** | -9.7080 | -0.1317 | 0.2612 |
| **C** | -9.0324 | 1.0395 | 0.4377 | **C** | -9.0649 | 0.9712 | -0.2135 |
| **C** | -7.6101 | 1.1547 | 0.3970 | **C** | -7.6462 | 1.0831 | -0.3232 |
| **C** | 1.4214 | 1.1198 | -0.0804 | **C** | 1.4204 | 1.1240 | -0.0298 |
| **C** | 2.8372 | 1.1716 | -0.1376 | **C** | 2.8364 | 1.1789 | -0.0841 |
| **C** | 3.6389 | -0.0217 | -0.3832 | **C** | 3.6387 | -0.0023 | -0.3837 |
| **C** | 2.9006 | -1.2676 | -0.5338 | **C** | 2.9000 | -1.2406 | -0.5910 |
| **C** | 1.4817 | -1.3020 | -0.4742 | **C** | 1.4813 | -1.2779 | -0.5337 |
| **N** | 5.0381 | 0.0301 | -0.4595 | **N** | 5.0369 | 0.0528 | -0.4571 |
| **C** | 5.7566 | 1.3326 | -0.6489 | **C** | 5.7564 | 1.3631 | -0.5848 |
| **C** | 5.8547 | -1.2222 | -0.5634 | **C** | 5.8540 | -1.1937 | -0.6200 |
| **C** | 6.3409 | 1.9529 | 0.6816 | **C** | 6.3398 | 1.9192 | 0.7741 |
| **C** | 7.1298 | 3.3046 | 0.4616 | **C** | 7.1347 | 3.2763 | 0.6186 |
| **C** | 6.2300 | 4.5440 | 0.0805 | **C** | 6.2416 | 4.5354 | 0.2898 |
| **C** | 6.0021 | -2.0182 | 0.7959 | **C** | 6.0005 | -2.0530 | 0.7003 |
| **C** | 6.7015 | -3.4253 | 0.6342 | **C** | 6.7011 | -3.4505 | 0.4724 |
| **C** | 8.2138 | -3.3673 | 0.1868 | **C** | 8.2142 | -3.3698 | 0.0314 |
| **H** | -6.9953 | -2.1860 | -0.3537 | **H** | -6.9327 | -2.0779 | 0.9435 |
| **H** | -9.5356 | -2.1778 | -0.2202 | **H** | -9.4733 | -2.0787 | 1.0420 |
| **H** | -9.6567 | 1.9401 | 0.6624 | **H** | -9.7156 | 1.8225 | -0.5344 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **H** | -7.1387 | 2.1463 | 0.6066 | **H** | -7.2058 | 2.0201 | -0.7440 |
| **H** | 0.8575 | 2.0626 | 0.1226 | **H** | 0.8571 | 2.0567 | 0.2173 |
| **H** | 3.3248 | 2.1566 | 0.0443 | **H** | 3.3234 | 2.1547 | 0.1430 |
| **H** | 3.4304 | -2.2305 | -0.7107 | **H** | 3.4299 | -2.1943 | -0.8117 |
| **H** | 0.9823 | -2.2922 | -0.6268 | **H** | 0.9819 | -2.2598 | -0.7326 |
| **H** | 6.6097 | 1.1482 | -1.3698 | **H** | 6.6096 | 1.2117 | -1.3126 |
| **H** | 5.0675 | 2.0568 | -1.1676 | **H** | 5.0677 | 2.1112 | -1.0690 |
| **H** | 5.4296 | -1.9009 | -1.3685 | **H** | 5.4296 | -1.8334 | -1.4565 |
| **H** | 6.8730 | -0.9125 | -0.9281 | **H** | 6.8723 | -0.8666 | -0.9683 |
| **H** | 5.5004 | 2.1177 | 1.4280 | **H** | 5.4983 | 2.0534 | 1.5256 |
| **H** | 7.0397 | 1.1931 | 1.1510 | **H** | 7.0352 | 1.1361 | 1.2090 |
| **H** | 7.6924 | 3.5452 | 1.4170 | **H** | 7.6934 | 3.4710 | 1.5867 |
| **H** | 7.9232 | 3.1510 | -0.3393 | **H** | 7.9311 | 3.1555 | -0.1848 |
| **H** | 5.4291 | 4.7206 | 0.8658 | **H** | 5.4356 | 4.6774 | 1.0769 |
| **H** | 6.8549 | 5.4874 | 0.0111 | **H** | 6.8705 | 5.4786 | 0.2692 |
| **H** | 5.7111 | 4.4116 | -0.9181 | **H** | 5.7293 | 4.4514 | -0.7174 |
| **H** | 6.5914 | -1.3822 | 1.5293 | **H** | 6.5888 | -1.4524 | 1.4636 |
| **H** | 4.9796 | -2.1706 | 1.2575 | **H** | 4.9776 | -2.2290 | 1.1528 |
| **H** | 6.6357 | -3.9675 | 1.6287 | **H** | 6.6340 | -4.0395 | 1.4399 |
| **H** | 6.1120 | -4.0553 | -0.1074 | **H** | 6.1133 | -4.0441 | -0.2996 |
| **H** | 8.8237 | -2.7255 | 0.8981 | **H** | 8.8219 | -2.7621 | 0.7739 |
| **H** | 8.6716 | -4.4043 | 0.1827 | **H** | 8.6727 | -4.4053 | -0.0213 |
| **H** | 8.3388 | -2.9412 | -0.8559 | **H** | 8.3407 | -2.8939 | -0.9893 |

## Ph2N-TTz-Py in absorption state

| toluene | | | | chloroform | | | |
|---|---|---|---|---|---|---|---|
| **C** | 1.2273 | -0.1019 | -0.0628 | **C** | 1.2282 | -0.1005 | -0.0616 |
| **N** | 1.9800 | 0.9599 | 0.2033 | **N** | 1.9821 | 0.9680 | 0.1758 |
| **C** | 3.3190 | 0.6227 | 0.1452 | **C** | 3.3213 | 0.6279 | 0.1280 |
| **C** | 3.6715 | -0.6999 | -0.1693 | **C** | 3.6721 | -0.7030 | -0.1506 |
| **S** | 2.1727 | -1.6581 | -0.4046 | **S** | 2.1723 | -1.6657 | -0.3608 |
| **S** | 4.8124 | 1.5817 | 0.3778 | **S** | 4.8153 | 1.5915 | 0.3348 |
| **C** | 5.7585 | 0.0405 | 0.0131 | **C** | 5.7601 | 0.0408 | 0.0124 |
| **N** | 5.0108 | -1.0240 | -0.2449 | **N** | 5.0114 | -1.0299 | -0.2174 |
| **C** | 7.2675 | 0.0118 | 0.0160 | **C** | 7.2693 | 0.0110 | 0.0159 |
| **C** | -0.2749 | -0.0872 | -0.0602 | **C** | -0.2739 | -0.0858 | -0.0591 |
| **C** | 8.0661 | 1.1758 | 0.2731 | **C** | 8.0683 | 1.1787 | 0.2554 |
| **C** | 9.4892 | 1.0543 | 0.2546 | **C** | 9.4913 | 1.0567 | 0.2389 |
| **N** | 10.1531 | -0.1076 | 0.0056 | **N** | 10.1547 | -0.1101 | 0.0078 |
| **C** | 9.3909 | -1.2124 | -0.2385 | **C** | 9.3921 | -1.2189 | -0.2193 |
| **C** | 7.9649 | -1.2181 | -0.2471 | **C** | 7.9662 | -1.2234 | -0.2280 |
| **C** | -1.0553 | -1.1042 | -0.7121 | **C** | -1.0539 | -1.1101 | -0.7007 |
| **C** | -2.4784 | -1.0652 | -0.6972 | **C** | -2.4770 | -1.0716 | -0.6863 |
| **C** | -3.1786 | -0.0050 | -0.0175 | **C** | -3.1788 | -0.0046 | -0.0177 |
| **C** | -2.3983 | 1.0162 | 0.6382 | **C** | -2.3985 | 1.0238 | 0.6279 |
| **C** | -0.9774 | 0.9772 | 0.6117 | **C** | -0.9774 | 0.9849 | 0.6021 |
| **N** | -4.6137 | 0.0339 | 0.0076 | **N** | -4.6125 | 0.0338 | 0.0068 |
| **C** | -5.3872 | -1.1982 | 0.0911 | **C** | -5.3873 | -1.1988 | 0.0822 |
| **C** | -5.3217 | 1.3060 | -0.0570 | **C** | -5.3223 | 1.3060 | -0.0499 |
| **C** | -6.3194 | 1.6279 | 0.9224 | **C** | -6.3073 | 1.6278 | 0.9421 |
| **C** | -7.0277 | 2.8683 | 0.8461 | **C** | -7.0179 | 2.8678 | 0.8736 |
| **C** | -6.7368 | 3.8066 | -0.1952 | **C** | -6.7416 | 3.8048 | -0.1733 |
| **C** | -5.7359 | 3.4878 | -1.1686 | **C** | -5.7532 | 3.4855 | -1.1598 |
| **C** | -5.0381 | 2.2414 | -1.1080 | **C** | -5.0532 | 2.2397 | -1.1062 |
| **C** | -5.1234 | -2.1499 | 1.1327 | **C** | -5.1370 | -2.1486 | 1.1288 |
| **C** | -5.8854 | -3.3568 | 1.2137 | **C** | -5.9009 | -3.3552 | 1.2023 |
| **C** | -6.9307 | -3.6191 | 0.2704 | **C** | -6.9345 | -3.6183 | 0.2459 |
| **C** | -7.2014 | -2.6643 | -0.7611 | **C** | -7.1917 | -2.6650 | -0.7909 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | -6.4297 | -1.4636 | -0.8580 | **C** | -6.4179 | -1.4647 | -0.8797 |
| **H** | 7.6104 | 2.1755 | 0.4868 | **H** | 7.6140 | 2.1817 | 0.4544 |
| **H** | 10.1275 | 1.9528 | 0.4530 | **H** | 10.1289 | 1.9583 | 0.4238 |
| **H** | 9.9533 | -2.1595 | -0.4411 | **H** | 9.9530 | -2.1697 | -0.4072 |
| **H** | 7.4049 | -2.1615 | -0.4542 | **H** | 7.4075 | -2.1704 | -0.4210 |
| **H** | -0.5545 | -1.9313 | -1.2776 | **H** | -0.5533 | -1.9428 | -1.2580 |
| **H** | -3.0538 | -1.8632 | -1.2280 | **H** | -3.0507 | -1.8753 | -1.2102 |
| **H** | -2.9133 | 1.8465 | 1.1819 | **H** | -2.9126 | 1.8590 | 1.1646 |
| **H** | -0.3961 | 1.7722 | 1.1401 | **H** | -0.3982 | 1.7851 | 1.1250 |
| **H** | -6.5452 | 0.9003 | 1.7429 | **H** | -6.5209 | 0.9018 | 1.7673 |
| **H** | -7.8055 | 3.1068 | 1.6165 | **H** | -7.7857 | 3.1068 | 1.6539 |
| **H** | -7.2879 | 4.7802 | -0.2492 | **H** | -7.2944 | 4.7777 | -0.2216 |
| **H** | -5.5042 | 4.2093 | -1.9940 | **H** | -5.5335 | 4.2058 | -1.9895 |
| **H** | -4.2640 | 1.9918 | -1.8777 | **H** | -4.2899 | 1.9893 | -1.8864 |
| **H** | -4.3149 | -1.9435 | 1.8796 | **H** | -4.3386 | -1.9411 | 1.8861 |
| **H** | -5.6690 | -4.0913 | 2.0319 | **H** | -5.6956 | -4.0882 | 2.0245 |
| **H** | -7.5320 | -4.5615 | 0.3408 | **H** | -7.5372 | -4.5602 | 0.3102 |
| **H** | -8.0141 | -2.8585 | -1.5077 | **H** | -7.9947 | -2.8600 | -1.5476 |
| **H** | -6.6410 | -0.7229 | -1.6705 | **H** | -6.6177 | -0.7257 | -1.6968 |

