

## Supporting Information

# Theoretical Investigation of the $\alpha$ -Substitution Effect on $\gamma$ -C( $sp^3$ )-H Arylation of Amines: Structure-Reactivity Relationship (SRR) Studies

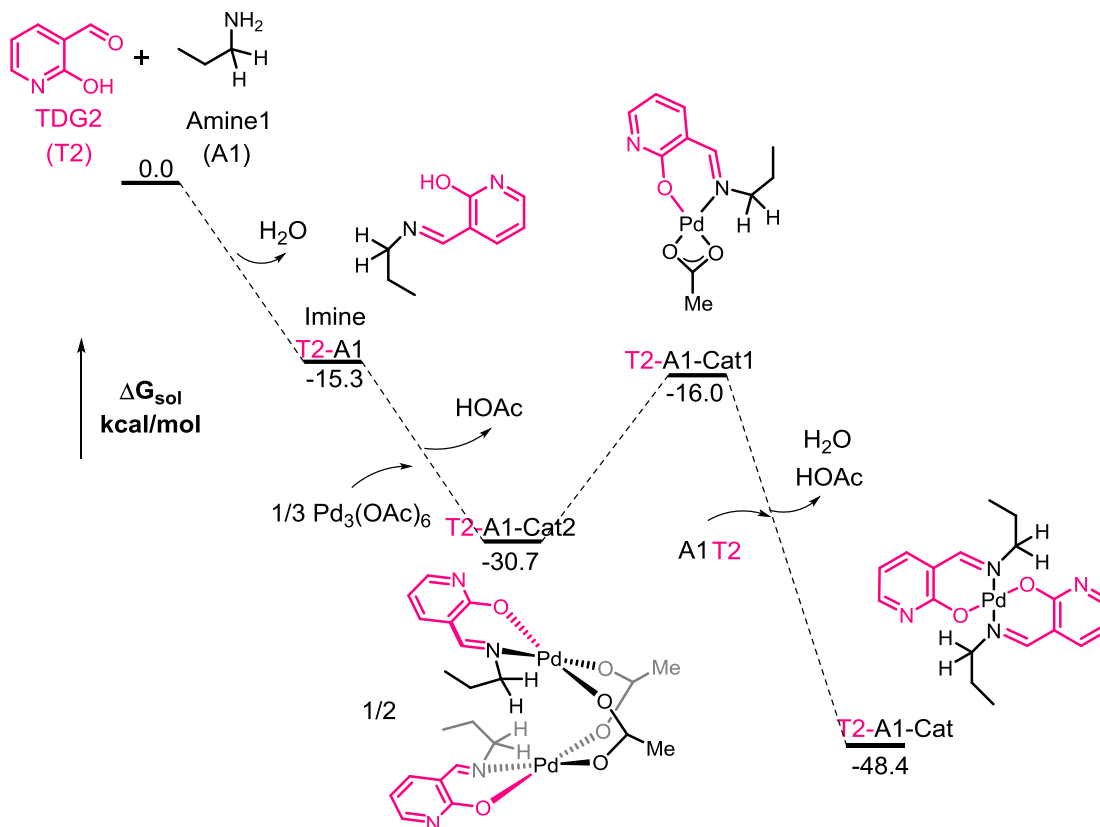
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<sup>a</sup> Department of Chemistry and Key Laboratory for Preparation and Application of Ordered Structural Materials of Guangdong Province, Shantou University, Shantou, Guangdong 515063, PR China

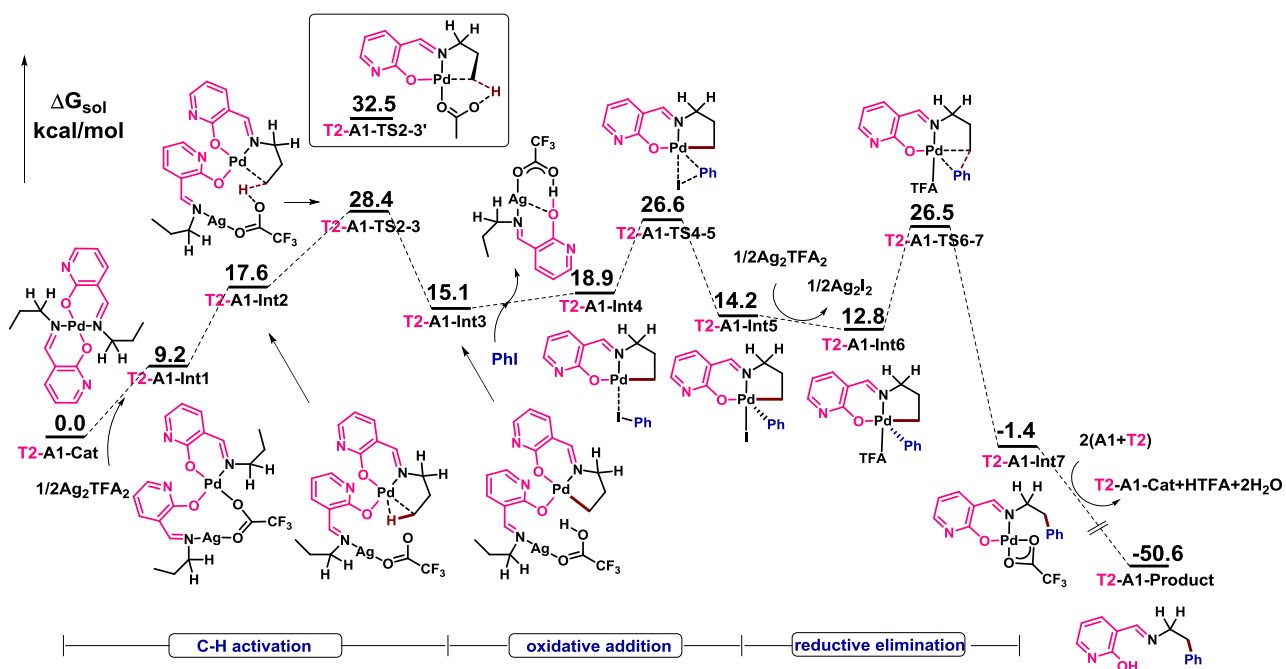
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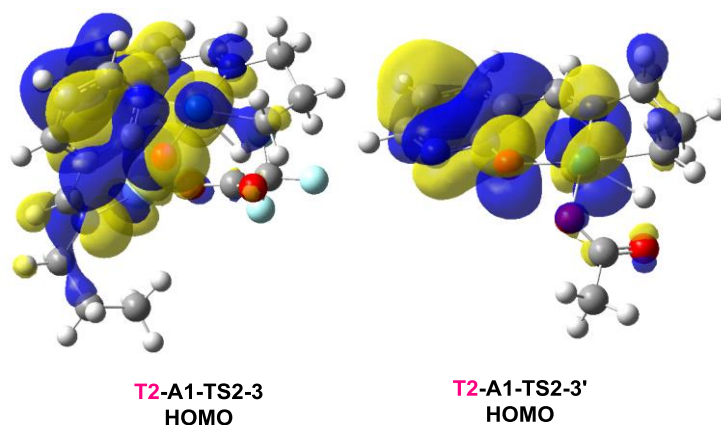
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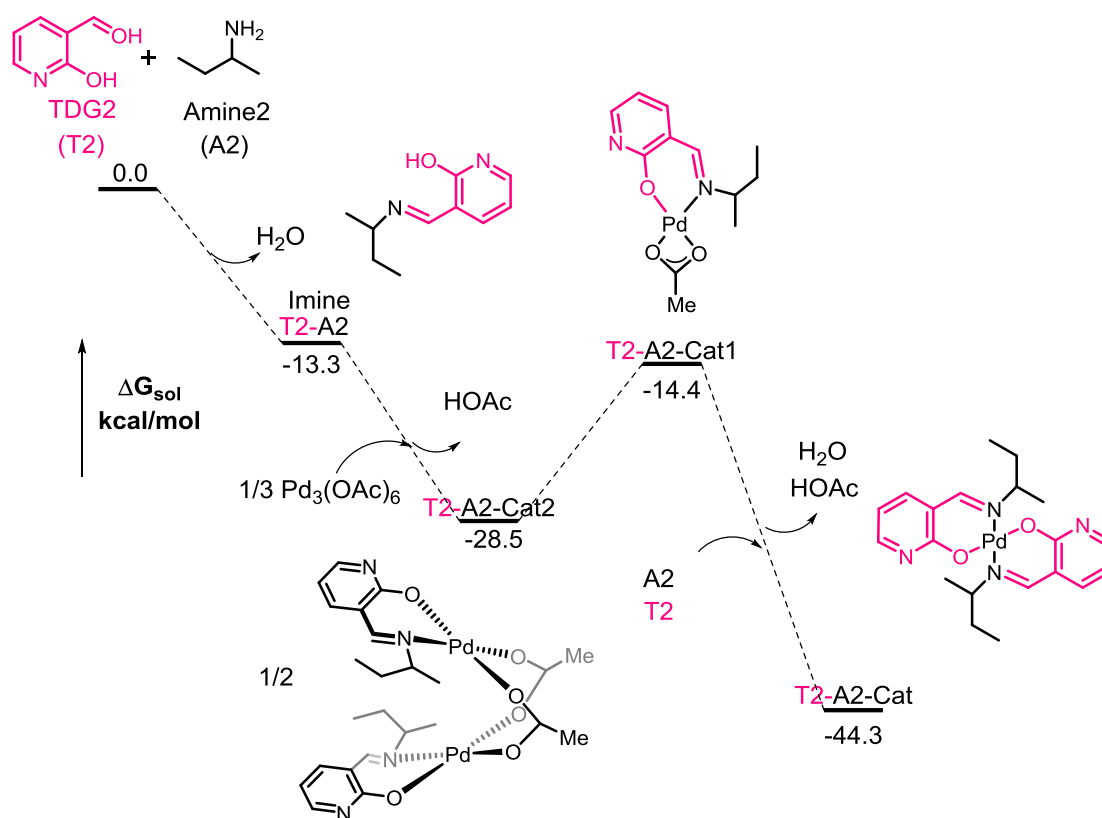
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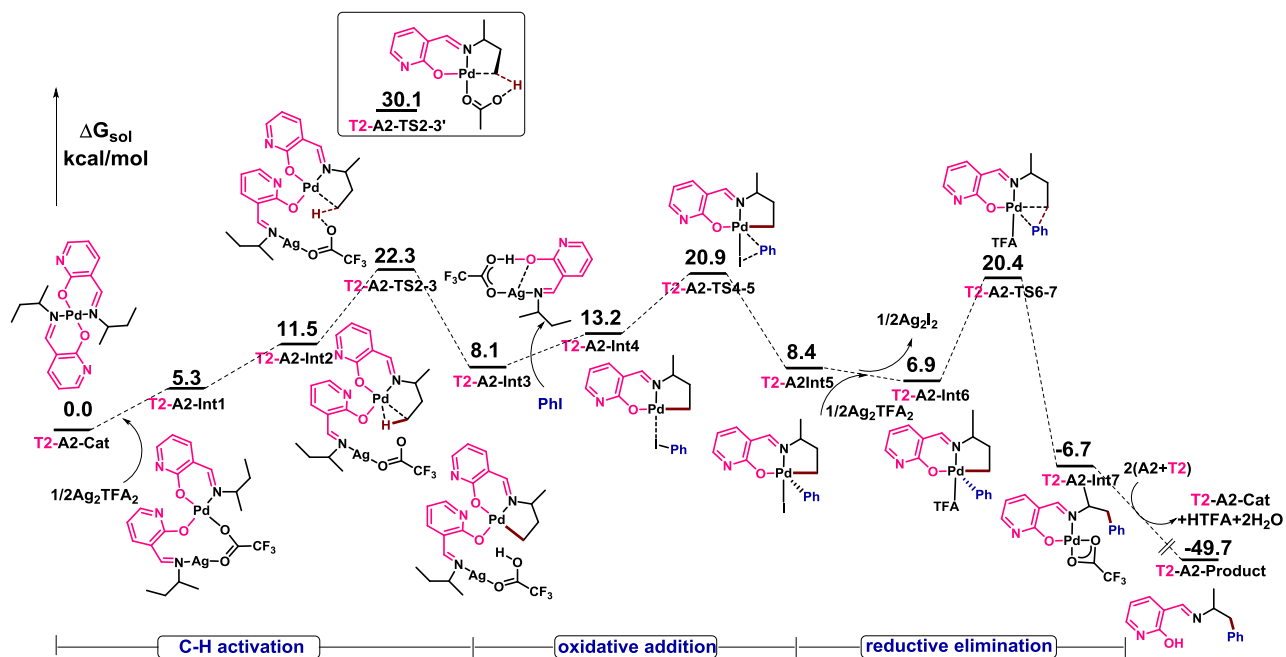
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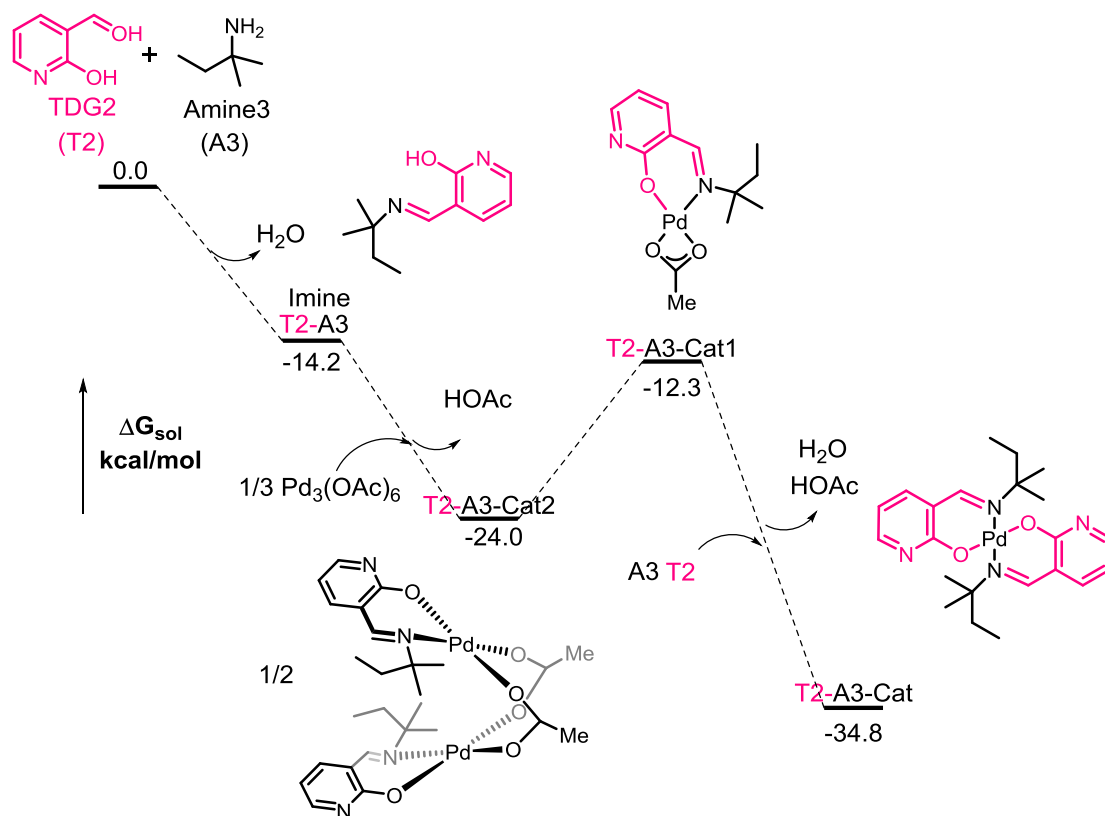
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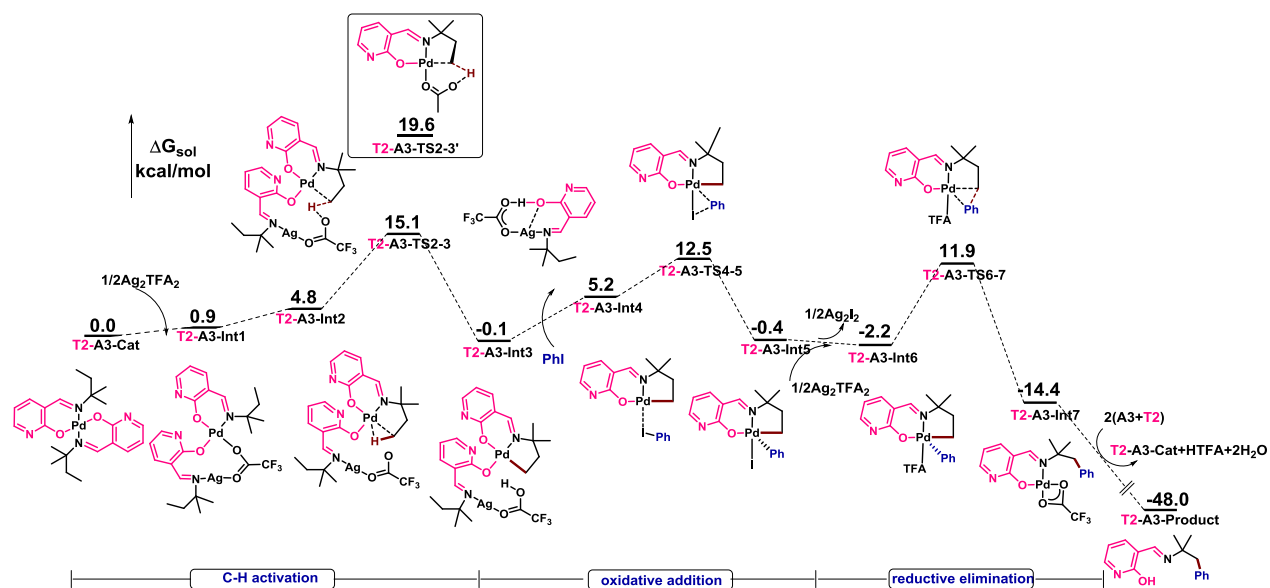
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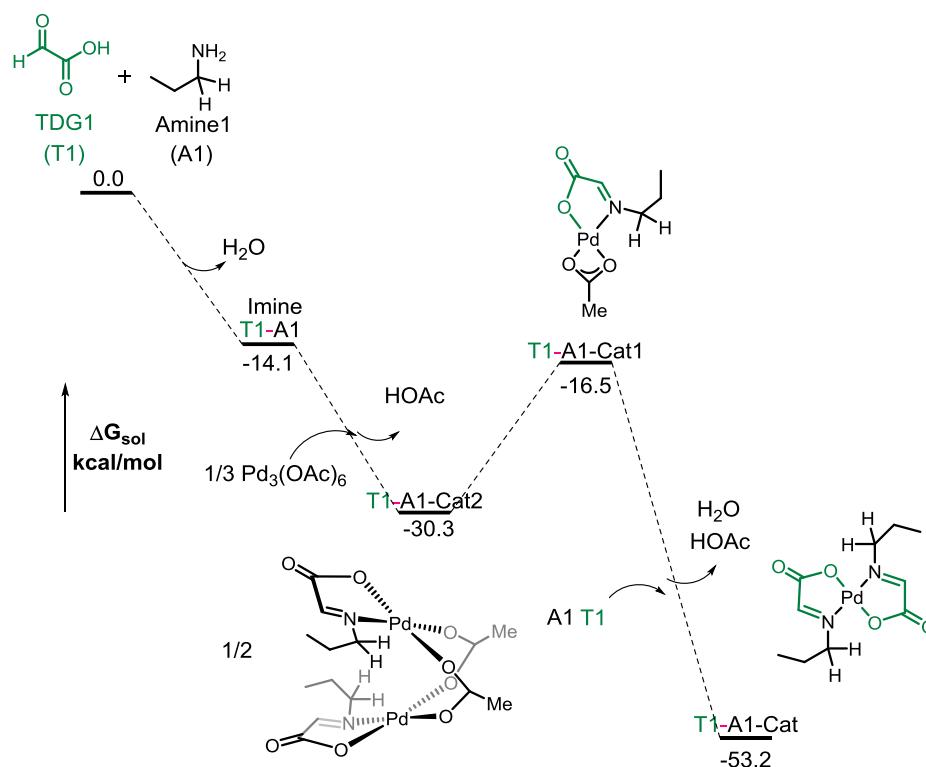
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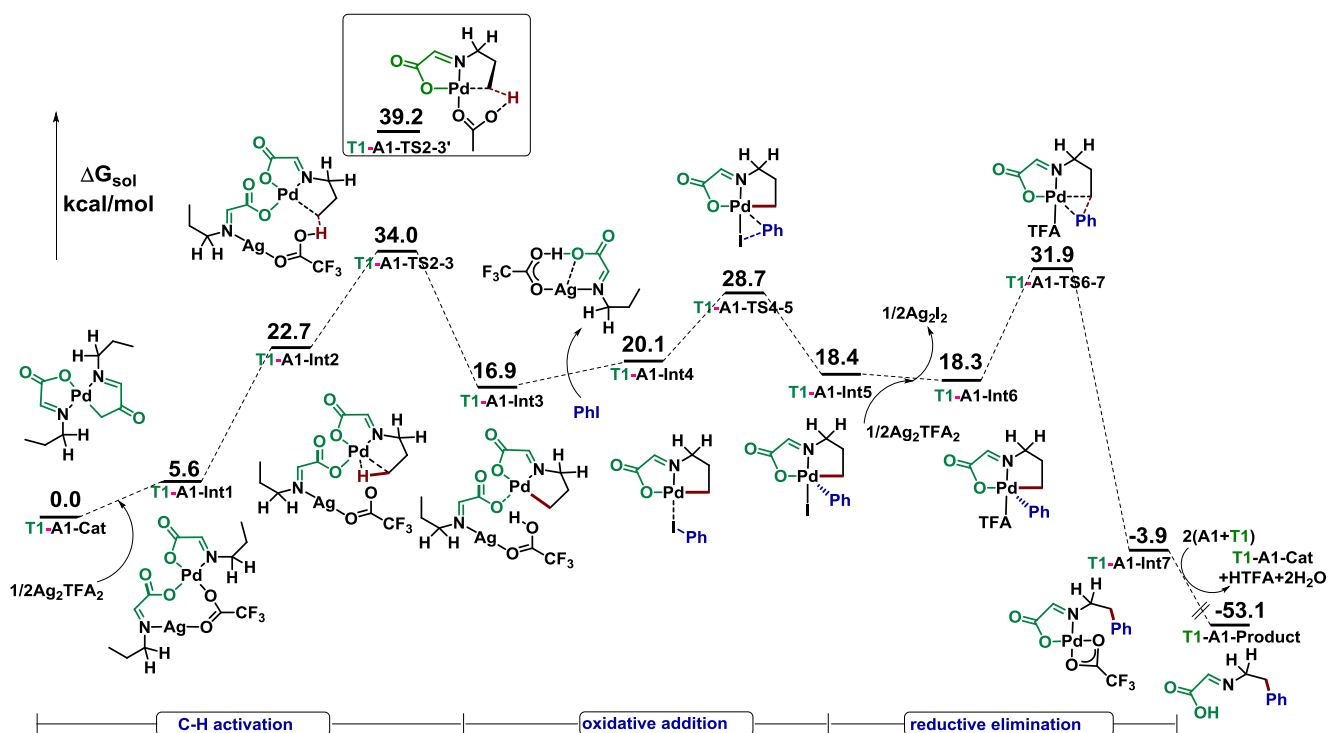
**Figure S6.** The calculated Gibbs free energy profiles for the condensation reaction between Amine and TDG and the formation of catalyst **T2-A3-Cat2**, **T2-A3-Cat1** and **T2-A3-Cat**. (Gibbs free energies in solvent are given in kcal/mol)