## Ph2N-TTz-Py in absorption state

| DCM | | | | methanol | | | |
|---|---|---|---|---|---|---|---|
| **C** | 1.2293 | -0.1104 | -0.0385 | **C** | 1.2308 | -0.1027 | -0.0520 |
| **N** | 1.9842 | 0.9652 | 0.1616 | **N** | 1.9871 | 0.9697 | 0.1614 |
| **C** | 3.3237 | 0.6233 | 0.1231 | **C** | 3.3268 | 0.6263 | 0.1196 |
| **C** | 3.6731 | -0.7163 | -0.1115 | **C** | 3.6738 | -0.7109 | -0.1306 |
| **S** | 2.1724 | -1.6852 | -0.2847 | **S** | 2.1719 | -1.6746 | -0.3200 |
| **S** | 4.8187 | 1.5933 | 0.2908 | **S** | 4.8239 | 1.5917 | 0.2988 |
| **C** | 5.7611 | 0.0318 | 0.0261 | **C** | 5.7626 | 0.0365 | -0.0052 |
| **N** | 5.0130 | -1.0463 | -0.1692 | **N** | 5.0138 | -1.0409 | -0.2012 |
| **C** | 7.2702 | 0.0083 | 0.0155 | **C** | 7.2719 | 0.0091 | 0.0010 |
| **C** | -0.2728 | -0.0947 | -0.0374 | **C** | -0.2712 | -0.0877 | -0.0465 |
| **C** | 8.0638 | 1.1013 | 0.5000 | **C** | 8.0652 | 1.1876 | -0.2006 |
| **C** | 9.4872 | 0.9949 | 0.4496 | **C** | 9.4887 | 1.0707 | -0.1791 |
| **N** | 10.1543 | -0.0919 | -0.0301 | **N** | 10.1544 | -0.1024 | 0.0172 |
| **C** | 9.3964 | -1.1314 | -0.4869 | **C** | 9.3961 | -1.2223 | 0.2044 |
| **C** | 7.9703 | -1.1403 | -0.4927 | **C** | 7.9699 | -1.2303 | 0.2100 |
| **C** | -1.0530 | -1.1333 | -0.6557 | **C** | -1.0517 | -1.1076 | -0.6953 |
| **C** | -2.4761 | -1.0918 | -0.6466 | **C** | -2.4748 | -1.0684 | -0.6818 |
| **C** | -3.1785 | -0.0071 | -0.0069 | **C** | -3.1779 | -0.0050 | -0.0068 |
| **C** | -2.3976 | 1.0347 | 0.6172 | **C** | -2.3963 | 1.0179 | 0.6480 |
| **C** | -0.9766 | 0.9923 | 0.5967 | **C** | -0.9752 | 0.9778 | 0.6230 |
| **N** | -4.6113 | 0.0361 | 0.0110 | **N** | -4.6095 | 0.0351 | 0.0162 |
| **C** | -5.3918 | -1.1933 | 0.0904 | **C** | -5.3898 | -1.1977 | 0.0349 |
| **C** | -5.3180 | 1.3094 | -0.0671 | **C** | -5.3201 | 1.3092 | 0.0001 |
| **C** | -6.2998 | 1.6508 | 0.9215 | **C** | -6.2887 | 1.6062 | 1.0156 |
| **C** | -7.0085 | 2.8909 | 0.8323 | **C** | -7.0028 | 2.8464 | 0.9870 |
| **C** | -6.7329 | 3.8081 | -0.2325 | **C** | -6.7454 | 3.8070 | -0.0437 |
| **C** | -5.7474 | 3.4691 | -1.2157 | **C** | -5.7728 | 3.5119 | -1.0541 |
| **C** | -5.0496 | 2.2230 | -1.1410 | **C** | -5.0698 | 2.2663 | -1.0397 |
| **C** | -5.1663 | -2.1257 | 1.1579 | **C** | -5.1767 | -2.1729 | 1.0660 |
| **C** | -5.9360 | -3.3285 | 1.2360 | **C** | -5.9468 | -3.3781 | 1.0851 |
| **C** | -6.9506 | -3.6044 | 0.2625 | **C** | -6.9490 | -3.6137 | 0.0881 |
| **C** | -7.1828 | -2.6681 | -0.7958 | **C** | -7.1687 | -2.6347 | -0.9339 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | -6.4029 | -1.4716 | -0.8883 | **C** | -6.3882 | -1.4352 | -0.9672 |
| **H** | 7.6030 | 2.0267 | 0.9279 | **H** | 7.6037 | 2.1885 | -0.3912 |
| **H** | 10.1215 | 1.8377 | 0.8246 | **H** | 10.1237 | 1.9790 | -0.3366 |
| **H** | 9.9604 | -2.0155 | -0.8792 | **H** | 9.9590 | -2.1763 | 0.3671 |
| **H** | 7.4150 | -2.0236 | -0.8903 | **H** | 7.4140 | -2.1834 | 0.3820 |
| **H** | -0.5527 | -1.9801 | -1.1913 | **H** | -0.5516 | -1.9368 | -1.2579 |
| **H** | -3.0488 | -1.9068 | -1.1536 | **H** | -3.0465 | -1.8680 | -1.2135 |
| **H** | -2.9110 | 1.8831 | 1.1335 | **H** | -2.9086 | 1.8486 | 1.1932 |
| **H** | -0.3984 | 1.8036 | 1.1035 | **H** | -0.3978 | 1.7732 | 1.1555 |
| **H** | -6.5120 | 0.9407 | 1.7608 | **H** | -6.4858 | 0.8623 | 1.8288 |
| **H** | -7.7737 | 3.1456 | 1.6100 | **H** | -7.7572 | 3.0666 | 1.7854 |
| **H** | -7.2840 | 4.7810 | -0.2972 | **H** | -7.3005 | 4.7795 | -0.0612 |
| **H** | -5.5288 | 4.1736 | -2.0590 | **H** | -5.5691 | 4.2507 | -1.8714 |
| **H** | -4.2893 | 1.9566 | -1.9188 | **H** | -4.3205 | 2.0341 | -1.8389 |
| **H** | -4.3833 | -1.9075 | 1.9283 | **H** | -4.4039 | -1.9861 | 1.8546 |
| **H** | -5.7508 | -4.0482 | 2.0746 | **H** | -5.7721 | -4.1317 | 1.8956 |
| **H** | -7.5579 | -4.5430 | 0.3301 | **H** | -7.5566 | -4.5543 | 0.1094 |
| **H** | -7.9704 | -2.8735 | -1.5657 | **H** | -7.9461 | -2.8086 | -1.7216 |
| **H** | -6.5823 | -0.7464 | -1.7222 | **H** | -6.5567 | -0.6769 | -1.7735 |

## Ph2N-TTz-CHO in absorption state

| toluene | | | | chloroform | | | |
|---|---|---|---|---|---|---|---|
| **C** | -3.8513 | -0.0002 | -0.0139 | **C** | -3.8518 | 0.0007 | -0.0183 |
| **C** | -3.0633 | 1.0319 | 0.6153 | **C** | -3.0635 | 1.0395 | 0.6005 |
| **C** | -1.6425 | 0.9844 | 0.5856 | **C** | -1.6425 | 0.9927 | 0.5694 |
| **C** | -0.9477 | -0.0997 | -0.0631 | **C** | -0.9472 | -0.0962 | -0.0711 |
| **C** | -1.7360 | -1.1275 | -0.6885 | **C** | -1.7356 | -1.1305 | -0.6866 |
| **C** | -3.1591 | -1.0800 | -0.6704 | **C** | -3.1587 | -1.0843 | -0.6665 |
| **C** | 0.5546 | -0.1231 | -0.0692 | **C** | 0.5551 | -0.1194 | -0.0783 |
| **N** | 1.3146 | 0.9374 | 0.1807 | **N** | 1.3163 | 0.9460 | 0.1482 |
| **C** | 2.6518 | 0.5927 | 0.1206 | **C** | 2.6539 | 0.5989 | 0.0964 |
| **C** | 2.9962 | -0.7355 | -0.1795 | **C** | 2.9966 | -0.7357 | -0.1747 |
| **S** | 1.4912 | -1.6893 | -0.3946 | **S** | 1.4906 | -1.6925 | -0.3695 |
| **S** | 4.1525 | 1.5455 | 0.3375 | **S** | 4.1557 | 1.5541 | 0.2957 |
| **C** | 5.0897 | -0.0103 | 0.0021 | **C** | 5.0909 | -0.0093 | -0.0036 |
| **N** | 4.3335 | -1.0717 | -0.2487 | **N** | 4.3342 | -1.0752 | -0.2338 |
| **C** | 6.5979 | -0.0404 | -0.0091 | **C** | 6.5995 | -0.0396 | -0.0114 |
| **C** | 7.3816 | 1.0088 | 0.5968 | **C** | 7.3801 | 0.9914 | 0.6292 |
| **C** | 8.8028 | 0.9580 | 0.5705 | **C** | 8.8015 | 0.9406 | 0.6069 |
| **C** | 9.4755 | -0.1462 | -0.0568 | **C** | 9.4765 | -0.1451 | -0.0504 |
| **C** | 8.6986 | -1.1936 | -0.6558 | **C** | 8.7024 | -1.1744 | -0.6841 |
| **C** | 7.2742 | -1.1460 | -0.6378 | **C** | 7.2778 | -1.1262 | -0.6705 |
| **C** | 10.9954 | -0.2252 | -0.0943 | **C** | 10.9955 | -0.2260 | -0.0847 |
| **O** | 11.7510 | 0.6091 | 0.3848 | **O** | 11.7516 | 0.5940 | 0.4219 |
| **N** | -5.2865 | 0.0473 | 0.0147 | **N** | -5.2859 | 0.0462 | 0.0124 |
| **C** | -6.0657 | -1.1784 | 0.1331 | **C** | -6.0645 | -1.1804 | 0.1322 |
| **C** | -5.9881 | 1.3207 | -0.0832 | **C** | -5.9903 | 1.3192 | -0.0791 |
| **C** | -5.8041 | -2.1029 | 1.1997 | **C** | -5.8087 | -2.0986 | 1.2057 |
| **C** | -6.5717 | -3.3037 | 1.3150 | **C** | -6.5761 | -3.2997 | 1.3227 |
| **C** | -7.6204 | -3.5866 | 0.3812 | **C** | -7.6186 | -3.5886 | 0.3832 |
| **C** | -7.8888 | -2.6588 | -0.6756 | **C** | -7.8810 | -2.6668 | -0.6807 |
| **C** | -7.1117 | -1.4647 | -0.8066 | **C** | -7.1038 | -1.4723 | -0.8129 |
| **C** | -6.9845 | 1.6729 | 0.8874 | **C** | -6.9737 | 1.6728 | 0.9042 |
| **C** | -7.6869 | 2.9145 | 0.7786 | **C** | -7.6791 | 2.9137 | 0.8015 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | -7.3914 | 3.8241 | -0.2868 | **C** | -7.3992 | 3.8203 | -0.2711 |
| **C** | -6.3917 | 3.4752 | -1.2514 | **C** | -6.4123 | 3.4696 | -1.2486 |
| **C** | -5.6998 | 2.2273 | -1.1582 | **C** | -5.7176 | 2.2225 | -1.1609 |
| **H** | -3.5722 | 1.8780 | 1.1406 | **H** | -3.5713 | 1.8893 | 1.1206 |
| **H** | -1.0551 | 1.7885 | 1.0934 | **H** | -1.0568 | 1.8015 | 1.0717 |
| **H** | -1.2417 | -1.9709 | -1.2357 | **H** | -1.2420 | -1.9783 | -1.2273 |
| **H** | -3.7407 | -1.8874 | -1.1804 | **H** | -3.7392 | -1.8967 | -1.1694 |
| **H** | 6.8797 | 1.8671 | 1.1113 | **H** | 6.8762 | 1.8325 | 1.1689 |
| **H** | 9.4050 | 1.7724 | 1.0453 | **H** | 9.4001 | 1.7407 | 1.1094 |
| **H** | 9.2138 | -2.0586 | -1.1506 | **H** | 9.2192 | -2.0238 | -1.2031 |
| **H** | 6.6760 | -1.9605 | -1.1132 | **H** | 6.6825 | -1.9252 | -1.1751 |
| **H** | 11.4150 | -1.1535 | -0.6206 | **H** | 11.4158 | -1.1382 | -0.6349 |
| **H** | -4.9929 | -1.8800 | 1.9392 | **H** | -5.0033 | -1.8707 | 1.9499 |
| **H** | -6.3571 | -4.0168 | 2.1526 | **H** | -6.3665 | -4.0078 | 2.1657 |
| **H** | -8.2262 | -4.5240 | 0.4783 | **H** | -8.2240 | -4.5260 | 0.4815 |
| **H** | -8.7040 | -2.8694 | -1.4152 | **H** | -8.6909 | -2.8823 | -1.4247 |
| **H** | -7.3212 | -0.7451 | -1.6387 | **H** | -7.3079 | -0.7582 | -1.6511 |
| **H** | -7.2139 | 0.9680 | 1.7268 | **H** | -7.1902 | 0.9709 | 1.7495 |
| **H** | -8.4638 | 3.1767 | 1.5426 | **H** | -8.4455 | 3.1774 | 1.5754 |
| **H** | -7.9379 | 4.7988 | -0.3663 | **H** | -7.9479 | 4.7941 | -0.3461 |
| **H** | -6.1564 | 4.1741 | -2.0953 | **H** | -6.1897 | 4.1658 | -2.0981 |
| **H** | -4.9266 | 1.9541 | -1.9211 | **H** | -4.9556 | 1.9473 | -1.9343 |