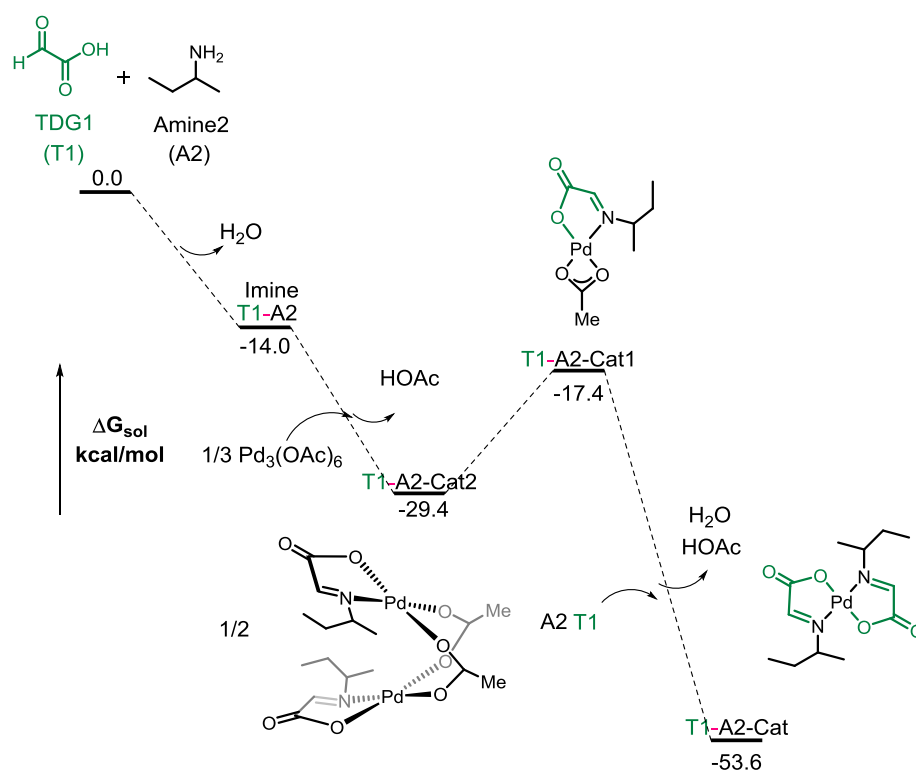
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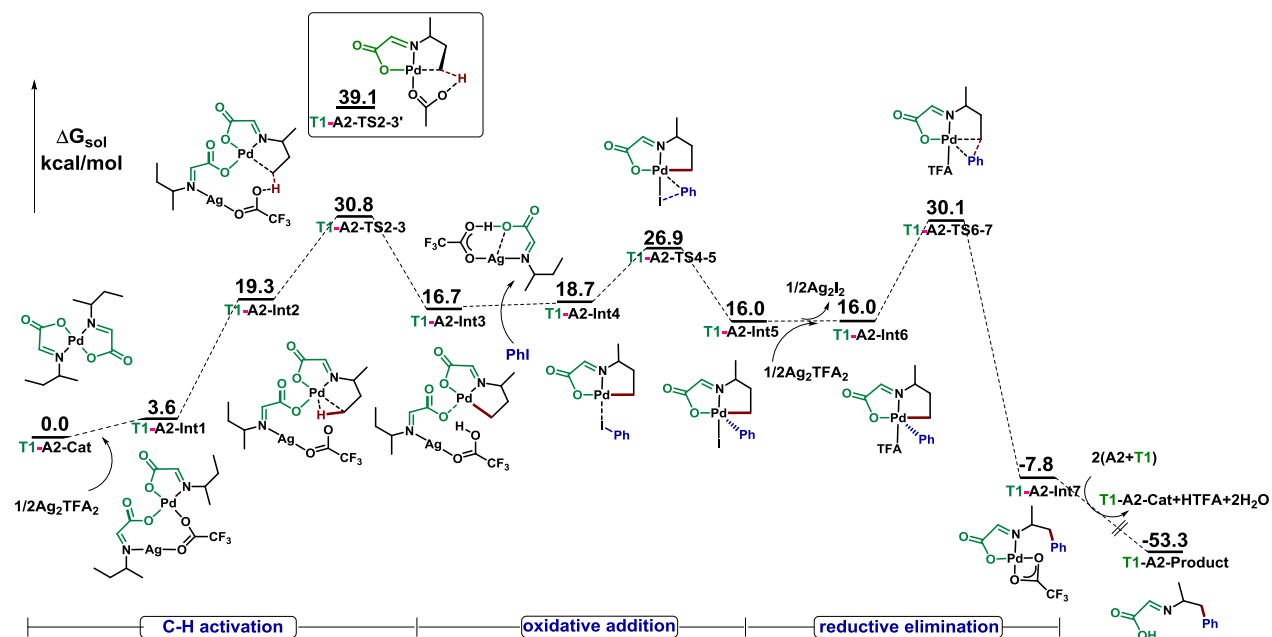
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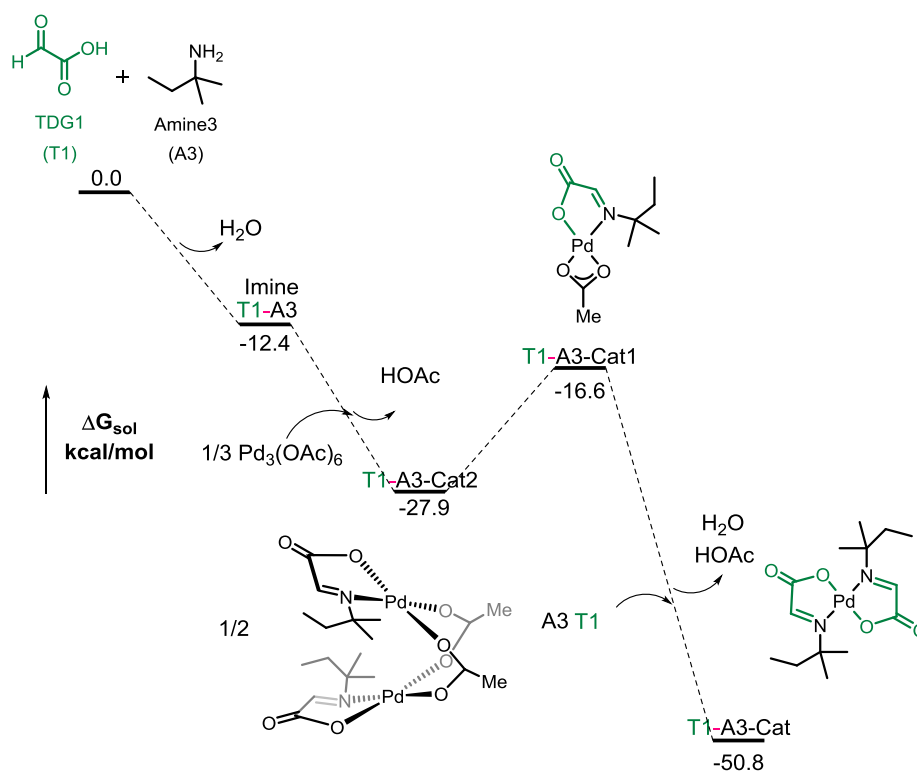
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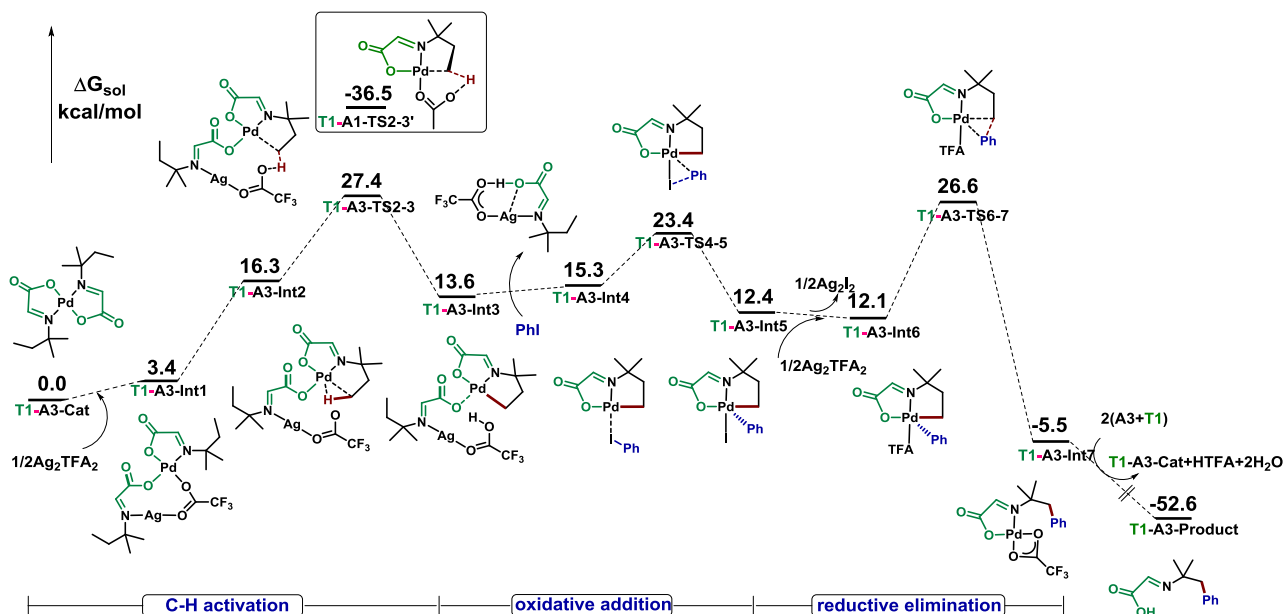


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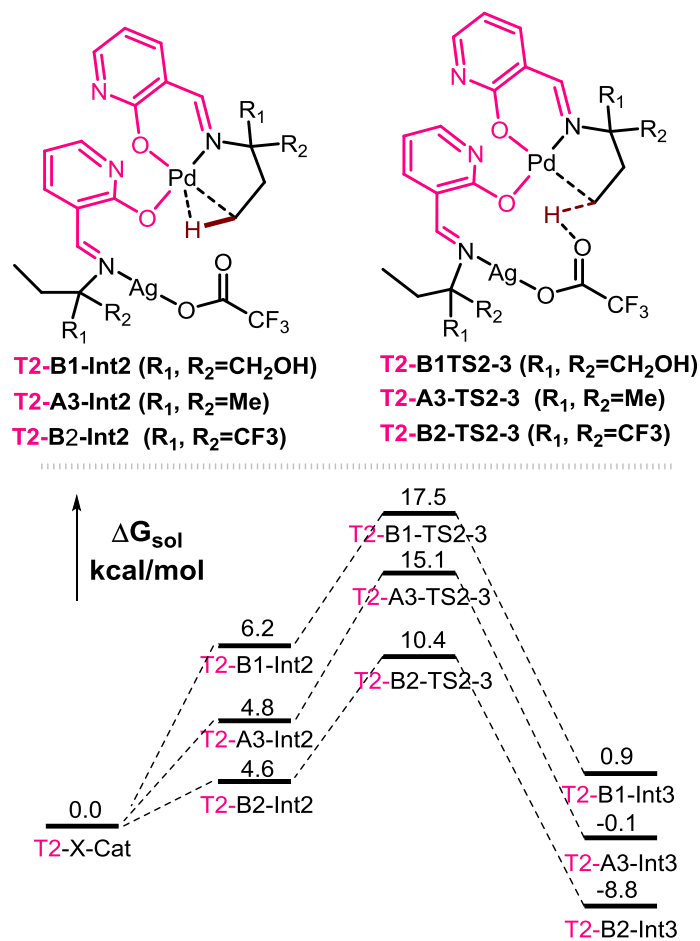


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**Figure S14.** The calculated Gibbs free energy profiles for the mechanism of **TDG2** co-catalyzed C-H bond activation processes for amines with two  $\text{CH}_2\text{OH}$  or two  $\text{CH}_3$  or two  $\text{CF}_3$  groups at the  $\alpha$ -position. (Gibbs free energies in solvent are given in kcal/mol)

**Table S1.**  $\Delta E_{\text{gas}}$ ,  $\Delta G_{\text{gas}}$ ,  $\Delta E_{\text{sol}}$  calculated for all species in the reaction

| species      | $\Delta G_{\text{gas}}$ | $\Delta E_{\text{gas}}$ | $\Delta E_{\text{sol}}$ |
|--------------|-------------------------|-------------------------|-------------------------|
| T1-A3        | -1.7                    | -2.3                    | -12.9                   |
| T1-A2        | -3.3                    | -3.6                    | -14.9                   |
| T1-A1        | -3.4                    | -3.7                    | -14.3                   |
| T2-A3        | -7.7                    | -8.3                    | -14.7                   |
| T2-A2        | -7.8                    | -8.3                    | -14.7                   |
| T2-A1        | -9.1                    | -9.6                    | -15.9                   |
| T1-A3-Cat2   | -15.0                   | -16.7                   | -29.7                   |
| T1-A2-Cat2   | -16.2                   | -17.3                   | -30.5                   |
| T1-A1-Cat2   | -16.7                   | -16.9                   | -30.6                   |
| T2-A3-Cat2   | -14.0                   | -16.3                   | -26.3                   |
| T2-A2-Cat2   | -18.0                   | -19.7                   | -30.2                   |
| T2-A1-Cat2   | -20.0                   | -21.1                   | -31.9                   |
| T1-A3-Cat1   | -0.6                    | 6.7                     | -9.3                    |
| T1-A2-Cat1   | -1.5                    | 6.2                     | -9.8                    |
| T1-A1-Cat1   | -0.3                    | 7.6                     | -8.5                    |
| T2-A3-Cat1   | -0.1                    | 6.8                     | -5.3                    |
| T2-A2-Cat1   | -1.4                    | 6.1                     | -6.9                    |
| T2-A1-Cat1   | -3.5                    | 4.3                     | -8.2                    |
| T1-A3-Cat    | -23.3                   | -20.0                   | -47.4                   |
| T1-A2-Cat    | -26.2                   | -22.2                   | -49.7                   |
| T1-A1-Cat    | -24.7                   | -19.4                   | -48.3                   |
| T2-A3-Cat    | -15.4                   | -11.6                   | -31.0                   |
| T2-A2-Cat    | -23.3                   | -18.7                   | -39.7                   |
| T2-A1-Cat    | -28.1                   | -23.4                   | -43.6                   |
| T1-A3-TS2-3' | 39.9                    | 45.7                    | 42.3                    |
| T1-A2-TS2-3' | 42.5                    | 47.9                    | 44.5                    |
| T1-A1-TS2-3' | 68.9                    | 73.3                    | 43.5                    |
| T2-A3-TS2-3' | 22.9                    | 27.9                    | 24.6                    |
| T2-A2-TS2-3' | 31.8                    | 35.6                    | 33.9                    |
| T2-A1-TS2-3' | 34.3                    | 38.5                    | 36.7                    |
| T1-A3-Int1   | 0.7                     | -6.6                    | -3.9                    |
| T1-A2-Int1   | 1.5                     | -5.4                    | -3.3                    |
| T1-A1-Int1   | 2.5                     | -4.4                    | -1.3                    |
| T2-A3-Int1   | -1.6                    | -9.2                    | -6.8                    |
| T2-A2-Int1   | 1.9                     | -6.1                    | -2.7                    |
| T2-A1-Int1   | 6.2                     | -0.4                    | 2.6                     |
| T1-A3-Int2   | 18.9                    | 13.4                    | 10.7                    |
| T1-A2-Int2   | 21.7                    | 16.3                    | 13.9                    |
| T1-A1-Int2   | 22.0                    | 15.5                    | 16.1                    |
| T2-A3-Int2   | 7.0                     | 0.8                     | -1.5                    |
| T2-A2-Int2   | 12.8                    | 6.7                     | 5.3                     |

|                    |      |      |       |
|--------------------|------|------|-------|
| <b>T2-A1-Int2</b>  | 19.5 | 13.3 | 11.3  |
| <b>T1-A3-TS2-3</b> | 27.7 | 24.0 | 23.7  |
| <b>T1-A2-TS2-3</b> | 31.3 | 27.4 | 27.0  |
| <b>T1-A1-TS2-3</b> | 32.3 | 28.5 | 30.2  |
| <b>T2-A3-TS2-3</b> | 14.1 | 10.7 | 11.6  |
| <b>T2-A2-TS2-3</b> | 20.5 | 16.9 | 18.6  |
| <b>T2-A1-TS2-3</b> | 27.3 | 24.3 | 25.4  |
| <b>T1-A3-Int3</b>  | 13.6 | 10.4 | 10.4  |
| <b>T1-A2-Int3</b>  | 17.1 | 13.7 | 13.3  |
| <b>T1-A1-Int3</b>  | 12.9 | 8.8  | 12.9  |
| <b>T2-A3-Int3</b>  | -4.7 | -9.2 | -4.6  |
| <b>T2-A2-Int3</b>  | 1.6  | -3.0 | 3.4   |
| <b>T2-A1-Int3</b>  | 8.5  | 3.4  | 9.9   |
| <b>T2-A3-Int4</b>  | 9.2  | 6.1  | 2.0   |
| <b>T2-A2-Int4</b>  | 15.3 | 11.6 | 9.4   |
| <b>T2-A1-Int4</b>  | 21.3 | 17.7 | 15.3  |
| <b>T2-A3-TS4-5</b> | 18.3 | 14.3 | 8.6   |
| <b>T2-A3-TS4-5</b> | 24.7 | 20.1 | 16.2  |
| <b>T2-A3-TS4-5</b> | 30.7 | 26.1 | 22.0  |
| <b>T2-A3-Int5</b>  | 9.3  | 4.5  | -5.2  |
| <b>T2-A2-Int5</b>  | 16.3 | 10.8 | 2.8   |
| <b>T2-A1-Int5</b>  | 22.4 | 17.0 | 8.7   |
| <b>T2-A3-Int6</b>  | 3.8  | -1.4 | -7.4  |
| <b>T2-A2-Int6</b>  | 11.1 | 5.0  | 0.8   |
| <b>T2-A1-Int6</b>  | 17.7 | 11.8 | 6.9   |
| <b>T2-A3-TS6-7</b> | 20.5 | 14.6 | 5.9   |
| <b>T2-A2-TS6-7</b> | 27.2 | 20.6 | 13.8  |
| <b>T2-A1-TS6-7</b> | 34.1 | 27.8 | 20.1  |
| <b>T2-A3-Int7</b>  | -4.1 | -9.5 | -19.9 |
| <b>T2-A2-Int7</b>  | 1.7  | -4.2 | -12.6 |
| <b>T2-A1-Int7</b>  | 7.9  | 2.9  | -6.5  |
| <b>T1-A3-Int4</b>  | 20.9 | 19.2 | 13.6  |
| <b>T1-A2-Int4</b>  | 24.3 | 22.4 | 16.8  |
| <b>T1-A1-Int4</b>  | 23.8 | 21.2 | 17.5  |
| <b>T1-A3-TS4-5</b> | 30.0 | 27.1 | 20.5  |
| <b>T1-A2-TS4-5</b> | 33.4 | 30.2 | 23.7  |
| <b>T1-A1-TS4-5</b> | 33.5 | 29.2 | 24.5  |
| <b>T1-A3-Int5</b>  | 21.9 | 18.9 | 9.4   |
| <b>T1-A2-Int5</b>  | 25.5 | 22.3 | 12.9  |
| <b>T1-A1-Int5</b>  | 26.1 | 21.6 | 14.0  |
| <b>T1-A3-Int6</b>  | 18.0 | 14.2 | 8.3   |
| <b>T1-A2-Int6</b>  | 22.2 | 18.2 | 12.1  |
| <b>T1-A1-Int6</b>  | 22.9 | 17.8 | 13.3  |
| <b>T1-A3-TS6-7</b> | 33.9 | 29.3 | 21.9  |

|                      |       |       |       |
|----------------------|-------|-------|-------|
| <b>T1-A2-TS6-7</b>   | 37.8  | 33.1  | 25.4  |
| <b>T1-A1-TS6-7</b>   | 38.1  | 32.4  | 26.2  |
| <b>T1-A3-Int7</b>    | -5.8  | -12.3 | -12.0 |
| <b>T1-A2-Int7</b>    | 0.4   | -6.4  | -14.5 |
| <b>T1-A1-Int7</b>    | -5.4  | -12.1 | -10.6 |
| <b>T1-A3-Product</b> | -32.7 | -42.4 | -62.3 |
| <b>T1-A2-Product</b> | -31.3 | -40.8 | -62.8 |
| <b>T1-A1-Product</b> | -33.5 | -42.1 | -61.6 |
| <b>T2-A3-Product</b> | -33.7 | -42.6 | -57.0 |
| <b>T2-A2-Product</b> | -36.8 | -45.1 | -57.9 |
| <b>T2-A1-Product</b> | -36.6 | -44.6 | -58.6 |
| <b>T2-B1-Int2</b>    | 6.8   | 1.7   | 1.0   |
| <b>T2-B2-Int2</b>    | -13.3 | -0.4  | -1.4  |
| <b>T2-B1-TS2-3</b>   | 14.2  | 11.2  | 14.5  |
| <b>T2-B2-TS2-3</b>   | 9.9   | 6.9   | 7.4   |
| <b>T2-B1-Int3</b>    | -4.3  | -8.6  | -3.3  |
| <b>T2-B2-Int3</b>    | -13.3 | -18.2 | -13.7 |

**Table S2.** Absolute Calculation Energies and imaginary frequencies.

| species                                | $E_{(\text{gas-BP86-D3(BJ)})}^1$ | $G_{(\text{corr-BP86-D3(BJ)})}^2$ | $H_{(\text{corr-BP86-D3(BJ)})}^3$ | $E_{(\text{solv-BP86-D3(BJ)})}^4$ | IF <sup>5</sup> |
|--|----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------|
| <b>H<sub>2</sub>O</b>                  | -76.4183734                      | 0.002455                          | 0.024573                          | -76.4677454                       | -               |
| <b>TDG1</b>                            | -303.0829784                     | 0.013500                          | 0.047568                          | -303.1878547                      | -               |
| <b>TDG2</b>                            | -436.8649753                     | 0.067785                          | 0.108048                          | -437.0003014                      | -               |
| <b>Amine-3</b>                         | -253.1385307                     | 0.141508                          | 0.181778                          | -253.2113021                      | -               |
| <b>Amine-2</b>                         | -213.8182239                     | 0.115758                          | 0.153414                          | -213.8823147                      | -               |
| <b>Amine-1</b>                         | -174.49652                       | 0.090437                          | 0.124908                          | -174.5522075                      | -               |
| <b>T1-A3</b>                           | -479.8067358                     | 0.153336                          | 0.204136                          | -479.9519655                      | -               |
| <b>T1-A2</b>                           | -440.488604                      | 0.127252                          | 0.175620                          | -440.6251393                      | -               |
| <b>T1-A1</b>                           | -401.1670737                     | 0.101943                          | 0.146972                          | -401.2951746                      | -               |
| <b>T2-A3</b>                           | -613.5983374                     | 0.207768                          | 0.263781                          | -613.767338                       | -               |
| <b>T2-A2</b>                           | -574.2766855                     | 0.182264                          | 0.235490                          | -574.4373086                      | -               |
| <b>T2-A1</b>                           | -534.958423                      | 0.156606                          | 0.206730                          | -535.1100278                      | -               |
| <b>HOAc</b>                            | -229.0947452                     | 0.032725                          | 0.065688                          | -229.1760099                      | -               |
| <b>Pd<sub>3</sub>(OAc)<sub>6</sub></b> | -1751.683922                     | 0.231927                          | 0.341591                          | -1752.104344                      | -               |
| <b>T1-A3-Cat2</b>                      | -1669.259327                     | 0.399860                          | 0.505407                          | -1669.674882                      | -               |
| <b>T1-A2-Cat2</b>                      | -1590.62074                      | 0.346550                          | 0.448098                          | -1591.019727                      | -               |
| <b>T1-A1-Cat2</b>                      | -1511.976061                     | 0.292936                          | 0.390580                          | -1512.35966                       | -               |
| <b>T2-A3-Cat2</b>                      | -1936.822102                     | 0.510025                          | 0.626491                          | -1937.289052                      | -               |
| <b>T2-A2-Cat2</b>                      | -1858.192361                     | 0.457010                          | 0.569669                          | -1858.643666                      | -               |
| <b>T2-A1-Cat2</b>                      | -1779.553351                     | 0.404306                          | 0.511799                          | -1779.988611                      | -               |
| <b>T1-A3-Cat1</b>                      | -834.592302                      | 0.185466                          | 0.251216                          | -834.804979                       | -               |
| <b>T1-A2-Cat1</b>                      | -795.2728813                     | 0.159182                          | 0.222667                          | -795.4767508                      | -               |
| <b>T1-A1-Cat1</b>                      | -755.9488666                     | 0.133442                          | 0.193955                          | -756.1446867                      | -               |
| <b>T2-A3-Cat1</b>                      | -968.3741702                     | 0.240340                          | 0.311866                          | -968.611138                       | -               |
| <b>T2-A2-Cat1</b>                      | -929.0550329                     | 0.213678                          | 0.283371                          | -929.2845924                      | -               |