## Ph2N-TTz-CHO in absorption state

| DCM | | | | methanol | | | |
|---|---|---|---|---|---|---|---|
| **C** | -3.8520 | 0.0005 | -0.0175 | **C** | -3.8520 | -0.0004 | -0.0120 |
| **C** | -3.0635 | 1.0427 | 0.5959 | **C** | -3.0630 | 1.0459 | 0.5947 |
| **C** | -1.6425 | 0.9956 | 0.5654 | **C** | -1.6419 | 0.9981 | 0.5648 |
| **C** | -0.9468 | -0.0965 | -0.0694 | **C** | -0.9460 | -0.0983 | -0.0626 |
| **C** | -1.7351 | -1.1345 | -0.6792 | **C** | -1.7345 | -1.1408 | -0.6648 |
| **C** | -3.1582 | -1.0883 | -0.6595 | **C** | -3.1577 | -1.0942 | -0.6456 |
| **C** | 0.5555 | -0.1198 | -0.0768 | **C** | 0.5562 | -0.1216 | -0.0708 |
| **N** | 1.3173 | 0.9490 | 0.1333 | **N** | 1.3186 | 0.9519 | 0.1133 |
| **C** | 2.6552 | 0.6005 | 0.0872 | **C** | 2.6567 | 0.6019 | 0.0750 |
| **C** | 2.9969 | -0.7381 | -0.1636 | **C** | 2.9974 | -0.7423 | -0.1442 |
| **S** | 1.4904 | -1.6971 | -0.3438 | **S** | 1.4903 | -1.7048 | -0.3005 |
| **S** | 4.1575 | 1.5579 | 0.2717 | **S** | 4.1595 | 1.5629 | 0.2353 |
| **C** | 5.0918 | -0.0098 | -0.0040 | **C** | 5.0930 | -0.0108 | -0.0040 |
| **N** | 4.3347 | -1.0790 | -0.2179 | **N** | 4.3354 | -1.0848 | -0.1916 |
| **C** | 6.6005 | -0.0398 | -0.0124 | **C** | 6.6018 | -0.0403 | -0.0137 |
| **C** | 7.3802 | 0.9900 | 0.6316 | **C** | 7.3810 | 0.9940 | 0.6236 |
| **C** | 8.8017 | 0.9392 | 0.6096 | **C** | 8.8026 | 0.9433 | 0.6013 |
| **C** | 9.4772 | -0.1446 | -0.0507 | **C** | 9.4782 | -0.1444 | -0.0528 |
| **C** | 8.7039 | -1.1723 | -0.6884 | **C** | 8.7053 | -1.1763 | -0.6846 |
| **C** | 7.2791 | -1.1240 | -0.6749 | **C** | 7.2803 | -1.1281 | -0.6705 |
| **C** | 10.9957 | -0.2262 | -0.0851 | **C** | 10.9963 | -0.2268 | -0.0875 |
| **O** | 11.7524 | 0.5924 | 0.4255 | **O** | 11.7536 | 0.5946 | 0.4199 |
| **N** | -5.2854 | 0.0463 | 0.0125 | **N** | -5.2844 | 0.0468 | 0.0172 |
| **C** | -6.0652 | -1.1803 | 0.1284 | **C** | -6.0672 | -1.1794 | 0.1222 |
| **C** | -5.9901 | 1.3196 | -0.0763 | **C** | -5.9886 | 1.3210 | -0.0705 |
| **C** | -5.8186 | -2.0959 | 1.2062 | **C** | -5.8366 | -2.0945 | 1.2039 |
| **C** | -6.5876 | -3.2966 | 1.3198 | **C** | -6.6087 | -3.2943 | 1.3075 |
| **C** | -7.6224 | -3.5873 | 0.3721 | **C** | -7.6307 | -3.5841 | 0.3452 |
| **C** | -7.8757 | -2.6678 | -0.6964 | **C** | -7.8680 | -2.6648 | -0.7274 |
| **C** | -7.0968 | -1.4738 | -0.8248 | **C** | -7.0857 | -1.4716 | -0.8452 |
| **C** | -6.9656 | 1.6756 | 0.9138 | **C** | -6.9559 | 1.6806 | 0.9264 |
| **C** | -7.6717 | 2.9166 | 0.8138 | **C** | -7.6623 | 2.9218 | 0.8279 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | -7.4000 | 3.8205 | -0.2635 | **C** | -7.3986 | 3.8219 | -0.2548 |
| **C** | -6.4207 | 3.4671 | -1.2482 | **C** | -6.4274 | 3.4647 | -1.2464 |
| **C** | -5.7256 | 2.2200 | -1.1626 | **C** | -5.7321 | 2.2173 | -1.1620 |
| **H** | -3.5707 | 1.8950 | 1.1125 | **H** | -3.5694 | 1.9013 | 1.1066 |
| **H** | -1.0578 | 1.8068 | 1.0652 | **H** | -1.0581 | 1.8124 | 1.0608 |
| **H** | -1.2417 | -1.9852 | -1.2154 | **H** | -1.2413 | -1.9955 | -1.1948 |
| **H** | -3.7379 | -1.9034 | -1.1588 | **H** | -3.7366 | -1.9128 | -1.1400 |
| **H** | 6.8760 | 1.8293 | 1.1737 | **H** | 6.8768 | 1.8364 | 1.1607 |
| **H** | 9.3988 | 1.7385 | 1.1152 | **H** | 9.3986 | 1.7462 | 1.1023 |
| **H** | 9.2208 | -2.0195 | -1.2103 | **H** | 9.2220 | -2.0258 | -1.2024 |
| **H** | 6.6850 | -1.9213 | -1.1838 | **H** | 6.6871 | -1.9281 | -1.1761 |
| **H** | 11.4162 | -1.1355 | -0.6380 | **H** | 11.4167 | -1.1377 | -0.6361 |
| **H** | -5.0198 | -1.8663 | 1.9570 | **H** | -5.0484 | -1.8651 | 1.9659 |
| **H** | -6.3855 | -4.0027 | 2.1662 | **H** | -6.4195 | -4.0002 | 2.1570 |
| **H** | -8.2290 | -4.5242 | 0.4675 | **H** | -8.2398 | -4.5202 | 0.4326 |
| **H** | -8.6792 | -2.8849 | -1.4467 | **H** | -8.6610 | -2.8815 | -1.4889 |
| **H** | -7.2929 | -0.7621 | -1.6669 | **H** | -7.2684 | -0.7608 | -1.6910 |
| **H** | -7.1750 | 0.9763 | 1.7631 | **H** | -7.1580 | 0.9847 | 1.7803 |
| **H** | -8.4318 | 3.1825 | 1.5930 | **H** | -8.4157 | 3.1910 | 1.6125 |
| **H** | -7.9491 | 4.7942 | -0.3367 | **H** | -7.9477 | 4.7956 | -0.3270 |
| **H** | -6.2050 | 4.1610 | -2.1013 | **H** | -6.2185 | 4.1554 | -2.1037 |
| **H** | -4.9703 | 1.9424 | -1.9418 | **H** | -4.9840 | 1.9362 | -1.9467 |

## Ph2N-TTz-COOH in absorption state

| **toluene** | | | | **chloroform** | | | |
|---|---|---|---|---|---|---|---|
| **C** | 0.1992 | -0.0931 | -0.0684 | **C** | 0.2000 | -0.0971 | -0.0531 |
| **N** | 0.9508 | 0.9610 | 0.2295 | **N** | 0.9529 | 0.9761 | 0.1644 |
| **C** | 2.2913 | 0.6278 | 0.1602 | **C** | 2.2937 | 0.6374 | 0.1213 |
| **C** | 2.6455 | -0.6838 | -0.1952 | **C** | 2.6462 | -0.6975 | -0.1336 |
| **S** | 1.1476 | -1.6364 | -0.4608 | **S** | 1.1473 | -1.6669 | -0.3230 |
| **S** | 3.7856 | 1.5821 | 0.4185 | **S** | 3.7891 | 1.6060 | 0.3114 |
| **C** | 4.7342 | 0.0558 | -0.0119 | **C** | 4.7357 | 0.0449 | 0.0329 |
| **N** | 3.9863 | -1.0034 | -0.2925 | **N** | 3.9873 | -1.0287 | -0.1863 |
| **C** | 6.2434 | 0.0341 | -0.0048 | **C** | 6.2453 | 0.0264 | 0.0276 |
| **C** | -1.3041 | -0.0814 | -0.0628 | **C** | -1.3033 | -0.0841 | -0.0525 |
| **C** | 7.0185 | 1.2436 | -0.0753 | **C** | 7.0172 | 1.0570 | 0.6688 |
| **C** | 8.4442 | 1.1948 | -0.0633 | **C** | 8.4432 | 1.0163 | 0.6461 |
| **C** | 8.3529 | -1.2785 | 0.0772 | **C** | 8.3577 | -1.0946 | -0.6514 |
| **C** | 6.9306 | -1.2319 | 0.0708 | **C** | 6.9351 | -1.0538 | -0.6343 |
| **C** | -2.0834 | -1.0771 | -0.7489 | **C** | -2.0817 | -1.1269 | -0.6666 |
| **C** | -3.5071 | -1.0410 | -0.7315 | **C** | -3.5055 | -1.0897 | -0.6544 |
| **C** | -4.2084 | -0.0060 | -0.0149 | **C** | -4.2090 | -0.0056 | -0.0158 |
| **C** | -3.4296 | 0.9934 | 0.6753 | **C** | -3.4307 | 1.0414 | 0.6021 |
| **C** | -2.0079 | 0.9581 | 0.6463 | **C** | -2.0090 | 1.0037 | 0.5788 |
| **N** | -5.6450 | 0.0296 | 0.0126 | **N** | -5.6442 | 0.0314 | 0.0067 |
| **C** | -6.4151 | -1.2063 | 0.0684 | **C** | -6.4156 | -1.1995 | 0.1316 |
| **C** | -6.3547 | 1.3019 | -0.0244 | **C** | -6.3558 | 1.2990 | -0.1044 |
| **C** | -7.3596 | 1.5978 | 0.9566 | **C** | -7.3515 | 1.6558 | 0.8657 |
| **C** | -8.0693 | 2.8393 | 0.9072 | **C** | -8.0640 | 2.8912 | 0.7439 |
| **C** | -7.7729 | 3.8048 | -0.1080 | **C** | -7.7790 | 3.7897 | -0.3346 |
| **C** | -6.7647 | 3.5119 | -1.0828 | **C** | -6.7798 | 3.4359 | -1.2989 |
| **C** | -6.0655 | 2.2648 | -1.0495 | **C** | -6.0780 | 2.1940 | -1.1923 |
| **C** | -6.1424 | -2.1850 | 1.0832 | **C** | -6.1603 | -2.1073 | 1.2144 |
| **C** | -6.9005 | -3.3965 | 1.1364 | **C** | -6.9200 | -3.3131 | 1.3364 |
| **C** | -7.9511 | -3.6371 | 0.1925 | **C** | -7.9546 | -3.6171 | 0.3926 |
| **C** | -8.2308 | -2.6556 | -0.8119 | **C** | -8.2168 | -2.7056 | -0.6806 |
| **C** | -7.4630 | -1.4501 | -0.8816 | **C** | -7.4471 | -1.5066 | -0.8177 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **H** | 6.5144 | 2.2398 | -0.1597 | **H** | 6.5112 | 1.8944 | 1.2128 |
| **H** | 9.0278 | 2.1455 | -0.1223 | **H** | 9.0235 | 1.8243 | 1.1540 |
| **H** | 8.8806 | -2.2623 | 0.1392 | **H** | 8.8856 | -1.9327 | -1.1700 |
| **H** | 6.3388 | -2.1776 | 0.1303 | **H** | 6.3466 | -1.8567 | -1.1415 |
| **H** | -1.5812 | -1.8837 | -1.3431 | **H** | -1.5794 | -1.9744 | -1.2003 |
| **H** | -4.0822 | -1.8216 | -1.2890 | **H** | -4.0783 | -1.9087 | -1.1562 |
| **H** | -3.9462 | 1.8038 | 1.2479 | **H** | -3.9471 | 1.8909 | 1.1151 |
| **H** | -1.4273 | 1.7357 | 1.2017 | **H** | -1.4309 | 1.8191 | 1.0801 |
| **H** | -7.5900 | 0.8491 | 1.7572 | **H** | -7.5722 | 0.9605 | 1.7157 |
| **H** | -8.8529 | 3.0571 | 1.6788 | **H** | -8.8401 | 3.1574 | 1.5076 |
| **H** | -8.3251 | 4.7793 | -0.1407 | **H** | -8.3333 | 4.7593 | -0.4245 |
| **H** | -6.5283 | 4.2549 | -1.8882 | **H** | -6.5530 | 4.1256 | -2.1529 |
| **H** | -5.2857 | 2.0361 | -1.8207 | **H** | -5.3063 | 1.9165 | -1.9555 |
| **H** | -5.3297 | -1.9961 | 1.8308 | **H** | -5.3608 | -1.8677 | 1.9619 |
| **H** | -6.6767 | -4.1520 | 1.9338 | **H** | -6.7106 | -4.0130 | 2.1866 |
| **H** | -8.5494 | -4.5833 | 0.2413 | **H** | -8.5542 | -4.5582 | 0.4947 |
| **H** | -9.0476 | -2.8325 | -1.5591 | **H** | -9.0206 | -2.9331 | -1.4281 |
| **H** | -7.6813 | -0.6886 | -1.6735 | **H** | -7.6509 | -0.8008 | -1.6633 |
| **C** | 9.1230 | -0.0673 | 0.0129 | **C** | 9.1250 | -0.0604 | -0.0143 |
| **C** | 10.6506 | -0.1713 | 0.0267 | **C** | 10.6532 | -0.1474 | -0.0631 |
| **O** | 11.2714 | -1.2225 | 0.0858 | **O** | 11.2763 | -1.0461 | -0.6120 |
| **O** | 11.2667 | 1.0435 | -0.0342 | **O** | 11.2649 | 0.8887 | 0.5733 |
| **H** | 12.2419 | 0.8897 | -0.0207 | **H** | 12.2418 | 0.7631 | 0.4985 |