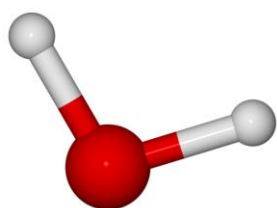
|                                       |              |           |          |              |          |
|---------------------------------------|--------------|-----------|----------|--------------|----------|
| <b>T2-A1-Cat1</b>                     | -889.7362191 | 0.187900  | 0.254502 | -889.9565741 | -        |
| <b>T1-A3-Cat</b>                      | -1085.343277 | 0.311632  | 0.390821 | -1085.621145 | -        |
| <b>T1-A2-Cat</b>                      | -1006.706228 | 0.259197  | 0.333635 | -1006.966819 | -        |
| <b>T1-A1-Cat</b>                      | -928.058362  | 0.206430  | 0.276056 | -928.3043197 | -        |
| <b>T2-A3-Cat</b>                      | -1352.893976 | 0.419564  | 0.511008 | -1353.219904 | -        |
| <b>T2-A2-Cat</b>                      | -1274.264641 | 0.366721  | 0.454919 | -1274.575727 | -        |
| <b>T2-A1-Cat</b>                      | -1195.628694 | 0.315873  | 0.397335 | -1195.921837 | -        |
| <b>T1-A3-TS2-3'</b>                   | -834.5584099 | 0.181699  | 0.245025 | -834.7777404 | -922.24  |
| <b>T1-A2-TS2-3'</b>                   | -795.2360401 | 0.156084  | 0.216601 | -795.4468147 | -920.22  |
| <b>T1-A1-TS2-3'</b>                   | -755.8692948 | 0.130341  | 0.187653 | -756.1158422 | -966.88  |
| <b>T2-A3-TS2-3'</b>                   | -968.3459021 | 0.236524  | 0.305660 | -968.5893842 | -886.80  |
| <b>T2-A2-TS2-3'</b>                   | -929.0259361 | 0.211020  | 0.277231 | -929.2603614 | -906.45  |
| <b>T2-A1-TS2-3'</b>                   | -889.7036694 | 0.185401  | 0.248506 | -889.9293788 | -901.65  |
| <b>Ag<sub>2</sub>TFA<sub>2</sub></b>  | -1344.166807 | 0.001896  | 0.073709 | -1344.537633 | -        |
| <b>T1-A3-Int1</b>                     | -1757.437227 | 0.324259  | 0.428003 | -1757.896222 | -        |
| <b>T1-A2-Int1</b>                     | -1678.798159 | 0.271134  | 0.370848 | -1679.2409   | -        |
| <b>T1-A1-Int1</b>                     | -1600.148813 | 0.218445  | 0.313506 | -1600.575247 | -        |
| <b>T2-A3-Int1</b>                     | -2024.991977 | 0.432616  | 0.548073 | -2025.4995   | -        |
| <b>T2-A2-Int1</b>                     | -1946.357706 | 0.380329  | 0.491457 | -1946.848817 | -        |
| <b>T2-A1-Int1</b>                     | -1867.712704 | 0.327231  | 0.433934 | -1868.186531 | -        |
| <b>T1-A3-Int2</b>                     | -1757.405366 | 0.321430  | 0.426445 | -1757.872907 | -        |
| <b>T1-A2-Int2</b>                     | -1678.763669 | 0.268824  | 0.369494 | -1679.213439 | -        |
| <b>T1-A1-Int2</b>                     | -1600.117114 | 0.217823  | 0.311866 | -1600.547485 | -        |
| <b>T2-A3-Int2</b>                     | -2024.976075 | 0.430420  | 0.546680 | -2025.491067 | -        |
| <b>T2-A2-Int2</b>                     | -1946.337303 | 0.377395  | 0.489782 | -1946.836042 | -        |
| <b>T2-A1-Int2</b>                     | -1867.690887 | 0.326754  | 0.432525 | -1868.172598 | -        |
| <b>T1-A3-TS2-3</b>                    | -1757.388366 | 0.318420  | 0.420505 | -1757.852195 | -1000.50 |
| <b>T1-A2-TS2-3</b>                    | -1678.745908 | 0.266255  | 0.363558 | -1679.192593 | -1001.39 |
| <b>T1-A1-TS2-3</b>                    | -1600.096356 | 0.213483  | 0.305935 | -1600.525044 | -1021.66 |
| <b>T2-A3-TS2-3</b>                    | -2024.96037  | 0.425983  | 0.540963 | -2025.470249 | -966.79  |
| <b>T2-A2-TS2-3</b>                    | -1946.321137 | 0.373450  | 0.484039 | -1946.814917 | -994.55  |
| <b>T2-A1-TS2-3</b>                    | -1867.673379 | 0.321672  | 0.426739 | -1868.150224 | -983.23  |
| <b>T1-A3-Int3</b>                     | -1757.410108 | 0.317683  | 0.425286 | -1757.873385 | -        |
| <b>T1-A2-Int3</b>                     | -1678.767845 | 0.265587  | 0.368258 | -1679.214404 | -        |
| <b>T1-A1-Int3</b>                     | -1600.127808 | 0.213935  | 0.311114 | -1600.55262  | -        |
| <b>T2-A3-Int3</b>                     | -2024.991988 | 0.427599  | 0.546035 | -2025.496085 | -        |
| <b>T2-A2-Int3</b>                     | -1946.352865 | 0.375080  | 0.489284 | -1946.839116 | -        |
| <b>T2-A1-Int3</b>                     | -1867.70675  | 0.324986  | 0.432097 | -1868.174867 | -        |
| <b>PhI</b>                            | -243.0855557 | 0.055681  | 0.094532 | -243.1464722 | -        |
| <b>1/2Ag<sub>2</sub>I<sub>2</sub></b> | -314.66484   | -0.037067 | 0.009583 | -314.6785375 | -        |
| <b>T2-A3-Int4</b>                     | -982.3579602 | 0.262134  | 0.339883 | -982.5859012 | -        |
| <b>T2-A2-Int4</b>                     | -943.0378034 | 0.236354  | 0.311421 | -943.2568813 | -        |
| <b>T2-A1-Int4</b>                     | -903.7152191 | 0.210685  | 0.282658 | -903.9255191 | -        |
| <b>T2-A3-TS4-5</b>                    | -982.3448369 | 0.263425  | 0.338424 | -982.5754824 | -133.61  |

|                      |              |          |          |              |         |
|----------------------|--------------|----------|----------|--------------|---------|
| <b>T2-A3-TS4-5</b>   | -943.0242686 | 0.237810 | 0.309964 | -943.246038  | -134.74 |
| <b>T2-A3-TS4-5</b>   | -903.7018652 | 0.212315 | 0.281202 | -903.9148396 | -133.61 |
| <b>T2-A3-Int5</b>    | -982.360497  | 0.264754 | 0.340036 | -982.5974329 | -       |
| <b>T2-A2-Int5</b>    | -943.0390875 | 0.239210 | 0.311599 | -943.2673368 | -       |
| <b>T2-A1-Int5</b>    | -903.7164731 | 0.213598 | 0.282834 | -903.9359962 | -       |
| <b>T2-A3-Int6</b>    | -1497.120853 | 0.284977 | 0.372639 | -1497.530538 | -       |
| <b>T2-A2-Int6</b>    | -1457.79925  | 0.259596 | 0.344215 | -1458.200176 | -       |
| <b>T2-A1-Int6</b>    | -1418.475669 | 0.233812 | 0.315444 | -1418.868366 | -       |
| <b>T2-A3-TS6-7</b>   | -1497.095417 | 0.286065 | 0.371431 | -1497.509234 | -299.35 |
| <b>T2-A2-TS6-7</b>   | -1457.774342 | 0.260294 | 0.342997 | -1458.179398 | -294.97 |
| <b>T2-A1-TS6-7</b>   | -1418.450251 | 0.234644 | 0.314304 | -1418.847389 | -304.29 |
| <b>T2-A3-Int7</b>    | -1497.133803 | 0.285294 | 0.372948 | -1497.55035  | -       |
| <b>T2-A2-Int7</b>    | -1457.813904 | 0.259299 | 0.344486 | -1458.221537 | -       |
| <b>T2-A1-Int7</b>    | -1418.489862 | 0.232419 | 0.315731 | -1418.889753 | -       |
| <b>HTFA</b>          | -526.7970985 | 0.005772 | 0.045065 | -526.9837296 | -       |
| <b>T1-A3-Int4</b>    | -848.5687467 | 0.206642 | 0.279335 | -848.7771011 | -       |
| <b>T1-A2-Int4</b>    | -809.2461469 | 0.180861 | 0.250845 | -809.4459807 | -       |
| <b>T1-A1-Int4</b>    | -769.9240479 | 0.154946 | 0.222072 | -770.114867  | -       |
| <b>T1-A3-TS4-5</b>   | -848.5561561 | 0.208572 | 0.277693 | -848.7661052 | -126.94 |
| <b>T1-A2-TS4-5</b>   | -809.2336585 | 0.182919 | 0.249219 | -809.4350057 | -126.06 |
| <b>T1-A1-TS4-5</b>   | -769.9111692 | 0.157386 | 0.220439 | -770.1036552 | -126.99 |
| <b>T1-A3-Int5</b>    | -848.5691248 | 0.208613 | 0.279243 | -848.7837016 | -       |
| <b>T1-A2-Int5</b>    | -809.2462412 | 0.182866 | 0.250794 | -809.4522558 | -       |
| <b>T1-A1-Int5</b>    | -769.9232865 | 0.157728 | 0.222013 | -770.1204552 | -       |
| <b>T1-A3-Int6</b>    | -1363.327691 | 0.229440 | 0.311866 | -1363.715104 | -       |
| <b>T1-A2-Int6</b>    | -1324.003758 | 0.203641 | 0.283372 | -1324.383151 | -       |
| <b>T1-A1-Int6</b>    | -1284.680361 | 0.178175 | 0.254595 | -1285.051109 | -       |
| <b>T1-A3-TS6-7</b>   | -1363.303675 | 0.230822 | 0.310721 | -1363.693414 | -280.10 |
| <b>T1-A2-TS6-7</b>   | -1323.980032 | 0.204849 | 0.282382 | -1324.361854 | -286.08 |
| <b>T1-A1-TS6-7</b>   | -1284.657162 | 0.179255 | 0.253590 | -1285.030554 | -282.00 |
| <b>T1-A3-Int7</b>    | -1363.369923 | 0.233717 | 0.314243 | -1363.747397 | -       |
| <b>T1-A2-Int7</b>    | -1324.04291  | 0.208039 | 0.285479 | -1324.425413 | -       |
| <b>T1-A1-Int7</b>    | -1284.728    | 0.180791 | 0.257071 | -1285.089053 | -       |
| <b>T1-A3-Product</b> | -710.8836902 | 0.226423 | 0.287746 | -711.0854579 | -       |
| <b>T1-A2-Product</b> | -671.5601409 | 0.201158 | 0.259303 | -671.7567715 | -       |
| <b>T1-A1-Product</b> | -632.2425872 | 0.174540 | 0.230554 | -632.4270188 | -       |
| <b>T2-A3-Product</b> | -844.6657267 | 0.279200 | 0.347533 | -844.8935407 | -       |
| <b>T2-A2-Product</b> | -805.3469233 | 0.252619 | 0.319132 | -805.5640192 | -       |
| <b>T2-A1-Product</b> | -766.0259885 | 0.227115 | 0.290388 | -766.2367173 | -       |
| <b>T1-B1-Cat</b>     | -1653.749319 | 0.433025 | 0.534970 | -1654.211006 | -       |
| <b>T1-B2-Cat</b>     | -2543.749191 | 0.316814 | 0.428377 | -2544.486022 | -       |
| <b>T2-B1-Int2</b>    | -2325.830027 | 0.442167 | 0.570476 | -2326.478211 | -       |
| <b>T2-B2-Int2</b>    | -3215.833247 | 0.327295 | 0.464022 | -3216.757116 | -       |
| <b>T2-B1-TS2-3</b>   | -2325.814799 | 0.438708 | 0.564788 | -2326.456697 | -968.39 |

|                    |              |          |          |              |         |
|--------------------|--------------|----------|----------|--------------|---------|
| <b>T2-B2-TS2-3</b> | -3215.821533 | 0.322482 | 0.458705 | -3216.743049 | -966.72 |
| <b>T2-B1-Int3</b>  | -2325.846396 | 0.440785 | 0.570119 | -2326.485155 | -       |
| <b>T2-B2-Int3</b>  | -3215.861567 | 0.325510 | 0.464095 | -3216.776606 | -       |

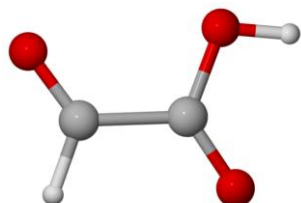
<sup>1</sup>The electronic energy calculated by BP86-D3(BJ) in gas phase. <sup>2</sup>The thermal correction to Gibbs free energy calculated by BP86-D3(BJ) in gas phase. <sup>3</sup>The thermal correction to enthalpy calculated by BP86-D3(BJ) in gas phase. <sup>4</sup>The electronic energy calculated by BP86-D3(BJ) in acetic acid solvent. <sup>5</sup>The BP86-D3(BJ) calculated imaginary frequencies for the transition states.

Cartesian coordinates for the complexes calculated in this study: [gas phase results optimized at the level of BP86-D3(BJ)/6-31G\*\* (LanI2dz for Pd Ag I)]:



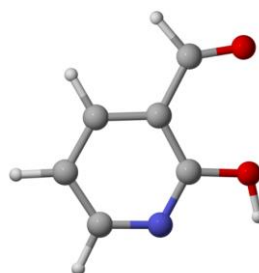
### H<sub>2</sub>O

|   |             |            |            |
|---|-------------|------------|------------|
| O | -1.67308300 | 2.66879000 | 0.00000000 |
| H | -0.70096000 | 2.72298100 | 0.00000000 |
| H | -1.94650300 | 3.60324400 | 0.00000000 |



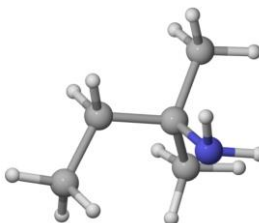
### TDG1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.70715800 | 1.76854000  | 0.00985400  |
| H | -2.81779200 | 1.65320100  | 0.08309200  |
| C | -1.00427300 | 0.40269100  | -0.08009100 |
| O | -1.12953200 | 2.83854600  | 0.00259300  |
| O | -1.63412600 | -0.64553100 | -0.06784000 |
| O | 0.34065700  | 0.51307100  | -0.17018100 |
| H | 0.68056700  | -0.40769600 | -0.22170800 |



### TDG2

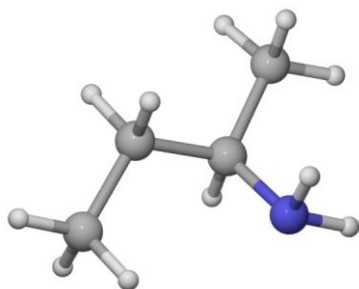
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.04781800 | -0.29934300 | -0.09077300 |
| C | 0.93397300  | 0.87802100  | -0.16521000 |
| C | 0.26533100  | 2.13226400  | -0.04729500 |
| C | -1.13765700 | 2.09037800  | 0.04991800  |
| C | -1.81768400 | 0.86810200  | 0.02946600  |
| H | -1.52817800 | -1.28543200 | -0.11219100 |
| H | -1.68283900 | 3.03764000  | 0.14189900  |
| H | -2.90643600 | 0.81364400  | 0.10363900  |
| N | 0.29577900  | -0.30539700 | -0.18647500 |
| O | 2.27644600  | 0.83741500  | -0.26271600 |
| H | 2.48584700  | -0.12118000 | -0.33129200 |
| C | 0.94385400  | 3.44702600  | -0.02170900 |
| H | 0.21461700  | 4.30170000  | 0.07803500  |
| O | 2.15017100  | 3.64903700  | -0.09604800 |



### Amine-3

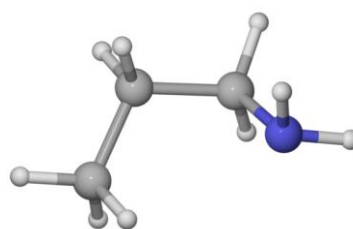
|   |             |            |             |
|---|-------------|------------|-------------|
| N | -1.48405800 | 3.57973500 | -0.09873600 |
| C | -2.59371100 | 4.19326300 | 0.67365600  |
| C | -2.30460200 | 3.95680600 | 2.17956500  |

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -3.89643200 | 3.49638800 | 0.23965800  |
| H | -3.80862800 | 2.40345100 | 0.33926100  |
| H | -4.74948400 | 3.84221700 | 0.84752300  |
| H | -4.12459100 | 3.72303500 | -0.81758100 |
| C | -2.71370100 | 5.71419600 | 0.42139900  |
| H | -2.88838400 | 5.92044300 | -0.64989300 |
| H | -3.54813200 | 6.16211800 | 0.99095600  |
| H | -1.78596300 | 6.23451200 | 0.72140900  |
| H | -1.36158700 | 4.48524500 | 2.42587200  |
| H | -3.09475000 | 4.45956700 | 2.76855300  |
| C | -2.18536500 | 2.48424500 | 2.59342200  |
| H | -1.47593100 | 1.96246200 | 1.93145100  |
| H | -1.83234500 | 2.39384500 | 3.63447000  |
| H | -3.15532100 | 1.96305300 | 2.52735700  |
| H | -0.62107000 | 4.10217700 | 0.10301000  |
| H | -1.66208100 | 3.72901400 | -1.10033400 |



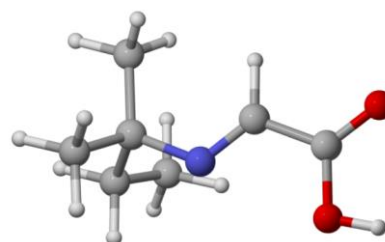
**Amine-2**

|   |             |            |             |
|---|-------------|------------|-------------|
| N | -1.47127800 | 3.58172000 | -0.09284800 |
| C | -2.54120800 | 4.21535300 | 0.70809400  |
| C | -2.25918400 | 3.97256300 | 2.20387500  |
| C | -2.73646000 | 5.71549300 | 0.41447800  |
| H | -2.94275500 | 5.88841200 | -0.65657600 |
| H | -3.57554900 | 6.14256800 | 0.99284200  |
| H | -1.82446800 | 6.28293000 | 0.67823200  |
| H | -1.29820700 | 4.46491100 | 2.45942700  |
| H | -3.03320100 | 4.49283900 | 2.79849500  |
| C | -2.20331000 | 2.48709000 | 2.58171600  |
| H | -1.46612900 | 1.96379300 | 1.95276200  |
| H | -1.93173300 | 2.34908600 | 3.64183400  |
| H | -3.18260500 | 2.00287900 | 2.41915400  |
| H | -0.59824700 | 4.10143300 | 0.07242300  |
| H | -1.67850800 | 3.71337500 | -1.09023800 |
| H | -3.47893300 | 3.68282400 | 0.44884400  |