## Ph2N-TTz-COOH in absorption state

| DCM | | | | methanol | | | |
|---|---|---|---|---|---|---|---|
| **C** | 0.2005 | -0.0984 | -0.0491 | **C** | 0.2015 | -0.1010 | -0.0410 |
| **N** | 0.9540 | 0.9788 | 0.1471 | **N** | 0.9557 | 0.9823 | 0.1175 |
| **C** | 2.2951 | 0.6385 | 0.1114 | **C** | 2.2970 | 0.6402 | 0.0941 |
| **C** | 2.6465 | -0.7013 | -0.1169 | **C** | 2.6473 | -0.7069 | -0.0873 |
| **S** | 1.1470 | -1.6735 | -0.2873 | **S** | 1.1470 | -1.6835 | -0.2236 |
| **S** | 3.7910 | 1.6099 | 0.2819 | **S** | 3.7934 | 1.6164 | 0.2289 |
| **C** | 4.7367 | 0.0438 | 0.0341 | **C** | 4.7380 | 0.0428 | 0.0354 |
| **N** | 3.9878 | -1.0340 | -0.1635 | **N** | 3.9889 | -1.0415 | -0.1234 |
| **C** | 6.2464 | 0.0256 | 0.0277 | **C** | 6.2479 | 0.0248 | 0.0274 |
| **C** | -1.3027 | -0.0853 | -0.0487 | **C** | -1.3016 | -0.0880 | -0.0402 |
| **C** | 7.0180 | 1.0592 | 0.6645 | **C** | 7.0195 | 1.0714 | 0.6427 |
| **C** | 8.4442 | 1.0188 | 0.6410 | **C** | 8.4458 | 1.0310 | 0.6182 |
| **C** | 8.3588 | -1.0974 | -0.6484 | **C** | 8.3600 | -1.1103 | -0.6296 |
| **C** | 6.9361 | -1.0569 | -0.6306 | **C** | 6.9372 | -1.0700 | -0.6108 |
| **C** | -2.0810 | -1.1325 | -0.6559 | **C** | -2.0797 | -1.1423 | -0.6355 |
| **C** | -3.5048 | -1.0950 | -0.6449 | **C** | -3.5036 | -1.1041 | -0.6264 |
| **C** | -4.2091 | -0.0060 | -0.0145 | **C** | -4.2089 | -0.0073 | -0.0096 |
| **C** | -3.4307 | 1.0450 | 0.5971 | **C** | -3.4301 | 1.0502 | 0.5915 |
| **C** | -2.0089 | 1.0067 | 0.5751 | **C** | -2.0083 | 1.0109 | 0.5711 |
| **N** | -5.6435 | 0.0317 | 0.0065 | **N** | -5.6421 | 0.0322 | 0.0088 |
| **C** | -6.4170 | -1.1991 | 0.1251 | **C** | -6.4195 | -1.1981 | 0.1130 |
| **C** | -6.3551 | 1.3001 | -0.1009 | **C** | -6.3531 | 1.3021 | -0.0926 |
| **C** | -7.3424 | 1.6591 | 0.8768 | **C** | -7.3291 | 1.6630 | 0.8957 |
| **C** | -8.0553 | 2.8949 | 0.7588 | **C** | -8.0423 | 2.8995 | 0.7839 |
| **C** | -7.7787 | 3.7911 | -0.3241 | **C** | -7.7769 | 3.7936 | -0.3037 |
| **C** | -6.7876 | 3.4349 | -1.2963 | **C** | -6.7971 | 3.4351 | -1.2867 |
| **C** | -6.0856 | 2.1926 | -1.1929 | **C** | -6.0949 | 2.1923 | -1.1890 |
| **C** | -6.1735 | -2.1049 | 1.2122 | **C** | -6.1973 | -2.1041 | 1.2043 |
| **C** | -6.9356 | -3.3100 | 1.3284 | **C** | -6.9640 | -3.3077 | 1.3070 |
| **C** | -7.9607 | -3.6148 | 0.3741 | **C** | -7.9723 | -3.6104 | 0.3339 |
| **C** | -8.2109 | -2.7049 | -0.7037 | **C** | -8.2012 | -2.7002 | -0.7486 |
| **C** | -7.4386 | -1.5066 | -0.8346 | **C** | -7.4241 | -1.5032 | -0.8652 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **H** | 6.5123 | 1.8986 | 1.2054 | **H** | 6.5142 | 1.9212 | 1.1674 |
| **H** | 9.0237 | 1.8292 | 1.1456 | **H** | 9.0249 | 1.8518 | 1.1061 |
| **H** | 8.8856 | -1.9374 | -1.1649 | **H** | 8.8855 | -1.9601 | -1.1309 |
| **H** | 6.3484 | -1.8615 | -1.1360 | **H** | 6.3500 | -1.8842 | -1.1013 |
| **H** | -1.5788 | -1.9838 | -1.1835 | **H** | -1.5773 | -1.9996 | -1.1529 |
| **H** | -4.0767 | -1.9172 | -1.1423 | **H** | -4.0742 | -1.9316 | -1.1162 |
| **H** | -3.9465 | 1.8976 | 1.1052 | **H** | -3.9450 | 1.9081 | 1.0912 |
| **H** | -1.4320 | 1.8251 | 1.0730 | **H** | -1.4324 | 1.8343 | 1.0621 |
| **H** | -7.5557 | 0.9660 | 1.7306 | **H** | -7.5326 | 0.9718 | 1.7534 |
| **H** | -8.8247 | 3.1631 | 1.5285 | **H** | -8.8026 | 3.1698 | 1.5618 |
| **H** | -8.3331 | 4.7608 | -0.4114 | **H** | -8.3314 | 4.7638 | -0.3863 |
| **H** | -6.5679 | 4.1226 | -2.1537 | **H** | -6.5866 | 4.1212 | -2.1477 |
| **H** | -5.3211 | 1.9128 | -1.9625 | **H** | -5.3400 | 1.9100 | -1.9671 |
| **H** | -5.3823 | -1.8643 | 1.9679 | **H** | -5.4198 | -1.8645 | 1.9746 |
| **H** | -6.7359 | -4.0085 | 2.1820 | **H** | -6.7815 | -4.0066 | 2.1641 |
| **H** | -8.5620 | -4.5552 | 0.4715 | **H** | -8.5772 | -4.5495 | 0.4204 |
| **H** | -9.0068 | -2.9332 | -1.4593 | **H** | -8.9834 | -2.9270 | -1.5187 |
| **H** | -7.6324 | -0.8025 | -1.6840 | **H** | -7.6000 | -0.7993 | -1.7187 |
| **C** | 9.1261 | -0.0604 | -0.0155 | **C** | 9.1275 | -0.0607 | -0.0179 |
| **C** | 10.6544 | -0.1460 | -0.0648 | **C** | 10.6560 | -0.1455 | -0.0673 |
| **O** | 11.2775 | -1.0470 | -0.6120 | **O** | 11.2788 | -1.0568 | -0.5992 |
| **O** | 11.2652 | 0.8915 | 0.5674 | **O** | 11.2662 | 0.9029 | 0.5443 |
| **H** | 12.2427 | 0.7691 | 0.4939 | **H** | 12.2443 | 0.7824 | 0.4730 |

We show XYZ coordinates of asymmetric TTz dyes for emission cases. These coordinates are obtained based on the dielectric DFT method of Eq. (2) with the 6-31+G* basis set.

### $Bu_2N$-TTz-Py in emission

| **toluene** | | | | **chloroform** | | | |
|---|---|---|---|---|---|---|---|
| **C** | -3.2332 | -0.7783 | -0.1413 | **C** | -3.2312 | -0.7802 | -0.1378 |
| **C** | -2.8478 | 0.6196 | -0.0045 | **C** | -2.8459 | 0.6209 | -0.0230 |
| **S** | -4.3393 | 1.6145 | 0.1661 | **S** | -4.3388 | 1.6167 | 0.1418 |
| **C** | -5.3056 | 0.0121 | 0.0499 | **C** | -5.3056 | 0.0131 | 0.0463 |
| **N** | -4.5364 | -1.1023 | -0.1123 | **N** | -4.5322 | -1.1046 | -0.1010 |
| **S** | -1.7533 | -1.7701 | -0.3224 | **S** | -1.7493 | -1.7725 | -0.3087 |
| **C** | -0.7738 | -0.1742 | -0.2155 | **C** | -0.7695 | -0.1754 | -0.2185 |
| **N** | -1.5492 | 0.9378 | -0.0457 | **N** | -1.5494 | 0.9394 | -0.0666 |
| **C** | -6.7663 | -0.0080 | 0.1145 | **C** | -6.7628 | -0.0090 | 0.1173 |
| **C** | 0.6764 | -0.1542 | -0.2673 | **C** | 0.6781 | -0.1529 | -0.2778 |
| **C** | -7.4993 | -1.2625 | 0.0200 | **C** | -7.4972 | -1.2663 | 0.0425 |
| **C** | -8.9167 | -1.2373 | 0.0881 | **C** | -8.9137 | -1.2425 | 0.1158 |
| **N** | -9.6711 | -0.1031 | 0.2381 | **N** | -9.6707 | -0.1069 | 0.2541 |
| **C** | -8.9862 | 1.0749 | 0.3239 | **C** | -8.9854 | 1.0739 | 0.3230 |
| **C** | -7.5693 | 1.1923 | 0.2702 | **C** | -7.5696 | 1.1924 | 0.2626 |
| **C** | 1.4055 | 1.1092 | -0.1449 | **C** | 1.4075 | 1.1137 | -0.1753 |
| **C** | 2.8078 | 1.1628 | -0.2137 | **C** | 2.8091 | 1.1681 | -0.2451 |
| **C** | 3.6217 | -0.0445 | -0.4125 | **C** | 3.6254 | -0.0424 | -0.4260 |
| **C** | 2.8899 | -1.3108 | -0.4969 | **C** | 2.8924 | -1.3115 | -0.4977 |
| **C** | 1.4829 | -1.3592 | -0.4297 | **C** | 1.4867 | -1.3596 | -0.4303 |
| **N** | 5.0087 | 0.0136 | -0.4969 | **N** | 5.0087 | 0.0138 | -0.5103 |
| **C** | 5.7282 | 1.3173 | -0.6964 | **C** | 5.7339 | 1.3191 | -0.6917 |
| **C** | 5.8433 | -1.2346 | -0.5288 | **C** | 5.8436 | -1.2368 | -0.5367 |
| **C** | 6.2820 | 1.9672 | 0.6346 | **C** | 6.2602 | 1.9640 | 0.6530 |
| **C** | 7.0440 | 3.3319 | 0.3967 | **C** | 7.0278 | 3.3290 | 0.4347 |
| **C** | 6.1197 | 4.5474 | -0.0014 | **C** | 6.1131 | 4.5476 | 0.0241 |
| **C** | 5.9917 | -1.9555 | 0.8734 | **C** | 5.9937 | -1.9497 | 0.8696 |
| **C** | 6.7180 | -3.3558 | 0.7831 | **C** | 6.7175 | -3.3516 | 0.7836 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | 8.2340 | -3.2913 | 0.3505 | **C** | 8.2331 | -3.2911 | 0.3488 |
| **H** | -6.9572 | -2.2301 | -0.1024 | **H** | -6.9567 | -2.2360 | -0.0697 |
| **H** | -9.4912 | -2.1959 | 0.0178 | **H** | -9.4857 | -2.2034 | 0.0600 |
| **H** | -9.6121 | 1.9956 | 0.4444 | **H** | -9.6109 | 1.9959 | 0.4347 |
| **H** | -7.1060 | 2.2073 | 0.3498 | **H** | -7.1089 | 2.2094 | 0.3281 |
| **H** | 0.8295 | 2.0515 | 0.0134 | **H** | 0.8327 | 2.0588 | -0.0299 |
| **H** | 3.2944 | 2.1556 | -0.0805 | **H** | 3.2934 | 2.1635 | -0.1282 |
| **H** | 3.4328 | -2.2742 | -0.6233 | **H** | 3.4353 | -2.2757 | -0.6151 |
| **H** | 0.9893 | -2.3592 | -0.5151 | **H** | 0.9946 | -2.3610 | -0.5051 |
| **H** | 6.5945 | 1.1144 | -1.3949 | **H** | 6.6136 | 1.1151 | -1.3712 |
| **H** | 5.0473 | 2.0244 | -1.2459 | **H** | 5.0651 | 2.0274 | -1.2541 |
| **H** | 5.4231 | -1.9551 | -1.2975 | **H** | 5.4197 | -1.9595 | -1.2998 |
| **H** | 6.8574 | -0.9316 | -0.9089 | **H** | 6.8562 | -0.9359 | -0.9209 |
| **H** | 5.4278 | 2.1260 | 1.3656 | **H** | 5.3919 | 2.1219 | 1.3672 |
| **H** | 6.9899 | 1.2311 | 1.1262 | **H** | 6.9588 | 1.2268 | 1.1550 |
| **H** | 7.5985 | 3.5945 | 1.3504 | **H** | 7.5635 | 3.5865 | 1.4004 |
| **H** | 7.8433 | 3.1841 | -0.3991 | **H** | 7.8419 | 3.1831 | -0.3461 |
| **H** | 5.3215 | 4.7258 | 0.7857 | **H** | 5.2986 | 4.7217 | 0.7953 |
| **H** | 6.7275 | 5.4995 | -0.0919 | **H** | 6.7241 | 5.4994 | -0.0481 |
| **H** | 5.5976 | 4.3901 | -0.9949 | **H** | 5.6117 | 4.3957 | -0.9808 |
| **H** | 6.5633 | -1.2743 | 1.5783 | **H** | 6.5680 | -1.2668 | 1.5701 |
| **H** | 4.9677 | -2.1012 | 1.3326 | **H** | 4.9704 | -2.0929 | 1.3312 |
| **H** | 6.6487 | -3.8506 | 1.8012 | **H** | 6.6491 | -3.8416 | 1.8041 |
| **H** | 6.1481 | -4.0309 | 0.0667 | **H** | 6.1453 | -4.0280 | 0.0704 |
| **H** | 8.8256 | -2.6088 | 1.0388 | **H** | 8.8261 | -2.6069 | 1.0341 |
| **H** | 8.7085 | -4.3191 | 0.3986 | **H** | 8.7054 | -4.3198 | 0.4000 |
| **H** | 8.3660 | -2.9121 | -0.7094 | **H** | 8.3638 | -2.9153 | -0.7125 |