**Amine-1**

|   |             |            |             |
|---|-------------|------------|-------------|
| N | -1.40618300 | 3.56771300 | -0.10514500 |
| C | -2.53844700 | 4.11387900 | 0.66553700  |
| C | -2.29703200 | 3.94607900 | 2.17477000  |
| H | -1.38332800 | 4.50895400 | 2.45304000  |
| H | -3.12876600 | 4.43026700 | 2.71994900  |
| C | -2.15493300 | 2.47933800 | 2.60327400  |
| H | -1.36084900 | 1.98841200 | 2.01892300  |
| H | -1.91387300 | 2.39131100 | 3.67602900  |
| H | -3.09288400 | 1.92490100 | 2.42140500  |
| H | -0.58551000 | 4.16766300 | 0.04277200  |
| H | -1.61397700 | 3.62615700 | -1.10789100 |
| H | -2.76359700 | 5.18483200 | 0.45300700  |
| H | -3.44209100 | 3.54192600 | 0.37982300  |

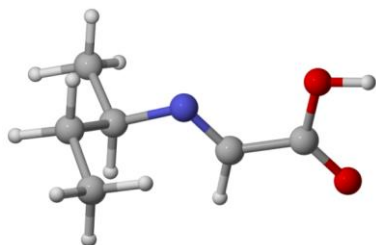


**T1-A3**

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 3.31863600  | -0.00765800 | 0.92350500  |
| C | 2.41689500  | 0.00902400  | 0.09147800  |
| O | 2.61731600  | 0.24292400  | -1.23267700 |
| C | 0.98263600  | -0.22944800 | 0.46064700  |
| H | 0.84955700  | -0.40685200 | 1.54320600  |
| N | 0.05528400  | -0.21891800 | -0.42194400 |
| C | -1.34843500 | -0.45289800 | -0.04009800 |
| C | -1.79033500 | -1.68685200 | -0.86038600 |
| C | -1.61082100 | -0.70168600 | 1.45726100  |
| C | -2.13038200 | 0.79267900  | -0.55323500 |
| H | -1.58095300 | -1.52992700 | -1.93031300 |
| H | -1.24776100 | -2.58836600 | -0.53016200 |
| H | -2.87133400 | -1.86231900 | -0.72832300 |
| H | -2.69137500 | -0.84030800 | 1.62592600  |
| H | -1.09894600 | -1.61401200 | 1.80875300  |
| H | -1.94849900 | 0.86907500  | -1.63984800 |
| H | -3.20883200 | 0.58745900  | -0.41815600 |

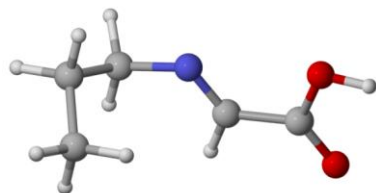


|   |             |            |             |
|---|-------------|------------|-------------|
| H | -1.27989500 | 0.14040200 | 2.08735000  |
| C | -1.75264100 | 2.11637700 | 0.12280300  |
| H | -1.98809400 | 2.11467400 | 1.20045800  |
| H | -0.67526400 | 2.32220600 | 0.00960300  |
| H | -2.30431500 | 2.95522700 | -0.33282300 |
| H | 3.58716500  | 0.37702900 | -1.31217300 |



### T1-A2

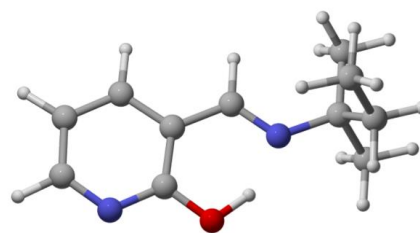
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 3.25239600  | 0.04587700  | 1.00985600  |
| C | 2.41034500  | 0.03167700  | 0.11789100  |
| O | 2.69889600  | 0.21425800  | -1.19768400 |
| C | 0.95379300  | -0.19050400 | 0.39508900  |
| H | 0.73088900  | -0.32997700 | 1.47232900  |
| N | 0.07672500  | -0.21330100 | -0.53763500 |
| C | -1.31668900 | -0.43119600 | -0.15137500 |
| C | -1.81051500 | -1.70912800 | -0.84988200 |
| C | -2.13845000 | 0.80425300  | -0.58268500 |
| H | -1.70462000 | -1.61159300 | -1.94284200 |
| H | -1.22837600 | -2.58664300 | -0.52488100 |
| H | -2.87227400 | -1.88633500 | -0.61017600 |
| H | -2.03382600 | 0.92246400  | -1.67666400 |
| H | -3.20300200 | 0.58334100  | -0.38117400 |
| C | -1.71905300 | 2.09353700  | 0.13358000  |
| H | -1.80796200 | 1.98849900  | 1.22961000  |
| H | -0.67173900 | 2.35060100  | -0.09550700 |
| H | -2.35071100 | 2.94305400  | -0.17413200 |
| H | 3.67234000  | 0.34433600  | -1.21962000 |
| H | -1.41475300 | -0.55348300 | 0.95342400  |



### T1-A1

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 3.27384600 | 0.06297700  | 0.98771900  |
| C | 2.41942000 | 0.01789500  | 0.10867300  |
| O | 2.68980600 | 0.14482200  | -1.21692400 |
| C | 0.96583100 | -0.18265800 | 0.41630800  |

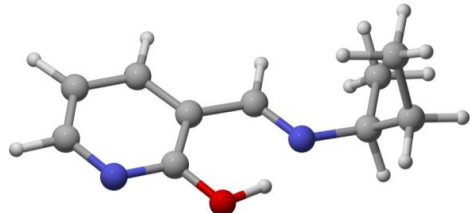
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.75872100  | -0.27659200 | 1.50177000  |
| N | 0.07451000  | -0.23682600 | -0.50177600 |
| C | -1.31019800 | -0.40898400 | -0.08212900 |
| C | -2.15682000 | 0.79327900  | -0.54896900 |
| H | -2.05941500 | 0.88451300  | -1.64528700 |
| H | -3.21657800 | 0.56406900  | -0.33498900 |
| C | -1.74828400 | 2.10674500  | 0.12962400  |
| H | -1.83640400 | 2.03250800  | 1.22829300  |
| H | -0.70270000 | 2.36491800  | -0.10684000 |
| H | -2.38597000 | 2.94222000  | -0.20299500 |
| H | 3.66359000  | 0.26744400  | -1.25840400 |
| H | -1.41151800 | -0.54275800 | 1.01921600  |
| H | -1.68655700 | -1.32561600 | -0.57391400 |



### T2-A3

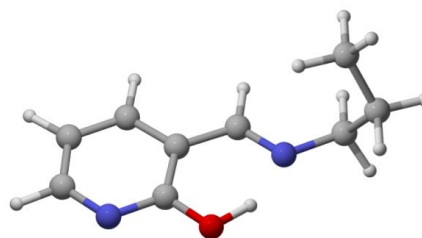
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.73565600 | 1.94701600  | 0.51481700  |
| C | -1.40568700 | 1.58769700  | 1.87135400  |
| C | -2.04228900 | 2.29291200  | 2.90959300  |
| C | -2.95701000 | 3.30164900  | 2.59943800  |
| C | -3.20017400 | 3.56476800  | 1.23709700  |
| N | -2.61908700 | 2.91948700  | 0.21212800  |
| H | -1.80942700 | 2.03817200  | 3.95065500  |
| H | -3.47078400 | 3.87108900  | 3.37804800  |
| H | -3.91362500 | 4.35064800  | 0.95380500  |
| O | -1.16657500 | 1.31403900  | -0.51084800 |
| C | -0.45120900 | 0.52679300  | 2.14767400  |
| H | -0.25313900 | 0.29645800  | 3.21038300  |
| N | 0.12884900  | -0.10970600 | 1.17633500  |
| C | 1.09390600  | -1.20208000 | 1.38681600  |
| C | 2.40430300  | -0.75440900 | 0.70127700  |
| C | 1.37121200  | -1.53516800 | 2.86410800  |
| H | 1.82002100  | -0.67658000 | 3.39258400  |
| H | 2.08515000  | -2.37272900 | 2.92366600  |
| C | 0.52526700  | -2.43726200 | 0.62917800  |
| H | 0.42332800  | -2.15435800 | -0.43437900 |
| H | 1.28572600  | -3.23912100 | 0.67315800  |
| H | 0.45888100  | -1.83536700 | 3.40554100  |
| C | -0.82181900 | -2.95162100 | 1.15096300  |
| H | -0.74984700 | -3.32772000 | 2.18551000  |
| H | -1.58232900 | -2.15341200 | 1.13090500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.18917900 | -3.78112900 | 0.52476100  |
| H | 3.15135800  | -1.56531800 | 0.73427300  |
| H | 2.21741200  | -0.49150800 | -0.35261200 |
| H | 2.82550400  | 0.13020400  | 1.20717800  |
| H | -0.52890600 | 0.61656400  | -0.08304900 |



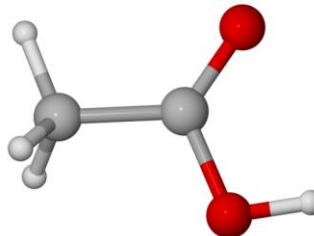
### T2-A2

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.72852800 | 1.97318800  | 0.51059800  |
| C | -1.42957700 | 1.60197600  | 1.87117300  |
| C | -2.08166200 | 2.30564300  | 2.90098800  |
| C | -2.98117500 | 3.32415900  | 2.57893000  |
| C | -3.19429300 | 3.59816500  | 1.21363000  |
| N | -2.59782500 | 2.95473300  | 0.19642700  |
| H | -1.87274400 | 2.04191600  | 3.94487800  |
| H | -3.50599600 | 3.89287100  | 3.35066200  |
| H | -3.89544300 | 4.39170600  | 0.92114900  |
| O | -1.14329300 | 1.34265900  | -0.50726300 |
| C | -0.49241900 | 0.52948700  | 2.15932500  |
| H | -0.32236900 | 0.28590600  | 3.22406100  |
| N | 0.10669300  | -0.10251600 | 1.19565900  |
| C | 1.02679400  | -1.21928100 | 1.43176500  |
| C | 0.49469800  | -2.44361600 | 0.64019200  |
| H | 0.41372000  | -2.14871700 | -0.42125000 |
| H | 1.25775000  | -3.24193800 | 0.69222400  |
| C | -0.86148600 | -2.96767700 | 1.13050200  |
| H | -0.81046200 | -3.34315100 | 2.16661500  |
| H | -1.62599000 | -2.17376200 | 1.09383400  |
| H | -1.20990700 | -3.79907400 | 0.49624300  |
| H | -0.52020600 | 0.63703800  | -0.07148400 |
| H | 1.97820700  | -0.92085600 | 0.94675900  |
| C | 1.32727000  | -1.54477600 | 2.90206800  |
| H | 2.05380300  | -2.37190000 | 2.95372400  |
| H | 1.76567900  | -0.67990300 | 3.42823600  |
| H | 0.42450100  | -1.85977400 | 3.45219100  |



### T2-A1

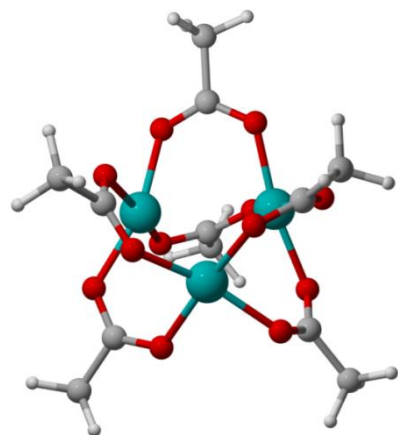
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.69857000 | 2.03556300  | 0.49241300  |
| C | -1.41358200 | 1.57978100  | 1.83019400  |
| C | -2.08012500 | 2.21410100  | 2.89566000  |
| C | -2.98006100 | 3.24750400  | 2.62815800  |
| C | -3.17843600 | 3.60749800  | 1.28052300  |
| N | -2.56767800 | 3.03232100  | 0.23151600  |
| H | -1.88180500 | 1.88546000  | 3.92289500  |
| H | -3.51615700 | 3.76413600  | 3.42817200  |
| H | -3.87912200 | 4.41587300  | 1.03094900  |
| O | -1.10073600 | 1.47383200  | -0.55833300 |
| C | -0.47417300 | 0.49697300  | 2.05558300  |
| H | -0.30042800 | 0.17545100  | 3.10303300  |
| N | 0.14054300  | -0.07622000 | 1.06516500  |
| C | 1.04392500  | -1.18867900 | 1.31992600  |
| C | 0.52585600  | -2.47861600 | 0.65287100  |
| H | 0.43107200  | -2.29967600 | -0.43352800 |
| H | 1.29597900  | -3.26106100 | 0.78123700  |
| C | -0.81545000 | -2.94983700 | 1.22839800  |
| H | -0.73792300 | -3.14177400 | 2.31364000  |
| H | -1.59997300 | -2.18997500 | 1.07697700  |
| H | -1.15133100 | -3.88215700 | 0.74574700  |
| H | -0.48066000 | 0.74338100  | -0.16977900 |
| H | 2.03291600  | -0.93017700 | 0.89744200  |
| H | 1.17603500  | -1.35412400 | 2.41194600  |



### HOAc

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 1.53857800 | 1.15966900  | 0.35306600  |
| C | 0.91642200 | 0.14672200  | 0.07149400  |
| O | 1.53412300 | -1.03773700 | -0.23346200 |

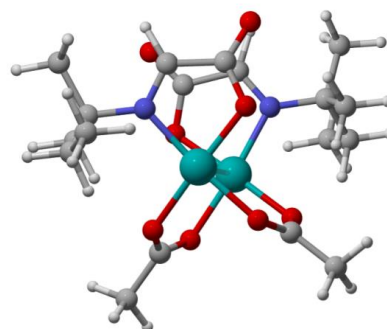
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.49433800  | -0.84269700 | -0.16410200 |
| C | -0.58885700 | 0.00850000  | 0.00725600  |
| H | -0.92759400 | -0.76844300 | 0.71207000  |
| H | -1.05534200 | 0.97012800  | 0.25539800  |
| H | -0.89637200 | -0.31098700 | -1.00194300 |



### Pd<sub>3</sub>(OAc)<sub>6</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| Pd | -1.54948400 | 0.87526800  | -0.01483200 |
| C  | 0.02385900  | 2.57195700  | 1.87668700  |
| O  | -1.04834300 | 2.45796800  | 1.19197900  |
| O  | 1.12987100  | 1.95242200  | 1.70468500  |
| C  | 2.28888100  | -1.21941200 | -1.85713400 |
| O  | 1.65164700  | -2.10437800 | -1.19327300 |
| O  | 2.26911000  | 0.04904700  | -1.68786800 |
| C  | 3.20423900  | -1.73311400 | -2.95259600 |
| C  | -0.02902500 | 3.55223400  | 3.03333400  |
| Pd | 0.01798700  | -1.77981900 | 0.00612600  |
| C  | 2.19250400  | -1.30679800 | 1.90579600  |
| O  | 2.63989300  | -0.32103600 | 1.22739000  |
| O  | 1.10614100  | -1.95520400 | 1.71715500  |
| C  | -0.07039100 | 2.55523100  | -1.89848200 |
| O  | -1.16427100 | 1.91591100  | -1.72141000 |
| O  | 1.00350500  | 2.46790800  | -1.21251800 |
| C  | -0.03595700 | 3.52654100  | -3.06335500 |
| C  | 3.04972300  | -1.75016900 | 3.07624600  |
| Pd | 1.53483000  | 0.90489600  | 0.00692400  |
| C  | -2.16474800 | -1.36238100 | -1.89694700 |
| O  | -2.63132900 | -0.38095400 | -1.22522100 |
| O  | -1.06625400 | -1.98859400 | -1.70349400 |
| C  | -3.01152800 | -1.82857400 | -3.06608500 |
| C  | -2.26237900 | -1.24786300 | 1.86625800  |
| O  | -2.26678400 | 0.01937100  | 1.68705500  |
| O  | -1.60931800 | -2.12575800 | 1.20843100  |
| C  | -3.16596300 | -1.77048300 | 2.96726100  |