## $Bu_2N$-TTz-Py in emission state

| DCM | | | | methanol | | | |
|---|---|---|---|---|---|---|---|
| **C** | -3.2329 | -0.7792 | -0.1332 | **C** | -3.2341 | -0.7794 | -0.1266 |
| **C** | -2.8474 | 0.6231 | -0.0220 | **C** | -2.8484 | 0.6243 | -0.0209 |
| **S** | -4.3413 | 1.6190 | 0.1401 | **S** | -4.3431 | 1.6208 | 0.1360 |
| **C** | -5.3086 | 0.0156 | 0.0461 | **C** | -5.3111 | 0.0175 | 0.0460 |
| **N** | -4.5328 | -1.1033 | -0.0971 | **N** | -4.5330 | -1.1029 | -0.0912 |
| **S** | -1.7501 | -1.7713 | -0.3001 | **S** | -1.7504 | -1.7718 | -0.2877 |
| **C** | -0.7697 | -0.1742 | -0.2110 | **C** | -0.7695 | -0.1743 | -0.2032 |
| **N** | -1.5523 | 0.9417 | -0.0637 | **N** | -1.5545 | 0.9429 | -0.0619 |
| **C** | -6.7641 | -0.0076 | 0.1153 | **C** | -6.7650 | -0.0066 | 0.1127 |
| **C** | 0.6762 | -0.1506 | -0.2723 | **C** | 0.6747 | -0.1497 | -0.2659 |
| **C** | -7.4994 | -1.2658 | 0.0410 | **C** | -7.5011 | -1.2658 | 0.0410 |
| **C** | -8.9157 | -1.2429 | 0.1120 | **C** | -8.9172 | -1.2436 | 0.1093 |
| **N** | -9.6744 | -0.1072 | 0.2478 | **N** | -9.6776 | -0.1076 | 0.2404 |
| **C** | -8.9888 | 1.0746 | 0.3168 | **C** | -8.9918 | 1.0754 | 0.3072 |
| **C** | -7.5735 | 1.1937 | 0.2585 | **C** | -7.5767 | 1.1949 | 0.2511 |
| **C** | 1.4065 | 1.1171 | -0.1748 | **C** | 1.4053 | 1.1195 | -0.1756 |
| **C** | 2.8073 | 1.1716 | -0.2468 | **C** | 2.8055 | 1.1746 | -0.2497 |
| **C** | 3.6242 | -0.0401 | -0.4251 | **C** | 3.6234 | -0.0385 | -0.4235 |
| **C** | 2.8902 | -1.3105 | -0.4926 | **C** | 2.8889 | -1.3106 | -0.4838 |
| **C** | 1.4855 | -1.3583 | -0.4236 | **C** | 1.4851 | -1.3583 | -0.4130 |
| **N** | 5.0051 | 0.0150 | -0.5125 | **N** | 5.0018 | 0.0161 | -0.5146 |
| **C** | 5.7332 | 1.3205 | -0.6898 | **C** | 5.7320 | 1.3224 | -0.6872 |
| **C** | 5.8401 | -1.2370 | -0.5410 | **C** | 5.8376 | -1.2370 | -0.5464 |
| **C** | 6.2613 | 1.9580 | 0.6576 | **C** | 6.2572 | 1.9548 | 0.6635 |
| **C** | 7.0435 | 3.3151 | 0.4433 | **C** | 7.0515 | 3.3056 | 0.4539 |
| **C** | 6.1453 | 4.5404 | 0.0169 | **C** | 6.1682 | 4.5354 | 0.0102 |
| **C** | 5.9929 | -1.9493 | 0.8652 | **C** | 5.9964 | -1.9478 | 0.8599 |
| **C** | 6.7144 | -3.3523 | 0.7773 | **C** | 6.7163 | -3.3514 | 0.7694 |
| **C** | 8.2285 | -3.2938 | 0.3371 | **C** | 8.2274 | -3.2945 | 0.3190 |
| **H** | -6.9596 | -2.2361 | -0.0695 | **H** | -6.9621 | -2.2370 | -0.0658 |
| **H** | -9.4862 | -2.2047 | 0.0562 | **H** | -9.4864 | -2.2063 | 0.0550 |
| **H** | -9.6143 | 1.9968 | 0.4268 | **H** | -9.6172 | 1.9979 | 0.4136 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **H** | -7.1142 | 2.2112 | 0.3241 | **H** | -7.1189 | 2.2131 | 0.3146 |
| **H** | 0.8328 | 2.0632 | -0.0314 | **H** | 0.8325 | 2.0666 | -0.0360 |
| **H** | 3.2914 | 2.1676 | -0.1340 | **H** | 3.2886 | 2.1714 | -0.1430 |
| **H** | 3.4327 | -2.2749 | -0.6087 | **H** | 3.4313 | -2.2753 | -0.5960 |
| **H** | 0.9937 | -2.3599 | -0.4954 | **H** | 0.9941 | -2.3605 | -0.4795 |
| **H** | 6.6114 | 1.1161 | -1.3703 | **H** | 6.6110 | 1.1176 | -1.3658 |
| **H** | 5.0654 | 2.0321 | -1.2486 | **H** | 5.0663 | 2.0359 | -1.2457 |
| **H** | 5.4132 | -1.9586 | -1.3029 | **H** | 5.4067 | -1.9578 | -1.3060 |
| **H** | 6.8513 | -0.9361 | -0.9277 | **H** | 6.8465 | -0.9354 | -0.9375 |
| **H** | 5.3922 | 2.1242 | 1.3690 | **H** | 5.3855 | 2.1282 | 1.3699 |
| **H** | 6.9516 | 1.2140 | 1.1607 | **H** | 6.9394 | 1.2058 | 1.1697 |
| **H** | 7.5695 | 3.5709 | 1.4149 | **H** | 7.5658 | 3.5612 | 1.4318 |
| **H** | 7.8654 | 3.1584 | -0.3269 | **H** | 7.8823 | 3.1394 | -0.3045 |
| **H** | 5.3191 | 4.7210 | 0.7741 | **H** | 5.3289 | 4.7212 | 0.7517 |
| **H** | 6.7653 | 5.4873 | -0.0454 | **H** | 6.7950 | 5.4786 | -0.0417 |
| **H** | 5.6600 | 4.3913 | -0.9961 | **H** | 5.7007 | 4.3874 | -1.0113 |
| **H** | 6.5707 | -1.2675 | 1.5638 | **H** | 6.5789 | -1.2663 | 1.5545 |
| **H** | 4.9708 | -2.0916 | 1.3299 | **H** | 4.9766 | -2.0895 | 1.3298 |
| **H** | 6.6492 | -3.8410 | 1.7987 | **H** | 6.6578 | -3.8375 | 1.7926 |
| **H** | 6.1385 | -4.0280 | 0.0667 | **H** | 6.1348 | -4.0279 | 0.0642 |
| **H** | 8.8243 | -2.6092 | 1.0195 | **H** | 8.8275 | -2.6073 | 0.9949 |
| **H** | 8.6997 | -4.3232 | 0.3879 | **H** | 8.6986 | -4.3241 | 0.3703 |
| **H** | 8.3555 | -2.9192 | -0.7250 | **H** | 8.3469 | -2.9235 | -0.7451 |

## Ph2N-TTz-Py in emission case

| toluene | | | | chloroform | | | |
|---|---|---|---|---|---|---|---|
| **C** | 1.1939 | -0.1222 | -0.0817 | **C** | 1.1938 | -0.1223 | -0.0843 |
| **N** | 1.9773 | 0.8486 | 0.4833 | **N** | 1.9806 | 0.8645 | 0.4548 |
| **C** | 3.2762 | 0.5681 | 0.3256 | **C** | 3.2774 | 0.5793 | 0.3059 |
| **C** | 3.6559 | -0.6466 | -0.3773 | **C** | 3.6582 | -0.6562 | -0.3634 |
| **S** | 2.1694 | -1.5112 | -0.8842 | **S** | 2.1708 | -1.5336 | -0.8472 |
| **S** | 4.7763 | 1.4269 | 0.8339 | **S** | 4.7781 | 1.4514 | 0.7918 |
| **C** | 5.7372 | 0.0358 | 0.0301 | **C** | 5.7403 | 0.0383 | 0.0286 |
| **N** | 4.9632 | -0.9279 | -0.5323 | **N** | 4.9637 | -0.9417 | -0.5089 |
| **C** | 7.2061 | 0.0139 | 0.0234 | **C** | 7.2065 | 0.0141 | 0.0244 |
| **C** | -0.2562 | -0.1022 | -0.0731 | **C** | -0.2537 | -0.1011 | -0.0759 |
| **C** | 8.0156 | 1.0510 | 0.6341 | **C** | 8.0181 | 1.0670 | 0.6086 |
| **C** | 9.4350 | 0.9453 | 0.5785 | **C** | 9.4368 | 0.9585 | 0.5586 |
| **N** | 10.1130 | -0.0787 | -0.0182 | **N** | 10.1160 | -0.0827 | -0.0095 |
| **C** | 9.3508 | -1.0598 | -0.5956 | **C** | 9.3527 | -1.0789 | -0.5621 |
| **C** | 7.9299 | -1.0760 | -0.6113 | **C** | 7.9324 | -1.0937 | -0.5798 |
| **C** | -1.0649 | -1.1562 | -0.6894 | **C** | -1.0641 | -1.1703 | -0.6664 |
| **C** | -2.4754 | -1.1095 | -0.6615 | **C** | -2.4734 | -1.1242 | -0.6375 |
| **C** | -3.1728 | -0.0100 | -0.0196 | **C** | -3.1729 | -0.0089 | -0.0212 |
| **C** | -2.3813 | 1.0458 | 0.5963 | **C** | -2.3795 | 1.0633 | 0.5668 |
| **C** | -0.9741 | 1.0037 | 0.5742 | **C** | -0.9732 | 1.0208 | 0.5444 |
| **N** | -4.5957 | 0.0329 | 0.0124 | **N** | -4.5916 | 0.0330 | 0.0116 |
| **C** | -5.3629 | -1.1880 | 0.1848 | **C** | -5.3615 | -1.1891 | 0.1782 |
| **C** | -5.2963 | 1.2964 | -0.1317 | **C** | -5.2964 | 1.2972 | -0.1246 |
| **C** | -6.3618 | 1.6392 | 0.7715 | **C** | -6.3451 | 1.6413 | 0.7964 |
| **C** | -7.0504 | 2.8804 | 0.6207 | **C** | -7.0389 | 2.8811 | 0.6522 |
| **C** | -6.6833 | 3.7936 | -0.4211 | **C** | -6.6926 | 3.7892 | -0.4013 |
| **C** | -5.6192 | 3.4520 | -1.3172 | **C** | -5.6453 | 3.4446 | -1.3164 |
| **C** | -4.9281 | 2.2101 | -1.1797 | **C** | -4.9496 | 2.2042 | -1.1850 |
| **C** | -5.0124 | -2.1187 | 1.2239 | **C** | -5.0269 | -2.1127 | 1.2281 |
| **C** | -5.7698 | -3.3175 | 1.3910 | **C** | -5.7873 | -3.3106 | 1.3909 |
| **C** | -6.8827 | -3.5985 | 0.5335 | **C** | -6.8872 | -3.5959 | 0.5177 |
| **C** | -7.2315 | -2.6685 | -0.4994 | **C** | -7.2205 | -2.6715 | -0.5256 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | -6.4768 | -1.4700 | -0.6796 | **C** | -6.4624 | -1.4738 | -0.7009 |
| **H** | 7.5575 | 1.9334 | 1.1487 | **H** | 7.5613 | 1.9637 | 1.0988 |
| **H** | 10.0675 | 1.7424 | 1.0479 | **H** | 10.0682 | 1.7679 | 1.0079 |
| **H** | 9.9197 | -1.8940 | -1.0817 | **H** | 9.9204 | -1.9270 | -1.0248 |
| **H** | 7.3804 | -1.9136 | -1.1048 | **H** | 7.3851 | -1.9449 | -1.0519 |
| **H** | -0.5714 | -2.0124 | -1.2144 | **H** | -0.5718 | -2.0381 | -1.1729 |
| **H** | -3.0618 | -1.9222 | -1.1569 | **H** | -3.0586 | -1.9485 | -1.1140 |
| **H** | -2.8980 | 1.8921 | 1.1130 | **H** | -2.8946 | 1.9218 | 1.0640 |
| **H** | -0.3866 | 1.8117 | 1.0724 | **H** | -0.3876 | 1.8416 | 1.0235 |
| **H** | -6.6439 | 0.9338 | 1.5929 | **H** | -6.6107 | 0.9395 | 1.6263 |
| **H** | -7.8747 | 3.1421 | 1.3323 | **H** | -7.8506 | 3.1449 | 1.3772 |
| **H** | -7.2249 | 4.7671 | -0.5338 | **H** | -7.2381 | 4.7610 | -0.5093 |
| **H** | -5.3311 | 4.1535 | -2.1414 | **H** | -5.3748 | 4.1415 | -2.1501 |
| **H** | -4.1080 | 1.9389 | -1.8910 | **H** | -4.1440 | 1.9294 | -1.9114 |
| **H** | -4.1540 | -1.8936 | 1.9055 | **H** | -4.1799 | -1.8831 | 1.9225 |
| **H** | -5.4953 | -4.0321 | 2.2085 | **H** | -5.5260 | -4.0202 | 2.2169 |
| **H** | -7.4762 | -4.5380 | 0.6698 | **H** | -7.4832 | -4.5343 | 0.6505 |
| **H** | -8.0940 | -2.8832 | -1.1809 | **H** | -8.0732 | -2.8893 | -1.2180 |
| **H** | -6.7457 | -0.7510 | -1.4937 | **H** | -6.7191 | -0.7591 | -1.5226 |

## Ph2N-TTz-Py in emission case

| DCM | | | | methanol | | | |
|---|---|---|---|---|---|---|---|
| **C** | 1.1938 | -0.1231 | -0.0840 | **C** | 1.1937 | -0.1257 | -0.0810 |
| **N** | 1.9827 | 0.8745 | 0.4363 | **N** | 1.9845 | 0.8812 | 0.4226 |
| **C** | 3.2782 | 0.5862 | 0.2934 | **C** | 3.2788 | 0.5909 | 0.2843 |
| **C** | 3.6594 | -0.6634 | -0.3517 | **C** | 3.6605 | -0.6707 | -0.3396 |
| **S** | 2.1715 | -1.5496 | -0.8187 | **S** | 2.1722 | -1.5649 | -0.7906 |
| **S** | 4.7792 | 1.4680 | 0.7619 | **S** | 4.7801 | 1.4813 | 0.7369 |
| **C** | 5.7421 | 0.0396 | 0.0278 | **C** | 5.7437 | 0.0405 | 0.0277 |
| **N** | 4.9637 | -0.9516 | -0.4909 | **N** | 4.9637 | -0.9607 | -0.4740 |
| **C** | 7.2065 | 0.0143 | 0.0245 | **C** | 7.2064 | 0.0147 | 0.0238 |
| **C** | -0.2522 | -0.1012 | -0.0755 | **C** | -0.2508 | -0.1029 | -0.0726 |
| **C** | 8.0198 | 1.0793 | 0.5864 | **C** | 8.0215 | 1.0901 | 0.5656 |
| **C** | 9.4382 | 0.9690 | 0.5392 | **C** | 9.4395 | 0.9790 | 0.5193 |
| **N** | 10.1177 | -0.0851 | -0.0062 | **N** | 10.1193 | -0.0855 | -0.0076 |
| **C** | 9.3534 | -1.0929 | -0.5380 | **C** | 9.3539 | -1.1032 | -0.5203 |
| **C** | 7.9333 | -1.1071 | -0.5557 | **C** | 7.9341 | -1.1175 | -0.5366 |
| **C** | -1.0636 | -1.1794 | -0.6498 | **C** | -1.0632 | -1.1888 | -0.6326 |
| **C** | -2.4721 | -1.1335 | -0.6209 | **C** | -2.4710 | -1.1425 | -0.6042 |
| **C** | -3.1728 | -0.0085 | -0.0208 | **C** | -3.1727 | -0.0089 | -0.0192 |
| **C** | -2.3784 | 1.0730 | 0.5505 | **C** | -2.3772 | 1.0805 | 0.5377 |
| **C** | -0.9726 | 1.0303 | 0.5280 | **C** | -0.9719 | 1.0370 | 0.5159 |
| **N** | -4.5890 | 0.0333 | 0.0115 | **N** | -4.5865 | 0.0337 | 0.0116 |
| **C** | -5.3612 | -1.1895 | 0.1727 | **C** | -5.3617 | -1.1891 | 0.1672 |
| **C** | -5.2958 | 1.2982 | -0.1198 | **C** | -5.2942 | 1.2997 | -0.1160 |
| **C** | -6.3349 | 1.6427 | 0.8113 | **C** | -6.3233 | 1.6466 | 0.8247 |
| **C** | -7.0313 | 2.8819 | 0.6716 | **C** | -7.0213 | 2.8856 | 0.6882 |
| **C** | -6.6967 | 3.7877 | -0.3879 | **C** | -6.6977 | 3.7877 | -0.3780 |
| **C** | -5.6590 | 3.4416 | -1.3136 | **C** | -5.6700 | 3.4382 | -1.3138 |
| **C** | -4.9610 | 2.2018 | -1.1863 | **C** | -4.9707 | 2.1986 | -1.1894 |
| **C** | -5.0390 | -2.1086 | 1.2299 | **C** | -5.0529 | -2.1041 | 1.2314 |
| **C** | -5.8017 | -3.3059 | 1.3883 | **C** | -5.8188 | -3.3003 | 1.3849 |
| **C** | -6.8913 | -3.5938 | 0.5029 | **C** | -6.8980 | -3.5900 | 0.4873 |
| **C** | -7.2124 | -2.6729 | -0.5474 | **C** | -7.2058 | -2.6723 | -0.5700 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | -6.4518 | -1.4758 | -0.7180 | **C** | -6.4418 | -1.4763 | -0.7354 |
| **H** | 7.5643 | 1.9868 | 1.0571 | **H** | 7.5672 | 2.0062 | 1.0203 |
| **H** | 10.0692 | 1.7878 | 0.9715 | **H** | 10.0702 | 1.8058 | 0.9361 |
| **H** | 9.9201 | -1.9513 | -0.9823 | **H** | 9.9196 | -1.9701 | -0.9494 |
| **H** | 7.3871 | -1.9686 | -1.0100 | **H** | 7.3888 | -1.9880 | -0.9746 |
| **H** | -0.5720 | -2.0541 | -1.1449 | **H** | -0.5723 | -2.0696 | -1.1173 |
| **H** | -3.0566 | -1.9644 | -1.0861 | **H** | -3.0548 | -1.9791 | -1.0597 |
| **H** | -2.8926 | 1.9383 | 1.0362 | **H** | -2.8905 | 1.9518 | 1.0132 |
| **H** | -0.3881 | 1.8585 | 0.9955 | **H** | -0.3884 | 1.8716 | 0.9731 |
| **H** | -6.5913 | 0.9426 | 1.6456 | **H** | -6.5706 | 0.9495 | 1.6642 |
| **H** | -7.8357 | 3.1468 | 1.4042 | **H** | -7.8179 | 3.1531 | 1.4283 |
| **H** | -7.2441 | 4.7587 | -0.4926 | **H** | -7.2462 | 4.7583 | -0.4804 |
| **H** | -5.3984 | 4.1363 | -2.1523 | **H** | -5.4186 | 4.1296 | -2.1580 |
| **H** | -4.1638 | 1.9251 | -1.9213 | **H** | -4.1824 | 1.9185 | -1.9326 |
| **H** | -4.2006 | -1.8763 | 1.9338 | **H** | -4.2233 | -1.8697 | 1.9449 |
| **H** | -5.5506 | -4.0124 | 2.2200 | **H** | -5.5785 | -4.0040 | 2.2221 |
| **H** | -7.4893 | -4.5314 | 0.6322 | **H** | -7.4985 | -4.5265 | 0.6127 |
| **H** | -8.0572 | -2.8928 | -1.2488 | **H** | -8.0425 | -2.8937 | -1.2805 |
| **H** | -6.6984 | -0.7639 | -1.5452 | **H** | -6.6774 | -0.7671 | -1.5681 |