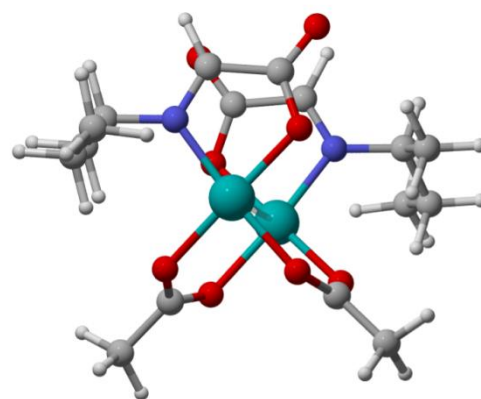
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.04076200 | 3.66555000  | -3.48358200 |
| H | 0.64230100  | 3.13090900  | -3.83711000 |
| H | 0.37417400  | 4.49001300  | -2.72345700 |
| H | -0.45974700 | 4.50401800  | 2.68609900  |
| H | -0.69756900 | 3.14902000  | 3.81162800  |
| H | 0.97332000  | 3.71564500  | 3.45065600  |
| H | -3.40508200 | -0.96743700 | 3.67784300  |
| H | -2.68729900 | -2.61813500 | 3.47815100  |
| H | -4.10462600 | -2.12811400 | 2.51099000  |
| H | 4.09687400  | -1.84131300 | 2.74906400  |
| H | 2.69039900  | -2.70527900 | 3.48146800  |
| H | 3.01200000  | -0.97435300 | 3.85859600  |
| H | 2.75047100  | -2.60367900 | -3.44724900 |
| H | 3.41610500  | -0.93515700 | -3.67750200 |
| H | 4.15543900  | -2.05277900 | -2.49405800 |
| H | -2.96944600 | -1.06580100 | -3.86107500 |
| H | -4.06097800 | -1.91764900 | -2.74616100 |
| H | -2.64516200 | -2.78856400 | -3.45312100 |



### T1-A3-Cat2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Pd | -0.87587900 | 0.71452200  | -0.27283600 |
| C  | 1.30185200  | -0.29245300 | -2.06401200 |
| O  | 1.34528900  | -1.44881600 | -1.50554500 |
| O  | 0.58240300  | 0.71228200  | -1.73988200 |
| C  | 2.18506800  | -0.11711400 | -3.28515400 |
| Pd | 0.26309000  | -1.82169100 | 0.21526400  |
| C  | 1.53299900  | 0.61611100  | 1.40131100  |
| O  | 0.60033700  | 1.40309500  | 0.99930200  |
| O  | 1.65636200  | -0.63615400 | 1.18050500  |
| C  | 2.59457900  | 1.24787900  | 2.28213400  |
| H  | 2.66788700  | 2.32600000  | 2.08410100  |
| H  | 3.56301300  | 0.75284100  | 2.12326200  |
| H  | 2.30401200  | 1.10044800  | 3.33652200  |
| H  | 3.03928200  | -0.80681600 | -3.24470600 |
| H  | 1.58641100  | -0.34776500 | -4.18309300 |
| H  | 2.52541600  | 0.92526700  | -3.36071500 |

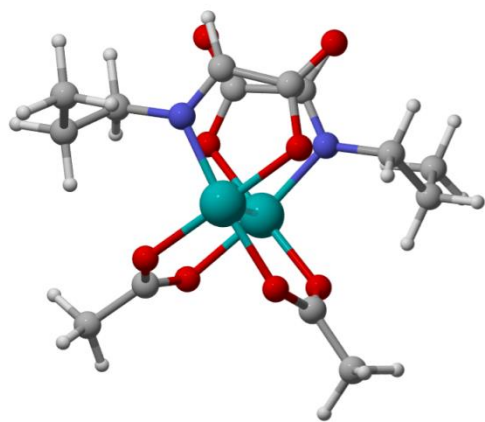
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.45729500 | 0.03480700  | 0.49437200  |
| C | -3.28935800 | -0.52809800 | -0.89434900 |
| C | -2.01385500 | -2.51873200 | 1.65902600  |
| C | -2.14180400 | -3.20701500 | 0.32366700  |
| O | -2.24470600 | -0.04212700 | -1.54314900 |
| O | -4.08128900 | -1.35904700 | -1.35546800 |
| N | -2.47317800 | 0.71485600  | 0.98903900  |
| N | -1.16403300 | -3.07639600 | -0.51447800 |
| O | -0.79705800 | -2.06664400 | 1.91072400  |
| O | -2.97767300 | -2.41376400 | 2.42738900  |
| H | -3.03791300 | -3.79498500 | 0.10376800  |
| H | -4.39278900 | -0.13570200 | 1.03554300  |
| C | -2.54966200 | 1.40195100  | 2.31444300  |
| C | -2.07572500 | 2.86288600  | 2.07865900  |
| H | -1.00900100 | 2.83067500  | 1.80184600  |
| H | -2.13680700 | 3.37230200  | 3.05790500  |
| C | -3.97827900 | 1.35784100  | 2.88717500  |
| H | -4.27848800 | 0.32536700  | 3.12968300  |
| H | -3.98962100 | 1.93621900  | 3.82449400  |
| H | -4.72328400 | 1.80235100  | 2.20704900  |
| C | -1.59913800 | 0.68063500  | 3.28981700  |
| H | -0.57022800 | 0.69543900  | 2.91192300  |
| C | -1.12897700 | -3.78025100 | -1.83276300 |
| C | 0.26134800  | -4.46766000 | -1.92610300 |
| C | -2.27349100 | -4.80332000 | -1.95300000 |
| C | -1.28269000 | -2.72720100 | -2.94752500 |
| H | -3.25528600 | -4.30261000 | -1.97064000 |
| H | -2.15599700 | -5.33812000 | -2.90873700 |
| H | -2.26213700 | -5.55162200 | -1.14365000 |
| H | -1.22376700 | -3.23975800 | -3.92227500 |
| H | -2.24895600 | -2.20885800 | -2.86235100 |
| H | -0.48043700 | -1.98227200 | -2.89157300 |
| H | 0.28597500  | -4.99045100 | -2.89987100 |
| H | -1.62890000 | 1.20631700  | 4.25889900  |
| C | -2.86492800 | 3.64442500  | 1.02064500  |
| H | -2.46340300 | 4.66622500  | 0.92296000  |
| H | -2.78500400 | 3.16182300  | 0.03136700  |
| H | -3.93501300 | 3.73201000  | 1.27418500  |
| H | -1.90638500 | -0.36607800 | 3.42954900  |
| H | 1.02676300  | -3.67532400 | -1.96997600 |
| C | 0.58681000  | -5.44375000 | -0.78840500 |
| H | -0.13659100 | -6.27442100 | -0.72746100 |
| H | 1.58551400  | -5.88519200 | -0.93858200 |
| H | 0.59748300  | -4.92580100 | 0.18602600  |



### T1-A2-Cat2

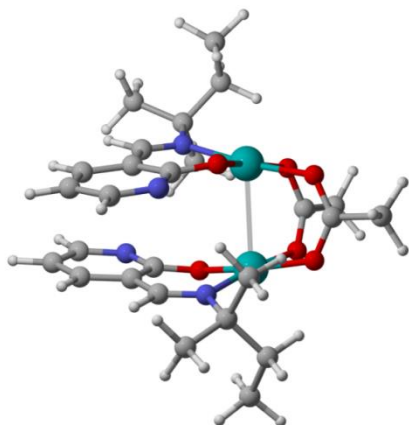
|    |             |             |             |
|----|-------------|-------------|-------------|
| Pd | -0.85105100 | 0.71891700  | -0.29436200 |
| C  | 1.31840800  | -0.32392400 | -2.08044400 |
| O  | 1.37634300  | -1.46608100 | -1.49476200 |
| O  | 0.59798400  | 0.68425200  | -1.77004900 |
| C  | 2.18873600  | -0.16967300 | -3.31381600 |
| Pd | 0.28823700  | -1.80505600 | 0.22554500  |
| C  | 1.52427800  | 0.64887600  | 1.41909200  |
| O  | 0.60335400  | 1.43226600  | 0.98454500  |
| O  | 1.65503100  | -0.60443100 | 1.20954300  |
| C  | 2.56269400  | 1.28823300  | 2.32205700  |
| H  | 2.62379000  | 2.36905100  | 2.13538000  |
| H  | 3.54042700  | 0.80868800  | 2.17204300  |
| H  | 2.26083300  | 1.12504300  | 3.37086500  |
| H  | 3.01508100  | -0.89321600 | -3.29662300 |
| H  | 1.56742800  | -0.35835100 | -4.20594400 |
| H  | 2.57105000  | 0.85909700  | -3.37882900 |
| C  | -3.43534100 | 0.09690900  | 0.51307500  |
| C  | -3.29575700 | -0.50990800 | -0.86103800 |
| C  | -2.02061700 | -2.53756800 | 1.61902600  |
| C  | -2.09334900 | -3.23483000 | 0.28334800  |
| O  | -2.24072800 | -0.06874600 | -1.52772000 |
| O  | -4.10585300 | -1.33661500 | -1.29457500 |
| N  | -2.42337800 | 0.76152300  | 0.96980500  |
| N  | -1.09481900 | -3.06993700 | -0.52298600 |
| O  | -0.82326900 | -2.04381700 | 1.89187500  |
| O  | -3.00275800 | -2.45185800 | 2.36458800  |
| H  | -2.95999300 | -3.85324700 | 0.01521700  |
| H  | -4.35973200 | -0.02413600 | 1.09296000  |
| C  | -2.48982500 | 1.44678600  | 2.27897100  |
| C  | -2.04018800 | 2.91057700  | 2.10777500  |
| H  | -0.96489000 | 2.91589900  | 1.86134500  |
| H  | -2.14838300 | 3.39121100  | 3.09721400  |

|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| C | -1.67462500 | 0.68090900  | 3.32769400  | H | 2.45281800  | 2.80736300  | 1.87994600  |
| H | -0.61023700 | 0.67182500  | 3.05657700  | H | 3.47725100  | 1.34073000  | 2.15336900  |
| C | -1.04866900 | -3.76122400 | -1.82987400 | H | 2.11003500  | 1.69115300  | 3.23871700  |
| C | 0.30706700  | -4.47827700 | -1.97720800 | H | 2.70697300  | -1.51105400 | -3.55567800 |
| C | -1.33942200 | -2.77526000 | -2.96761100 | H | 2.12363800  | 0.12674800  | -4.06065100 |
| H | -1.34851400 | -3.33013500 | -3.92060000 | H | 3.44764800  | -0.03941500 | -2.87162800 |
| H | -2.31035700 | -2.27984300 | -2.82116200 | C | -3.29725600 | -0.06460400 | 0.21375400  |
| H | -0.55991600 | -2.00287300 | -3.01588900 | C | -3.15568600 | -0.62445400 | -1.18228600 |
| H | 0.27705500  | -5.01328500 | -2.94393900 | C | -1.85467100 | -2.33422900 | 1.90935500  |
| H | -1.78854000 | 1.18746100  | 4.30062900  | C | -1.98714400 | -3.00557800 | 0.56239200  |
| C | -2.83994600 | 3.67982700  | 1.04909000  | O | -2.05720400 | -0.22855400 | -1.81082300 |
| H | -2.52897300 | 4.73643600  | 1.01315500  | O | -3.98432200 | -1.41482900 | -1.64185900 |
| H | -2.68128000 | 3.25076200  | 0.04473400  | N | -2.29698500 | 0.61035200  | 0.68157800  |
| H | -3.92372600 | 3.65402700  | 1.26213400  | N | -1.01164100 | -2.84572400 | -0.27292900 |
| H | -2.02037600 | -0.35973300 | 3.41215200  | O | -0.67158600 | -1.77080200 | 2.11434700  |
| H | 1.09713100  | -3.71234300 | -2.05583100 | O | -2.80071800 | -2.29365600 | 2.70041800  |
| C | 0.61385700  | -5.45466700 | -0.83499900 | H | -2.90239000 | -3.54507300 | 0.28441500  |
| H | -0.18672700 | -6.20721900 | -0.71931300 | H | -4.18226400 | -0.28374300 | 0.82594900  |
| H | 1.55735400  | -5.99278900 | -1.02113000 | C | -2.26526200 | 1.11608600  | 2.05649300  |
| H | 0.71822900  | -4.92002000 | 0.12479000  | C | -2.11666500 | 2.64557300  | 2.08407200  |
| H | -1.85546800 | -4.52246500 | -1.79801200 | H | -1.14635300 | 2.91087300  | 1.63258100  |
| H | -3.55957000 | 1.43240200  | 2.57375200  | H | -2.07033900 | 2.94247700  | 3.14739600  |



### T1-A1-Cat2

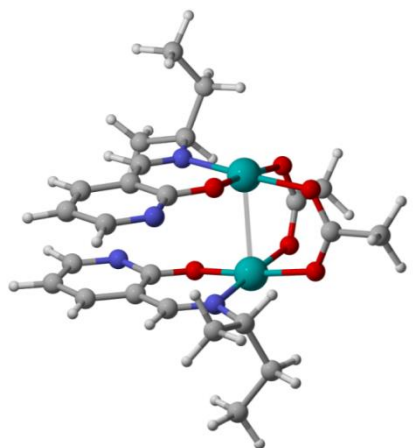
|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| Pd | -0.73802900 | 0.68008800  | -0.57226700 | H | 0.08742300  | -4.35048900 | -1.90365200 |
| C  | 1.50707300  | -0.48452600 | -2.08253300 | H | 0.00847400  | -4.66031800 | -2.96130300 |
| O  | 1.52575700  | -1.52589000 | -1.33022500 | C | -3.26411000 | 3.37228500  | 1.37208200  |
| O  | 0.77315300  | 0.55629000  | -1.96808500 | H | -3.14924900 | 4.46513100  | 1.45473800  |
| C  | 2.50201400  | -0.48219900 | -3.22805400 | H | -3.28743400 | 3.12008500  | 0.29817000  |
| Pd | 0.43325600  | -1.64856100 | 0.42240500  | H | -4.24419400 | 3.10300300  | 1.80462500  |
| C  | 1.52883100  | 0.93174700  | 1.32340100  | H | 1.04479700  | -3.81412000 | -1.79507800 |
| O  | 0.59502500  | 1.58281500  | 0.72838400  | C | 0.04167900  | -5.57336500 | -0.97950400 |
| O  | 1.75491400  | -0.32671900 | 1.29147100  | H | -0.91960500 | -6.11050900 | -1.06665700 |
| C  | 2.45960200  | 1.75487800  | 2.19413800  | H | 0.84704300  | -6.28388800 | -1.22625500 |
|    |             |             |             | H | 0.16978500  | -5.27816300 | 0.07589900  |
|    |             |             |             | H | -2.04730400 | -3.82456500 | -1.80921400 |
|    |             |             |             | H | -3.18724800 | 0.78588100  | 2.57014000  |
|    |             |             |             | H | -1.40960000 | 0.61595600  | 2.54197300  |
|    |             |             |             | H | -0.98568300 | -2.47450400 | -2.30034600 |



### T2-A3-Cat2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Pd | -0.80252400 | 0.88371100  | -0.44957300 |
| C  | 1.41391900  | -0.24092600 | -2.02347000 |
| O  | 1.65795200  | -1.09989800 | -1.11556800 |
| O  | 0.46934400  | 0.63004800  | -2.05945600 |
| C  | 2.31646200  | -0.27127800 | -3.24375300 |
| Pd | 0.52333100  | -1.42872000 | 0.59724700  |
| C  | 1.73235000  | 1.19464300  | 1.14974900  |
| O  | 0.85761500  | 1.77785700  | 0.43104900  |
| O  | 1.81503900  | -0.05409700 | 1.44325900  |
| C  | 2.78768400  | 2.08236600  | 1.78442400  |
| H  | 2.96495800  | 2.97010300  | 1.16150400  |
| H  | 3.71884200  | 1.52036500  | 1.94237400  |
| H  | 2.41126600  | 2.41790700  | 2.76632400  |
| H  | 3.31487800  | -0.64064400 | -2.97118000 |
| H  | 1.87864000  | -0.96796700 | -3.97950500 |
| H  | 2.37753600  | 0.72576500  | -3.70201500 |
| C  | -4.10977100 | 0.01515100  | 3.50696700  |
| C  | -2.77340600 | 0.59148600  | 1.69234200  |
| C  | -3.68510300 | -0.07147200 | 0.79125900  |
| C  | -4.85815900 | -0.64283500 | 1.33473300  |
| C  | -5.08479300 | -0.61783500 | 2.70766000  |
| H  | -4.23589700 | 0.04898800  | 4.59851400  |
| H  | -5.56769000 | -1.12997200 | 0.65710300  |
| H  | -5.97689300 | -1.06304200 | 3.15487700  |
| N  | -3.00475100 | 0.60700100  | 3.04082100  |
| O  | -1.70801300 | 1.22973800  | 1.30314400  |
| C  | -3.51897400 | -0.13717200 | -0.63499100 |
| H  | -4.39564500 | -0.53523800 | -1.15918100 |
| N  | -2.49393100 | 0.21344200  | -1.36519700 |
| C  | -2.62965700 | 0.19102100  | -2.87150900 |
| C  | -2.14612600 | 1.57003200  | -3.40125100 |
| H  | -2.27241600 | 1.54595900  | -4.49981000 |