## Ph2N-TTz-CHO in emission states

| toluene | | | | chloroform | | | |
|---|---|---|---|---|---|---|---|
| **C** | -3.8402 | -0.0043 | -0.0200 | **C** | -3.8396 | -0.0044 | -0.0147 |
| **C** | -3.0394 | 1.0711 | 0.5469 | **C** | -3.0374 | 1.0856 | 0.5255 |
| **C** | -1.6315 | 1.0211 | 0.5155 | **C** | -1.6303 | 1.0334 | 0.4981 |
| **C** | -0.9246 | -0.1105 | -0.0901 | **C** | -0.9217 | -0.1144 | -0.0769 |
| **C** | -1.7391 | -1.1818 | -0.6581 | **C** | -1.7372 | -1.2004 | -0.6177 |
| **C** | -3.1500 | -1.1300 | -0.6235 | **C** | -3.1469 | -1.1475 | -0.5867 |
| **C** | 0.5311 | -0.1380 | -0.1050 | **C** | 0.5314 | -0.1436 | -0.0907 |
| **N** | 1.3175 | 0.8503 | 0.4084 | **N** | 1.3213 | 0.8614 | 0.3915 |
| **C** | 2.6183 | 0.5593 | 0.2633 | **C** | 2.6199 | 0.5657 | 0.2548 |
| **C** | 2.9902 | -0.6892 | -0.3797 | **C** | 2.9919 | -0.7044 | -0.3495 |
| **S** | 1.4970 | -1.5666 | -0.8393 | **S** | 1.4975 | -1.5952 | -0.7797 |
| **S** | 4.1203 | 1.4366 | 0.7272 | **S** | 4.1225 | 1.4577 | 0.6883 |
| **C** | 5.0787 | -0.0022 | -0.0095 | **C** | 5.0818 | -0.0034 | -0.0032 |
| **N** | 4.2927 | -0.9905 | -0.5253 | **N** | 4.2922 | -1.0093 | -0.4870 |
| **C** | 6.5391 | -0.0346 | -0.0139 | **C** | 6.5388 | -0.0364 | -0.0104 |
| **C** | 7.3429 | 1.0462 | 0.5537 | **C** | 7.3459 | 1.0630 | 0.5205 |
| **C** | 8.7556 | 0.9867 | 0.5392 | **C** | 8.7579 | 1.0038 | 0.5020 |
| **C** | 9.4422 | -0.1489 | -0.0397 | **C** | 9.4453 | -0.1493 | -0.0443 |
| **C** | 8.6545 | -1.2221 | -0.6051 | **C** | 8.6548 | -1.2416 | -0.5721 |
| **C** | 7.2396 | -1.1782 | -0.5987 | **C** | 7.2406 | -1.1986 | -0.5614 |
| **C** | 10.9459 | -0.2265 | -0.0593 | **C** | 10.9455 | -0.2277 | -0.0700 |
| **O** | 11.7100 | 0.6272 | 0.3942 | **O** | 11.7151 | 0.6412 | 0.3528 |
| **N** | -5.2602 | 0.0445 | 0.0204 | **N** | -5.2555 | 0.0464 | 0.0194 |
| **C** | -6.0367 | -1.1735 | 0.1953 | **C** | -6.0384 | -1.1718 | 0.1808 |
| **C** | -5.9615 | 1.3119 | -0.1165 | **C** | -5.9581 | 1.3159 | -0.1115 |
| **C** | -5.7124 | -2.0884 | 1.2556 | **C** | -5.7426 | -2.0793 | 1.2547 |
| **C** | -6.4796 | -3.2810 | 1.4268 | **C** | -6.5165 | -3.2697 | 1.4140 |
| **C** | -7.5776 | -3.5687 | 0.5524 | **C** | -7.5925 | -3.5604 | 0.5133 |
| **C** | -7.9019 | -2.6525 | -0.5003 | **C** | -7.8885 | -2.6500 | -0.5531 |
| **C** | -7.1358 | -1.4608 | -0.6844 | **C** | -7.1152 | -1.4605 | -0.7247 |
| **C** | -6.9943 | 1.6687 | 0.8167 | **C** | -6.9781 | 1.6742 | 0.8341 |
| **C** | -7.6869 | 2.9094 | 0.6713 | **C** | -7.6735 | 2.9145 | 0.6937 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | -7.3542 | 3.8062 | -0.3956 | **C** | -7.3554 | 3.8073 | -0.3814 |
| **C** | -6.3225 | 3.4491 | -1.3233 | **C** | -6.3366 | 3.4470 | -1.3223 |
| **C** | -5.6295 | 2.2071 | -1.1910 | **C** | -5.6413 | 2.2054 | -1.1945 |
| **H** | -3.5469 | 1.9406 | 1.0331 | **H** | -3.5436 | 1.9675 | 0.9893 |
| **H** | -1.0378 | 1.8464 | 0.9773 | **H** | -1.0389 | 1.8707 | 0.9407 |
| **H** | -1.2528 | -2.0601 | -1.1531 | **H** | -1.2518 | -2.0914 | -1.0901 |
| **H** | -3.7409 | -1.9601 | -1.0831 | **H** | -3.7359 | -1.9889 | -1.0269 |
| **H** | 6.8459 | 1.9401 | 1.0102 | **H** | 6.8509 | 1.9705 | 0.9512 |
| **H** | 9.3576 | 1.8217 | 0.9776 | **H** | 9.3583 | 1.8541 | 0.9123 |
| **H** | 9.1731 | -2.1085 | -1.0581 | **H** | 9.1719 | -2.1416 | -0.9987 |
| **H** | 6.6459 | -2.0153 | -1.0392 | **H** | 6.6480 | -2.0508 | -0.9732 |
| **H** | 11.3700 | -1.1759 | -0.5456 | **H** | 11.3674 | -1.1905 | -0.5280 |
| **H** | -4.8652 | -1.8573 | 1.9498 | **H** | -4.9133 | -1.8450 | 1.9692 |
| **H** | -6.2248 | -3.9846 | 2.2603 | **H** | -6.2848 | -3.9684 | 2.2582 |
| **H** | -8.1794 | -4.5027 | 0.6919 | **H** | -8.1998 | -4.4922 | 0.6434 |
| **H** | -8.7540 | -2.8716 | -1.1935 | **H** | -8.7236 | -2.8715 | -1.2659 |
| **H** | -7.3866 | -0.7509 | -1.5126 | **H** | -7.3433 | -0.7551 | -1.5631 |
| **H** | -7.2503 | 0.9742 | 1.6562 | **H** | -7.2227 | 0.9825 | 1.6793 |
| **H** | -8.4870 | 3.1826 | 1.4061 | **H** | -8.4641 | 3.1898 | 1.4378 |
| **H** | -7.8981 | 4.7790 | -0.5044 | **H** | -7.9014 | 4.7793 | -0.4867 |
| **H** | -6.0621 | 4.1377 | -2.1675 | **H** | -6.0888 | 4.1319 | -2.1732 |
| **H** | -4.8344 | 1.9231 | -1.9261 | **H** | -4.8576 | 1.9179 | -1.9403 |

## Ph2N-TTz-CHO in emission states

| DCM | | | | methanol | | | |
|---|---|---|---|---|---|---|---|
| **C** | -3.8390 | -0.0049 | -0.0129 | **C** | -3.8384 | -0.0063 | -0.0111 |
| **C** | -3.0359 | 1.0930 | 0.5121 | **C** | -3.0338 | 1.0990 | 0.4984 |
| **C** | -1.6293 | 1.0395 | 0.4868 | **C** | -1.6279 | 1.0435 | 0.4756 |
| **C** | -0.9200 | -0.1170 | -0.0713 | **C** | -0.9182 | -0.1221 | -0.0646 |
| **C** | -1.7363 | -1.2106 | -0.5974 | **C** | -1.7357 | -1.2229 | -0.5754 |
| **C** | -3.1453 | -1.1571 | -0.5679 | **C** | -3.1440 | -1.1681 | -0.5481 |
| **C** | 0.5316 | -0.1473 | -0.0843 | **C** | 0.5317 | -0.1539 | -0.0761 |
| **N** | 1.3232 | 0.8658 | 0.3826 | **N** | 1.3248 | 0.8677 | 0.3748 |
| **C** | 2.6205 | 0.5684 | 0.2499 | **C** | 2.6209 | 0.5688 | 0.2464 |
| **C** | 2.9930 | -0.7120 | -0.3357 | **C** | 2.9941 | -0.7219 | -0.3192 |
| **S** | 1.4981 | -1.6091 | -0.7515 | **S** | 1.4991 | -1.6260 | -0.7194 |
| **S** | 4.1232 | 1.4673 | 0.6691 | **S** | 4.1232 | 1.4754 | 0.6503 |
| **C** | 5.0834 | -0.0036 | -0.0006 | **C** | 5.0848 | -0.0051 | 0.0032 |
| **N** | 4.2920 | -1.0180 | -0.4691 | **N** | 4.2920 | -1.0286 | -0.4487 |
| **C** | 6.5383 | -0.0370 | -0.0088 | **C** | 6.5377 | -0.0380 | -0.0069 |
| **C** | 7.3471 | 1.0707 | 0.5056 | **C** | 7.3477 | 1.0784 | 0.4902 |
| **C** | 8.7586 | 1.0116 | 0.4855 | **C** | 8.7587 | 1.0203 | 0.4675 |
| **C** | 9.4469 | -0.1492 | -0.0459 | **C** | 9.4485 | -0.1475 | -0.0490 |
| **C** | 8.6552 | -1.2499 | -0.5566 | **C** | 8.6559 | -1.2570 | -0.5417 |
| **C** | 7.2415 | -1.2074 | -0.5442 | **C** | 7.2426 | -1.2160 | -0.5266 |
| **C** | 10.9451 | -0.2281 | -0.0743 | **C** | 10.9447 | -0.2258 | -0.0810 |
| **O** | 11.7176 | 0.6477 | 0.3345 | **O** | 11.7195 | 0.6578 | 0.3120 |
| **N** | -5.2525 | 0.0471 | 0.0188 | **N** | -5.2493 | 0.0479 | 0.0175 |
| **C** | -6.0392 | -1.1708 | 0.1739 | **C** | -6.0412 | -1.1689 | 0.1659 |
| **C** | -5.9558 | 1.3178 | -0.1088 | **C** | -5.9520 | 1.3206 | -0.1068 |
| **C** | -5.7595 | -2.0731 | 1.2560 | **C** | -5.7800 | -2.0658 | 1.2565 |
| **C** | -6.5376 | -3.2618 | 1.4101 | **C** | -6.5638 | -3.2518 | 1.4049 |
| **C** | -7.6014 | -3.5548 | 0.4955 | **C** | -7.6145 | -3.5463 | 0.4756 |
| **C** | -7.8812 | -2.6488 | -0.5792 | **C** | -7.8759 | -2.6447 | -0.6076 |
| **C** | -7.1035 | -1.4610 | -0.7452 | **C** | -7.0924 | -1.4596 | -0.7674 |
| **C** | -6.9647 | 1.6795 | 0.8468 | **C** | -6.9466 | 1.6884 | 0.8609 |
| **C** | -7.6617 | 2.9195 | 0.7090 | **C** | -7.6439 | 2.9290 | 0.7257 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **C** | -7.3558 | 3.8073 | -0.3739 | **C** | -7.3518 | 3.8098 | -0.3667 |
| **C** | -6.3479 | 3.4428 | -1.3252 | **C** | -6.3578 | 3.4385 | -1.3301 |
| **C** | -5.6512 | 2.2015 | -1.1995 | **C** | -5.6610 | 2.1968 | -1.2068 |
| **H** | -3.5413 | 1.9814 | 0.9637 | **H** | -3.5381 | 1.9944 | 0.9370 |
| **H** | -1.0390 | 1.8832 | 0.9184 | **H** | -1.0383 | 1.8935 | 0.8958 |
| **H** | -1.2515 | -2.1081 | -1.0576 | **H** | -1.2517 | -2.1271 | -1.0229 |
| **H** | -3.7334 | -2.0043 | -0.9974 | **H** | -3.7315 | -2.0208 | -0.9668 |
| **H** | 6.8529 | 1.9840 | 0.9245 | **H** | 6.8540 | 1.9971 | 0.8974 |
| **H** | 9.3577 | 1.8688 | 0.8833 | **H** | 9.3562 | 1.8847 | 0.8521 |
| **H** | 9.1717 | -2.1557 | -0.9710 | **H** | 9.1722 | -2.1683 | -0.9441 |
| **H** | 6.6498 | -2.0664 | -0.9429 | **H** | 6.6522 | -2.0820 | -0.9117 |
| **H** | 11.3662 | -1.1964 | -0.5191 | **H** | 11.3655 | -1.1997 | -0.5119 |
| **H** | -4.9404 | -1.8364 | 1.9812 | **H** | -4.9716 | -1.8272 | 1.9931 |
| **H** | -6.3190 | -3.9568 | 2.2607 | **H** | -6.3599 | -3.9431 | 2.2621 |
| **H** | -8.2121 | -4.4849 | 0.6215 | **H** | -8.2296 | -4.4741 | 0.5969 |
| **H** | -8.7067 | -2.8722 | -1.3024 | **H** | -8.6911 | -2.8694 | -1.3420 |
| **H** | -7.3183 | -0.7591 | -1.5900 | **H** | -7.2921 | -0.7613 | -1.6190 |
| **H** | -7.1994 | 0.9916 | 1.6980 | **H** | -7.1694 | 1.0060 | 1.7195 |
| **H** | -8.4438 | 3.1983 | 1.4607 | **H** | -8.4150 | 3.2133 | 1.4866 |
| **H** | -7.9030 | 4.7788 | -0.4775 | **H** | -7.8992 | 4.7814 | -0.4684 |
| **H** | -6.1102 | 4.1236 | -2.1822 | **H** | -6.1313 | 4.1138 | -2.1945 |
| **H** | -4.8768 | 1.9099 | -1.9535 | **H** | -4.8982 | 1.8990 | -1.9700 |

## Ph2N-TTz-COOH in emission states

| toluene | | | | chloroform | | | |
|---|---|---|---|---|---|---|---|
| **C** | 0.1757 | -0.1129 | -0.0872 | **C** | 0.1754 | -0.1159 | -0.0822 |
| **N** | 0.9554 | 0.8804 | 0.4353 | **N** | 0.9586 | 0.8930 | 0.4120 |
| **C** | 2.2570 | 0.5987 | 0.2914 | **C** | 2.2581 | 0.6067 | 0.2765 |
| **C** | 2.6405 | -0.6448 | -0.3594 | **C** | 2.6421 | -0.6570 | -0.3383 |
| **S** | 1.1547 | -1.5321 | -0.8286 | **S** | 1.1552 | -1.5566 | -0.7817 |
| **S** | 3.7525 | 1.4829 | 0.7655 | **S** | 3.7543 | 1.5047 | 0.7236 |
| **C** | 4.7229 | 0.0560 | 0.0217 | **C** | 4.7257 | 0.0567 | 0.0228 |
| **N** | 3.9455 | -0.9336 | -0.5024 | **N** | 3.9453 | -0.9494 | -0.4726 |
| **C** | 6.1854 | 0.0357 | 0.0199 | **C** | 6.1854 | 0.0354 | 0.0205 |
| **C** | -1.2777 | -0.0961 | -0.0779 | **C** | -1.2754 | -0.0977 | -0.0732 |
| **C** | 6.9793 | 1.1114 | 0.6015 | **C** | 6.9821 | 1.1290 | 0.5680 |
| **C** | 8.3972 | 1.0612 | 0.5861 | **C** | 8.3994 | 1.0781 | 0.5522 |
| **C** | 8.3113 | -1.1311 | -0.5884 | **C** | 8.3125 | -1.1497 | -0.5542 |
| **C** | 6.8970 | -1.0933 | -0.5791 | **C** | 6.8986 | -1.1122 | -0.5445 |
| **C** | -2.0834 | -1.1746 | -0.6495 | **C** | -2.0825 | -1.1894 | -0.6203 |
| **C** | -3.4948 | -1.1323 | -0.6204 | **C** | -3.4928 | -1.1467 | -0.5926 |
| **C** | -4.1956 | -0.0111 | -0.0204 | **C** | -4.1958 | -0.0108 | -0.0188 |
| **C** | -3.4051 | 1.0707 | 0.5498 | **C** | -3.4037 | 1.0845 | 0.5265 |
| **C** | -1.9968 | 1.0315 | 0.5251 | **C** | -1.9962 | 1.0441 | 0.5034 |
| **N** | -5.6174 | 0.0278 | 0.0139 | **N** | -5.6137 | 0.0288 | 0.0128 |
| **C** | -6.3848 | -1.1939 | 0.2011 | **C** | -6.3854 | -1.1938 | 0.1900 |
| **C** | -6.3262 | 1.2885 | -0.1433 | **C** | -6.3248 | 1.2911 | -0.1362 |
| **C** | -7.3699 | 1.6493 | 0.7769 | **C** | -7.3548 | 1.6522 | 0.7983 |
| **C** | -8.0694 | 2.8838 | 0.6115 | **C** | -8.0576 | 2.8864 | 0.6403 |
| **C** | -7.7328 | 3.7715 | -0.4623 | **C** | -7.7372 | 3.7713 | -0.4410 |
| **C** | -6.6898 | 3.4111 | -1.3763 | **C** | -6.7079 | 3.4091 | -1.3701 |
| **C** | -5.9898 | 2.1749 | -1.2242 | **C** | -6.0049 | 2.1734 | -1.2249 |
| **C** | -6.0520 | -2.0973 | 1.2691 | **C** | -6.0732 | -2.0915 | 1.2682 |
| **C** | -6.8100 | -3.2943 | 1.4522 | **C** | -6.8357 | -3.2875 | 1.4426 |
| **C** | -7.9074 | -3.5984 | 0.5821 | **C** | -7.9167 | -3.5943 | 0.5528 |
| **C** | -8.2398 | -2.6941 | -0.4788 | **C** | -8.2288 | -2.6943 | -0.5182 |
| **C** | -7.4828 | -1.4983 | -0.6750 | **C** | -7.4670 | -1.4995 | -0.7051 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **H** | 6.4798 | 1.9965 | 1.0719 | **H** | 6.4842 | 2.0285 | 1.0121 |
| **H** | 8.9796 | 1.8998 | 1.0403 | **H** | 8.9807 | 1.9312 | 0.9800 |
| **H** | 8.8424 | -2.0003 | -1.0504 | **H** | 8.8408 | -2.0339 | -0.9904 |
| **H** | 6.3106 | -1.9293 | -1.0320 | **H** | 6.3138 | -1.9629 | -0.9712 |
| **H** | -1.5886 | -2.0499 | -1.1418 | **H** | -1.5887 | -2.0754 | -1.0940 |
| **H** | -4.0785 | -1.9673 | -1.0814 | **H** | -4.0750 | -1.9917 | -1.0361 |
| **H** | -3.9219 | 1.9371 | 1.0327 | **H** | -3.9191 | 1.9615 | 0.9907 |
| **H** | -1.4110 | 1.8615 | 0.9890 | **H** | -1.4124 | 1.8851 | 0.9498 |
| **H** | -7.6290 | 0.9625 | 1.6222 | **H** | -7.6011 | 0.9673 | 1.6488 |
| **H** | -8.8781 | 3.1597 | 1.3363 | **H** | -8.8560 | 3.1635 | 1.3758 |
| **H** | -8.2822 | 4.7397 | -0.5867 | **H** | -8.2891 | 4.7388 | -0.5599 |
| **H** | -6.4257 | 4.0924 | -2.2257 | **H** | -6.4575 | 4.0878 | -2.2257 |
| **H** | -5.1858 | 1.8883 | -1.9488 | **H** | -5.2129 | 1.8844 | -1.9617 |
| **H** | -5.2051 | -1.8538 | 1.9598 | **H** | -5.2401 | -1.8450 | 1.9744 |
| **H** | -6.5485 | -3.9887 | 2.2917 | **H** | -6.5910 | -3.9780 | 2.2902 |
| **H** | -8.5021 | -4.5359 | 0.7310 | **H** | -8.5151 | -4.5306 | 0.6947 |
| **H** | -9.0912 | -2.9262 | -1.1692 | **H** | -9.0675 | -2.9285 | -1.2231 |
| **H** | -7.7399 | -0.7981 | -1.5099 | **H** | -7.7077 | -0.8028 | -1.5476 |
| **C** | 9.0888 | -0.0585 | -0.0074 | **C** | 9.0921 | -0.0594 | -0.0078 |
| **C** | 10.6017 | -0.1519 | -0.0433 | **C** | 10.6037 | -0.1519 | -0.0425 |
| **O** | 11.2371 | -1.0823 | -0.5311 | **O** | 11.2399 | -1.0975 | -0.5045 |
| **O** | 11.2236 | 0.9240 | 0.5333 | **O** | 11.2255 | 0.9391 | 0.5007 |
| **H** | 12.1967 | 0.7757 | 0.4635 | **H** | 12.1997 | 0.7935 | 0.4362 |

## Ph2N-TTz-COOH in emission states

| DCM | | | | methanol | | | |
|---|---|---|---|---|---|---|---|
| **C** | 0.1752 | -0.1191 | -0.0749 | **C** | 0.1749 | -0.1224 | -0.0703 |
| **N** | 0.9604 | 0.8968 | 0.4062 | **N** | 0.9618 | 0.9010 | 0.3968 |
| **C** | 2.2586 | 0.6088 | 0.2741 | **C** | 2.2588 | 0.6115 | 0.2685 |
| **C** | 2.6429 | -0.6639 | -0.3246 | **C** | 2.6436 | -0.6706 | -0.3126 |
| **S** | 1.1554 | -1.5692 | -0.7552 | **S** | 1.1559 | -1.5819 | -0.7302 |
| **S** | 3.7552 | 1.5130 | 0.7085 | **S** | 3.7556 | 1.5222 | 0.6896 |
| **C** | 4.7272 | 0.0565 | 0.0260 | **C** | 4.7284 | 0.0568 | 0.0275 |
| **N** | 3.9449 | -0.9573 | -0.4560 | **N** | 3.9447 | -0.9649 | -0.4402 |
| **C** | 6.1851 | 0.0349 | 0.0220 | **C** | 6.1847 | 0.0349 | 0.0228 |
| **C** | -1.2742 | -0.0998 | -0.0668 | **C** | -1.2730 | -0.1020 | -0.0629 |
| **C** | 6.9838 | 1.1356 | 0.5552 | **C** | 6.9851 | 1.1436 | 0.5393 |
| **C** | 8.4008 | 1.0848 | 0.5370 | **C** | 8.4018 | 1.0927 | 0.5200 |
| **C** | 8.3128 | -1.1565 | -0.5424 | **C** | 8.3132 | -1.1645 | -0.5262 |
| **C** | 6.8991 | -1.1196 | -0.5305 | **C** | 6.8997 | -1.1281 | -0.5132 |
| **C** | -2.0820 | -1.1979 | -0.6015 | **C** | -2.0817 | -1.2063 | -0.5853 |
| **C** | -3.4917 | -1.1547 | -0.5754 | **C** | -3.4907 | -1.1625 | -0.5603 |
| **C** | -4.1957 | -0.0107 | -0.0164 | **C** | -4.1956 | -0.0111 | -0.0152 |
| **C** | -3.4029 | 1.0912 | 0.5164 | **C** | -3.4018 | 1.0972 | 0.5050 |
| **C** | -1.9958 | 1.0496 | 0.4955 | **C** | -1.9952 | 1.0545 | 0.4854 |
| **N** | -5.6114 | 0.0299 | 0.0123 | **N** | -5.6091 | 0.0304 | 0.0116 |
| **C** | -6.3861 | -1.1929 | 0.1833 | **C** | -6.3869 | -1.1924 | 0.1770 |
| **C** | -6.3232 | 1.2931 | -0.1343 | **C** | -6.3215 | 1.2948 | -0.1313 |
| **C** | -7.3468 | 1.6556 | 0.8063 | **C** | -7.3352 | 1.6601 | 0.8185 |
| **C** | -8.0511 | 2.8895 | 0.6501 | **C** | -8.0406 | 2.8941 | 0.6654 |
| **C** | -7.7382 | 3.7717 | -0.4358 | **C** | -7.7381 | 3.7724 | -0.4267 |
| **C** | -6.7154 | 3.4072 | -1.3715 | **C** | -6.7250 | 3.4045 | -1.3718 |
| **C** | -6.0112 | 2.1718 | -1.2278 | **C** | -6.0198 | 2.1690 | -1.2308 |
| **C** | -6.0887 | -2.0856 | 1.2695 | **C** | -6.1035 | -2.0805 | 1.2703 |
| **C** | -6.8543 | -3.2805 | 1.4387 | **C** | -6.8723 | -3.2743 | 1.4347 |
| **C** | -7.9234 | -3.5904 | 0.5355 | **C** | -7.9304 | -3.5865 | 0.5192 |
| **C** | -8.2206 | -2.6946 | -0.5435 | **C** | -8.2138 | -2.6945 | -0.5667 |
| **C** | -7.4556 | -1.5008 | -0.7250 | **C** | -7.4453 | -1.5017 | -0.7431 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **H** | 6.4872 | 2.0402 | 0.9899 | **H** | 6.4894 | 2.0545 | 0.9615 |
| **H** | 8.9817 | 1.9437 | 0.9538 | **H** | 8.9821 | 1.9584 | 0.9234 |
| **H** | 8.8393 | -2.0463 | -0.9692 | **H** | 8.8382 | -2.0612 | -0.9405 |
| **H** | 6.3152 | -1.9764 | -0.9460 | **H** | 6.3167 | -1.9919 | -0.9155 |
| **H** | -1.5888 | -2.0896 | -1.0649 | **H** | -1.5891 | -2.1031 | -1.0392 |
| **H** | -4.0730 | -2.0044 | -1.0103 | **H** | -4.0713 | -2.0167 | -0.9868 |
| **H** | -3.9176 | 1.9737 | 0.9703 | **H** | -3.9157 | 1.9849 | 0.9491 |
| **H** | -1.4133 | 1.8960 | 0.9331 | **H** | -1.4137 | 1.9062 | 0.9141 |
| **H** | -7.5871 | 0.9729 | 1.6604 | **H** | -7.5667 | 0.9805 | 1.6774 |
| **H** | -8.8445 | 3.1683 | 1.3902 | **H** | -8.8265 | 3.1757 | 1.4124 |
| **H** | -8.2911 | 4.7386 | -0.5536 | **H** | -8.2919 | 4.7391 | -0.5423 |
| **H** | -6.4715 | 4.0833 | -2.2309 | **H** | -6.4898 | 4.0774 | -2.2360 |
| **H** | -5.2252 | 1.8804 | -1.9700 | **H** | -5.2422 | 1.8742 | -1.9805 |
| **H** | -5.2655 | -1.8360 | 1.9862 | **H** | -5.2895 | -1.8284 | 1.9965 |
| **H** | -6.6216 | -3.9674 | 2.2926 | **H** | -6.6509 | -3.9580 | 2.2941 |
| **H** | -8.5242 | -4.5256 | 0.6733 | **H** | -8.5337 | -4.5206 | 0.6532 |
| **H** | -9.0500 | -2.9313 | -1.2585 | **H** | -9.0346 | -2.9331 | -1.2909 |
| **H** | -7.6841 | -0.8076 | -1.5737 | **H** | -7.6623 | -0.8116 | -1.5974 |
| **C** | 9.0940 | -0.0592 | -0.0110 | **C** | 9.0956 | -0.0591 | -0.0122 |
| **C** | 10.6046 | -0.1504 | -0.0479 | **C** | 10.6054 | -0.1495 | -0.0498 |
| **O** | 11.2410 | -1.1015 | -0.5015 | **O** | 11.2420 | -1.1077 | -0.4913 |
| **O** | 11.2269 | 0.9462 | 0.4812 | **O** | 11.2279 | 0.9538 | 0.4623 |
| **H** | 12.2017 | 0.8029 | 0.4172 | **H** | 12.2032 | 0.8122 | 0.3999 |