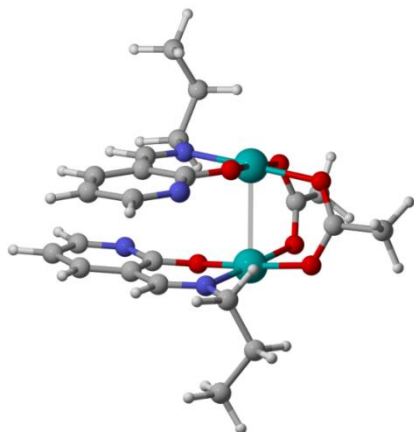
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.06519200 | 1.65227900  | -3.21223200 |
| C | -2.87078800 | 2.78751800  | -2.81193600 |
| H | -3.95485400 | 2.77509400  | -3.01787700 |
| H | -2.73024400 | 2.83686600  | -1.71858300 |
| H | -2.46378400 | 3.71815200  | -3.24051200 |
| C | -1.77068600 | -0.95529900 | -3.44003100 |
| H | -2.05707400 | -1.92120700 | -2.99240300 |
| H | -1.91872000 | -1.00237000 | -4.53256200 |
| H | -0.70942700 | -0.78192200 | -3.24134400 |
| C | -4.08705500 | -0.04707100 | -3.32666300 |
| H | -4.11504900 | 0.05777900  | -4.42282100 |
| H | -4.43067600 | -1.06852500 | -3.09122000 |
| H | -4.79794900 | 0.68019000  | -2.90149200 |
| C | -3.76080900 | -3.90533700 | -1.09811600 |
| C | -1.77679600 | -3.01399400 | -0.27400400 |
| C | -2.32238200 | -2.99459000 | 1.06179200  |
| C | -3.62171100 | -3.51621700 | 1.25588000  |
| C | -4.36832200 | -3.97204000 | 0.17341900  |
| H | -4.31495200 | -4.23972400 | -1.98671900 |
| H | -4.03773900 | -3.52623000 | 2.26916000  |
| H | -5.37941900 | -4.36850000 | 0.29407200  |
| N | -2.52132300 | -3.46057900 | -1.33150700 |
| O | -0.56338300 | -2.64386700 | -0.56481300 |
| C | -1.61338100 | -2.54026400 | 2.22668600  |
| H | -2.13439700 | -2.75595600 | 3.16671800  |
| N | -0.46076400 | -1.93045800 | 2.30829800  |
| C | 0.14618800  | -1.69749200 | 3.67404500  |
| C | 1.60742500  | -2.22547400 | 3.62777000  |
| H | 2.02973600  | -2.06898600 | 4.63799400  |
| H | 2.18443400  | -1.58410400 | 2.94463600  |
| C | 1.75869500  | -3.69506400 | 3.21292000  |
| H | 1.23511800  | -4.38388800 | 3.89790000  |
| H | 1.36438900  | -3.85846400 | 2.19535500  |
| H | 2.82313100  | -3.98199300 | 3.20575100  |
| C | 0.10966800  | -0.19049500 | 3.99435000  |
| H | -0.92028500 | 0.19888000  | 3.93986200  |
| H | 0.50452500  | -0.03395100 | 5.01286000  |
| H | 0.73094600  | 0.37168400  | 3.29175100  |
| C | -0.62579800 | -2.43140900 | 4.79348900  |
| H | -0.06248100 | -2.29590500 | 5.73030700  |
| H | -1.62807100 | -1.99947800 | 4.95390300  |
| H | -0.72360700 | -3.51463600 | 4.61435800  |



### T2-A2-Cat2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Pd | -0.70416000 | 0.98236300  | -0.21549900 |
| C  | 1.29983500  | 0.00759100  | -2.15464100 |
| O  | 1.52945700  | -1.03016400 | -1.45261700 |
| O  | 0.46597600  | 0.95937000  | -1.92004100 |
| C  | 2.07227000  | 0.12480400  | -3.45718700 |
| Pd | 0.55047000  | -1.48329600 | 0.32884600  |
| C  | 1.89764400  | 0.96904200  | 1.26697300  |
| O  | 0.98206600  | 1.70300700  | 0.77166600  |
| O  | 1.98100400  | -0.31518400 | 1.25732700  |
| C  | 3.01572200  | 1.68883500  | 2.00100600  |
| H  | 3.24207800  | 2.64223300  | 1.50249000  |
| H  | 3.91146500  | 1.05541900  | 2.05904200  |
| H  | 2.67256100  | 1.91505900  | 3.02518100  |
| H  | 3.08620600  | -0.28162500 | -3.33296400 |
| H  | 1.55691700  | -0.47841100 | -4.22430000 |
| H  | 2.10813600  | 1.17004700  | -3.79354200 |
| C  | -4.19055800 | -0.24616800 | 3.51037900  |
| C  | -2.74227700 | 0.45165900  | 1.82710500  |
| C  | -3.66152900 | -0.03362800 | 0.82012900  |
| C  | -4.88683200 | -0.59077700 | 1.25129100  |
| C  | -5.17317800 | -0.70288200 | 2.60854100  |
| H  | -4.35715300 | -0.34018000 | 4.59283100  |
| H  | -5.59111000 | -0.95811600 | 0.49697800  |
| H  | -6.10939400 | -1.13661700 | 2.96788300  |
| N  | -3.02469100 | 0.30860500  | 3.15807100  |
| O  | -1.61368800 | 1.04802400  | 1.56624500  |
| C  | -3.41270100 | -0.00867100 | -0.59500300 |
| H  | -4.23775300 | -0.37969800 | -1.21691500 |
| N  | -2.32590200 | 0.36788800  | -1.21097600 |
| C  | -2.26436900 | 0.36899400  | -2.69726500 |
| C  | -2.29894900 | 1.83693500  | -3.18892900 |
| H  | -2.17699600 | 1.81464000  | -4.28768200 |

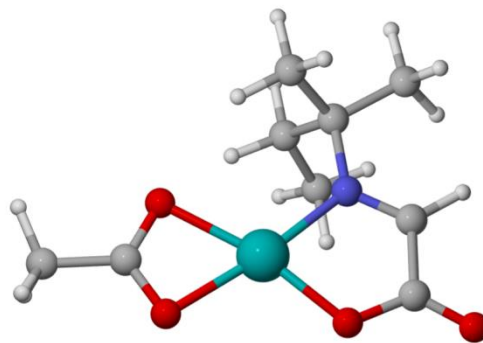
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.41198900 | 2.35113200  | -2.78184400 |
| C | -3.57021300 | 2.60505100  | -2.80816500 |
| H | -4.48095000 | 2.13347900  | -3.21624200 |
| H | -3.68115200 | 2.66835300  | -1.71250700 |
| H | -3.53033100 | 3.63543900  | -3.19768000 |
| C | -3.29850700 | -0.53798700 | -3.37418300 |
| H | -3.07102300 | -0.56389600 | -4.45244200 |
| H | -3.22262900 | -1.56586900 | -2.97971400 |
| H | -4.33505600 | -0.17344600 | -3.27162600 |
| C | -3.98148800 | -3.76528200 | -1.01390500 |
| C | -1.90740400 | -2.92212800 | -0.37750300 |
| C | -2.29030800 | -3.00315200 | 1.01595300  |
| C | -3.56164800 | -3.53682900 | 1.32666100  |
| C | -4.42930400 | -3.93095600 | 0.31253100  |
| H | -4.64186200 | -4.03429700 | -1.85047800 |
| H | -3.85988400 | -3.60494300 | 2.37849500  |
| H | -5.42026800 | -4.33877100 | 0.52568400  |
| N | -2.78169800 | -3.28695000 | -1.36447100 |
| O | -0.74302400 | -2.51532000 | -0.79754200 |
| C | -1.47713700 | -2.56084000 | 2.11516700  |
| H | -1.90734100 | -2.73673300 | 3.10972300  |
| N | -0.32179600 | -1.95686500 | 2.06485400  |
| C | 0.40344500  | -1.61292700 | 3.31739700  |
| C | 1.61541000  | -2.56627500 | 3.45992900  |
| H | 2.18058800  | -2.24228800 | 4.35336900  |
| H | 2.27616000  | -2.40561900 | 2.59130600  |
| C | 1.24696600  | -4.05054800 | 3.57037000  |
| H | 0.60325900  | -4.25687300 | 4.44290200  |
| H | 0.71638600  | -4.39515800 | 2.66677600  |
| H | 2.15438800  | -4.66705800 | 3.67765900  |
| C | -0.48487100 | -1.54524500 | 4.56493100  |
| H | 0.12559600  | -1.15039100 | 5.39349000  |
| H | -1.32887400 | -0.85424300 | 4.39695900  |
| H | -0.86592000 | -2.53007200 | 4.88557600  |
| H | -1.26977100 | -0.03532800 | -2.93359600 |
| H | 0.79764800  | -0.60199100 | 3.14122900  |



### T2-A1-Cat2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Pd | -0.57057000 | 1.02574100  | -0.27995400 |
| C  | 1.40915500  | -0.02493600 | -2.19358200 |
| O  | 1.80719500  | -0.90013100 | -1.35461900 |
| O  | 0.43834100  | 0.80923800  | -2.06863400 |
| C  | 2.14800100  | 0.02186100  | -3.51827700 |
| Pd | 0.67804000  | -1.41001700 | 0.31328100  |
| C  | 1.95307000  | 1.07635500  | 1.25503700  |
| O  | 1.18592900  | 1.78836900  | 0.52500600  |
| O  | 1.92305900  | -0.19733500 | 1.42940300  |
| C  | 3.01412600  | 1.82164800  | 2.04339100  |
| H  | 3.38173500  | 2.67916200  | 1.46166700  |
| H  | 3.84032100  | 1.15033000  | 2.31460900  |
| H  | 2.55108600  | 2.21143800  | 2.96599300  |
| H  | 3.21517200  | -0.19110500 | -3.36070900 |
| H  | 1.73860000  | -0.76692200 | -4.17225200 |
| H  | 2.01213800  | 0.99704500  | -4.00538100 |
| C  | -3.65618000 | 0.21526200  | 3.88003400  |
| C  | -2.40832400 | 0.73495200  | 1.98936900  |
| C  | -3.38782800 | 0.08605700  | 1.14455700  |
| C  | -4.53119600 | -0.47294600 | 1.76363500  |
| C  | -4.68151700 | -0.42086500 | 3.14529800  |
| H  | -3.72605700 | 0.27072200  | 4.97571800  |
| H  | -5.28014900 | -0.96578700 | 1.13334000  |
| H  | -5.55125700 | -0.84960600 | 3.64907200  |
| N  | -2.56543500 | 0.77437300  | 3.34721000  |
| O  | -1.32665500 | 1.31533800  | 1.54978600  |
| C  | -3.26346100 | -0.07008700 | -0.27837100 |
| H  | -4.11062200 | -0.56451100 | -0.78063800 |
| N  | -2.25371500 | 0.26859800  | -1.03540400 |
| C  | -2.32889700 | 0.00442400  | -2.48193400 |
| C  | -2.39151900 | 1.30851800  | -3.29198600 |
| H  | -2.41092400 | 1.02635100  | -4.36080300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.45546500 | 1.86755700  | -3.12767800 |
| C | -3.60779400 | 2.17492000  | -2.94395900 |
| H | -4.55362700 | 1.62406600  | -3.09691300 |
| H | -3.57325700 | 2.49981800  | -1.89031200 |
| H | -3.64219400 | 3.08038200  | -3.57158800 |
| C | -3.54072500 | -3.79850000 | -1.67322200 |
| C | -1.60336900 | -2.93097400 | -0.72664500 |
| C | -2.20979600 | -2.96658000 | 0.58671200  |
| C | -3.52590000 | -3.47526000 | 0.69607000  |
| C | -4.21580200 | -3.89562600 | -0.43606200 |
| H | -4.04983100 | -4.10903800 | -2.59673000 |
| H | -3.99440700 | -3.50766600 | 1.68627900  |
| H | -5.23476900 | -4.28640000 | -0.38062800 |
| N | -2.29414100 | -3.34344100 | -1.83231600 |
| O | -0.39041400 | -2.51640800 | -0.96606000 |
| C | -1.58543500 | -2.48399100 | 1.78750100  |
| H | -2.16715400 | -2.61401200 | 2.71438700  |
| N | -0.43330100 | -1.87845500 | 1.90176400  |
| C | 0.01713700  | -1.45082000 | 3.23659400  |
| C | 1.25201400  | -2.24102800 | 3.69613400  |
| H | 1.54794200  | -1.83710900 | 4.68184600  |
| H | 2.08208600  | -2.02688400 | 3.00265900  |
| C | 0.99981900  | -3.75062500 | 3.78916500  |
| H | 0.16542900  | -3.97938400 | 4.47683800  |
| H | 0.74742900  | -4.17110700 | 2.80103200  |
| H | 1.89325400  | -4.27986600 | 4.15882400  |
| H | -1.44433400 | -0.59102600 | -2.75340300 |
| H | 0.23191100  | -0.37317200 | 3.18038800  |
| H | -0.82133100 | -1.58752800 | 3.94482800  |
| H | -3.22228300 | -0.61888100 | -2.67352800 |

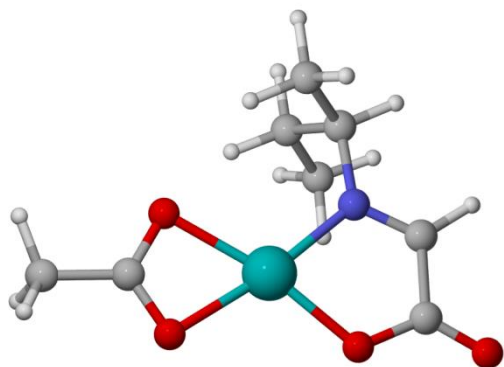


### T1-A3-Cat1

|   |             |            |            |
|---|-------------|------------|------------|
| O | -1.54211100 | 0.56583200 | 1.22677100 |
| C | 0.62026700  | 0.91264000 | 2.14388600 |
| H | 1.27324000  | 1.18357000 | 2.98158200 |
| N | 1.07283900  | 0.56680500 | 0.98305800 |



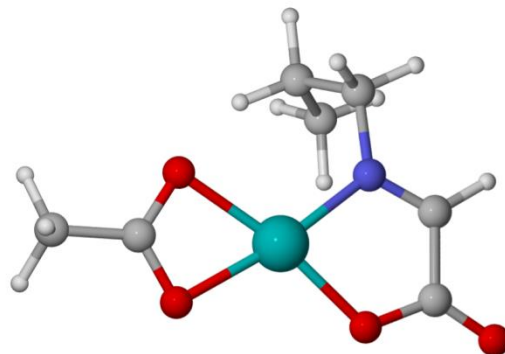
|    |             |             |             |
|----|-------------|-------------|-------------|
| Pd | -0.37390900 | 0.11249300  | -0.33884400 |
| C  | 2.51680800  | 0.47353300  | 0.62831200  |
| C  | 2.77556700  | -0.99396500 | 0.17994600  |
| H  | 2.19182900  | -1.17767500 | -0.73786700 |
| H  | 3.84217900  | -1.05036600 | -0.10495500 |
| O  | -1.70483500 | -0.40595700 | -1.87845900 |
| O  | 0.47567900  | -0.43660500 | -2.19960500 |
| C  | -0.71511800 | -0.62598100 | -2.67199200 |
| C  | -0.92729900 | -1.11001000 | -4.07590200 |
| H  | -0.05194700 | -0.87176900 | -4.69696900 |
| H  | -1.06513500 | -2.20493800 | -4.06463900 |
| H  | -1.83787500 | -0.65739100 | -4.49579300 |
| C  | 2.44363700  | -2.06339000 | 1.22755900  |
| H  | 3.04060900  | -1.95201200 | 2.14836500  |
| H  | 1.37651500  | -2.03121100 | 1.50483000  |
| H  | 2.64885000  | -3.06742200 | 0.82240000  |
| C  | -0.88133400 | 0.92857900  | 2.31674700  |
| O  | -1.40049800 | 1.25001700  | 3.38512800  |
| C  | 3.42337400  | 0.87240200  | 1.80416900  |
| H  | 4.47277000  | 0.77766800  | 1.48344100  |
| H  | 3.25913100  | 1.92072300  | 2.10506000  |
| H  | 3.28341100  | 0.22586500  | 2.68534100  |
| C  | 2.74108400  | 1.43171100  | -0.56093200 |
| H  | 2.09922400  | 1.15904700  | -1.41267100 |
| H  | 2.52390100  | 2.47210300  | -0.26837800 |
| H  | 3.79391700  | 1.37040300  | -0.88188200 |



**T1-A2-Cat1**

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.55052800 | 0.56376700  | 1.23225000  |
| C  | 0.63050000  | 0.87525900  | 2.10749900  |
| H  | 1.32791600  | 1.12432000  | 2.92011800  |
| N  | 1.04356700  | 0.53823100  | 0.93014600  |
| Pd | -0.41739200 | 0.11040000  | -0.36591900 |
| C  | 2.47036600  | 0.43834800  | 0.57475800  |
| C  | 2.79159100  | -1.02007700 | 0.18481400  |

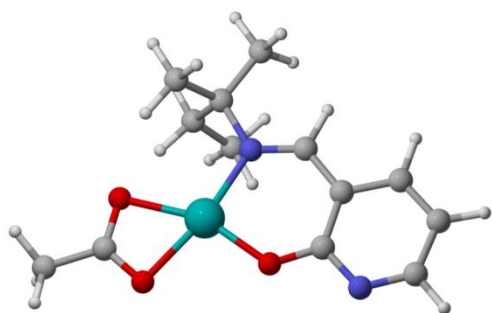
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.23136500  | -1.26558400 | -0.73464800 |
| H | 3.86514000  | -1.04888000 | -0.07619300 |
| O | -1.75683800 | -0.39172500 | -1.90766600 |
| O | 0.42498400  | -0.42735700 | -2.22310100 |
| C | -0.76601100 | -0.60943300 | -2.70022200 |
| C | -0.97454300 | -1.08258900 | -4.10813800 |
| H | -0.09444800 | -0.84695500 | -4.72344800 |
| H | -1.12101900 | -2.17644700 | -4.10472900 |
| H | -1.87965300 | -0.62024900 | -4.52929300 |
| C | 2.48128200  | -2.03322800 | 1.29268000  |
| H | 3.01267000  | -1.78578000 | 2.22893200  |
| H | 1.40120500  | -2.06453200 | 1.51375700  |
| H | 2.78845400  | -3.04759600 | 0.99153300  |
| C | -0.86673700 | 0.90727500  | 2.31507000  |
| O | -1.36188000 | 1.22263700  | 3.39630200  |
| C | 2.77448700  | 1.42994500  | -0.55739700 |
| H | 2.19750600  | 1.17096100  | -1.45950600 |
| H | 2.52351300  | 2.46023600  | -0.25876900 |
| H | 3.84827800  | 1.38697000  | -0.80213800 |
| H | 3.04802800  | 0.70851900  | 1.48299900  |



**T1-A1-Cat1**

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.57009900 | 0.47697900  | 1.25752300  |
| C  | 0.60961200  | 0.85426600  | 2.11111600  |
| H  | 1.30914300  | 1.11706100  | 2.91761800  |
| N  | 1.01741800  | 0.53053600  | 0.92786300  |
| Pd | -0.43762000 | 0.06454700  | -0.35489300 |
| C  | 2.43190800  | 0.43135500  | 0.56060300  |
| C  | 2.80070800  | -1.01962300 | 0.19674200  |
| H  | 2.21666600  | -1.31673100 | -0.69138600 |
| H  | 3.86340600  | -1.01306800 | -0.10529900 |
| O  | -1.75894700 | -0.47952400 | -1.89566700 |
| O  | 0.42286100  | -0.42685800 | -2.21021200 |
| C  | -0.75991500 | -0.64712100 | -2.69109100 |
| C  | -0.95450400 | -1.05078500 | -4.12228300 |

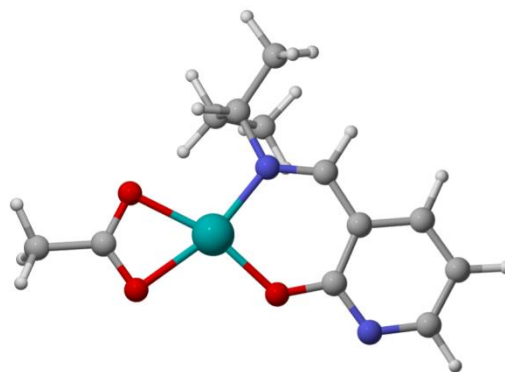
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.03295300 | -1.49884000 | -4.52054900 |
| H | -1.79633400 | -1.75466400 | -4.20217900 |
| H | -1.20073400 | -0.15668200 | -4.72046500 |
| C | 2.57171500  | -2.00457000 | 1.34904200  |
| H | 3.13520100  | -1.71047600 | 2.25245300  |
| H | 1.50367900  | -2.06159500 | 1.61856400  |
| H | 2.89718300  | -3.01847100 | 1.06622400  |
| C | -0.88681700 | 0.84407300  | 2.33241400  |
| O | -1.37843200 | 1.14625300  | 3.41905400  |
| H | 3.04618100  | 0.79919000  | 1.40546400  |
| H | 2.58844900  | 1.09254100  | -0.30900700 |



**T2-A3-Cat1**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.87388300 | 2.06620800  | 0.42053500  |
| C  | -1.42665500 | 1.56980400  | 1.70149900  |
| C  | -1.97424500 | 2.16670700  | 2.86609200  |
| C  | -2.90345900 | 3.19248400  | 2.75900100  |
| C  | -3.26665700 | 3.60122900  | 1.45468500  |
| N  | -2.78659700 | 3.07615500  | 0.32538100  |
| H  | -1.64915900 | 1.80280800  | 3.84817300  |
| H  | -3.34076700 | 3.67031200  | 3.63888300  |
| H  | -3.99811000 | 4.41096100  | 1.32302700  |
| O  | -1.45436300 | 1.60020100  | -0.72398500 |
| C  | -0.47214200 | 0.51486100  | 1.88012200  |
| H  | -0.26636300 | 0.26850900  | 2.92959400  |
| N  | 0.16766100  | -0.17184900 | 0.96679800  |
| Pd | -0.13017400 | 0.15924300  | -0.99292700 |
| C  | 1.12616500  | -1.26344900 | 1.35794200  |
| C  | 2.50755000  | -0.89927800 | 0.77290800  |
| C  | 1.27416300  | -1.41197700 | 2.88610100  |
| H  | 1.67627900  | -0.49650600 | 3.35211900  |
| H  | 1.99478400  | -2.22277500 | 3.07726100  |
| C  | 0.60515700  | -2.59604600 | 0.74674200  |
| H  | 0.67581700  | -2.52576500 | -0.35007800 |
| H  | 1.31163500  | -3.38791100 | 1.05800200  |
| O  | -0.18257200 | 0.22301400  | -3.10930800 |

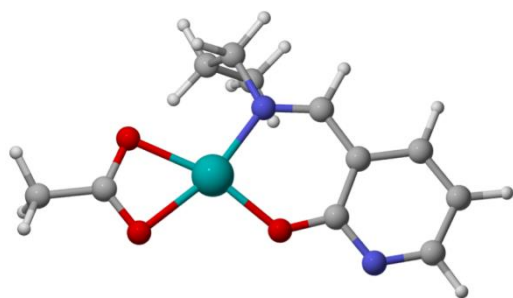
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.12517000  | -1.19871600 | -2.04774900 |
| C | 0.68317500  | -0.72322100 | -3.16935300 |
| C | 1.15048500  | -1.28605500 | -4.48046300 |
| H | 0.33162300  | -1.68391100 | 3.38834600  |
| C | -0.82691100 | -2.97298700 | 1.14658500  |
| H | -0.94253500 | -3.10491800 | 2.23609300  |
| H | -1.54305500 | -2.20102100 | 0.81883200  |
| H | -1.11904800 | -3.92232200 | 0.66864000  |
| H | 3.23368300  | -1.69020600 | 1.02546200  |
| H | 2.46658200  | -0.80441900 | -0.32125900 |
| H | 2.86476300  | 0.05190400  | 1.20154400  |
| H | 2.21051500  | -1.57329300 | -4.41285600 |
| H | 0.56576000  | -2.19183500 | -4.71642100 |
| H | 0.99752700  | -0.55067300 | -5.28318200 |



**T2-A2-Cat1**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.93049400 | 2.04754400  | 0.41418300  |
| C  | -1.48324300 | 1.50795100  | 1.68254400  |
| C  | -2.03349800 | 2.06180600  | 2.86703200  |
| C  | -2.96710900 | 3.08614800  | 2.79567800  |
| C  | -3.33433200 | 3.53602900  | 1.50576000  |
| N  | -2.85210800 | 3.05323500  | 0.35922100  |
| H  | -1.70753900 | 1.66401500  | 3.83557200  |
| H  | -3.40660500 | 3.53128600  | 3.69147700  |
| H  | -4.07217600 | 4.34417300  | 1.40247200  |
| O  | -1.50912200 | 1.63315100  | -0.75010300 |
| C  | -0.53472500 | 0.44258200  | 1.81966600  |
| H  | -0.32335700 | 0.12589400  | 2.85114200  |
| N  | 0.09639000  | -0.18351600 | 0.85902600  |
| Pd | -0.14366800 | 0.23474700  | -1.05953000 |
| C  | 0.98443700  | -1.34353300 | 1.12671700  |
| C  | 1.58848200  | -1.35165500 | 2.53769000  |
| H  | 2.07365100  | -0.38961200 | 2.77115000  |
| H  | 2.35528000  | -2.14128100 | 2.58536300  |
| C  | 0.22802700  | -2.65084800 | 0.77609700  |

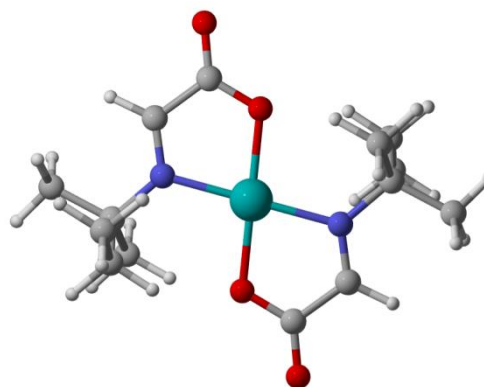
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.00081100  | -2.62480500 | -0.30347400 |
| H | 0.93478400  | -3.48705800 | 0.93018700  |
| O | -0.00263800 | 0.29275000  | -3.19415500 |
| O | 1.21183800  | -1.08142100 | -1.96425600 |
| C | 0.88041100  | -0.63575800 | -3.13884500 |
| C | 1.49479900  | -1.22041400 | -4.37837300 |
| H | 0.84577400  | -1.57096100 | 3.32278000  |
| C | -1.05895100 | -2.88114800 | 1.57675600  |
| H | -0.87348100 | -2.93526700 | 2.66354700  |
| H | -1.78964400 | -2.07536600 | 1.39541000  |
| H | -1.53207600 | -3.83074600 | 1.27826000  |
| H | 2.48259100  | -1.64656100 | -4.15029600 |
| H | 0.84527900  | -2.02707100 | -4.75992200 |
| H | 1.57466600  | -0.44874600 | -5.15810300 |
| H | 1.80888600  | -1.24187100 | 0.40042200  |



**T2-A1-Cat1**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.92525800 | 2.04350200  | 0.39997100  |
| C  | -1.42546700 | 1.52513400  | 1.65809300  |
| C  | -1.93939200 | 2.08532700  | 2.85605700  |
| C  | -2.88804800 | 3.09671100  | 2.80630800  |
| C  | -3.30747000 | 3.52682200  | 1.52525900  |
| N  | -2.86108700 | 3.03671100  | 0.36746100  |
| H  | -1.57321800 | 1.70330500  | 3.81643800  |
| H  | -3.30067500 | 3.54723700  | 3.71210300  |
| H  | -4.05865900 | 4.32464900  | 1.43991800  |
| O  | -1.54200500 | 1.62097400  | -0.77485000 |
| C  | -0.45880500 | 0.47498100  | 1.76683800  |
| H  | -0.19546100 | 0.15767800  | 2.78950500  |
| N  | 0.14285900  | -0.15007800 | 0.78569600  |
| Pd | -0.16780100 | 0.23970700  | -1.12703800 |
| C  | 1.04717700  | -1.27537600 | 1.06906800  |
| C  | 0.39437000  | -2.62767100 | 0.72883300  |
| H  | 0.19980400  | -2.65283800 | -0.35732200 |
| H  | 1.14498900  | -3.41264100 | 0.93540600  |
| O  | -0.10608100 | 0.27313100  | -3.26290100 |
| O  | 1.17662300  | -1.06201200 | -2.05932400 |

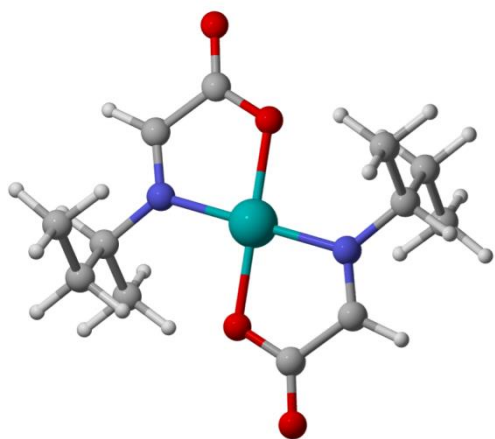
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.79426500  | -0.64020100 | -3.22745000 |
| C | 1.37168100  | -1.23372200 | -4.48001000 |
| C | -0.89432600 | -2.89496900 | 1.51460000  |
| H | -0.71724600 | -2.86695800 | 2.60507800  |
| H | -1.66719200 | -2.14462500 | 1.27799300  |
| H | -1.30683000 | -3.88697100 | 1.26876300  |
| H | 2.37753400  | -1.63306700 | -4.28460100 |
| H | 0.72659900  | -2.06214900 | -4.82023900 |
| H | 1.40203800  | -0.47503500 | -5.27577700 |
| H | 1.95808300  | -1.13584500 | 0.46437100  |
| H | 1.32880300  | -1.23947900 | 2.13972500  |



**T1-A3-Cat**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.13986100 | 1.81536700  | -0.17695900 |
| C  | -0.93165500 | 2.69150900  | 0.04385400  |
| C  | 0.93194200  | -2.69164200 | -0.04416000 |
| C  | 2.14009400  | -1.81548400 | 0.17694100  |
| Pd | 0.00012500  | -0.00008000 | -0.00020700 |
| O  | 0.20111200  | 2.01675800  | 0.16922500  |
| O  | -1.03827000 | 3.91672700  | 0.10133900  |
| N  | -1.96920700 | 0.53568600  | -0.23829500 |
| N  | 1.96939000  | -0.53580800 | 0.23827500  |
| O  | -0.20081400 | -2.01691000 | -0.16974700 |
| O  | 1.03858700  | -3.91685600 | -0.10167700 |
| H  | 3.12430500  | -2.28801500 | 0.27268400  |
| H  | -3.12408300 | 2.28792500  | -0.27246700 |
| C  | -3.09627600 | -0.42574300 | -0.42617000 |
| C  | -3.09378700 | -1.37492600 | 0.80729600  |
| H  | -2.17072700 | -1.97497900 | 0.76955300  |
| H  | -3.93840600 | -2.07328400 | 0.66263000  |
| C  | -4.45071800 | 0.29082400  | -0.56930800 |
| H  | -4.47422900 | 0.94868400  | -1.45461700 |

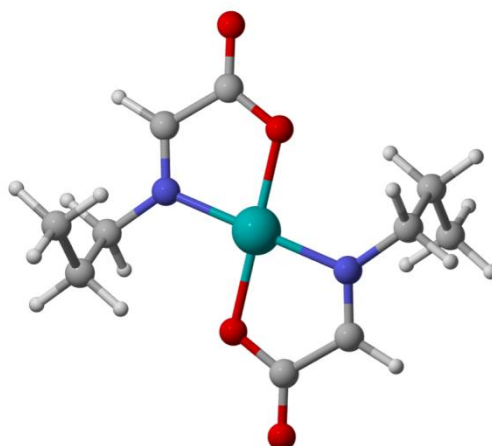
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.23106700 | -0.47444800 | -0.70398500 |
| H | -4.71731500 | 0.88467800  | 0.32007400  |
| C | -2.79361000 | -1.22268800 | -1.71281600 |
| H | -1.83739100 | -1.75811600 | -1.62321900 |
| C | 3.09633800  | 0.42569800  | 0.42645700  |
| C | 3.09396200  | 1.37499400  | -0.80692100 |
| C | 2.79336800  | 1.22248900  | 1.71312900  |
| C | 4.45081600  | -0.29076200 | 0.56978700  |
| H | 2.17081600  | 1.97492100  | -0.76927700 |
| H | 2.75912600  | 0.54923700  | 2.58593900  |
| H | 3.59572100  | 1.96109500  | 1.87461900  |
| H | 1.83715500  | 1.75789900  | 1.62337800  |
| H | 5.23108900  | 0.47456600  | 0.70460200  |
| H | 4.47423200  | -0.94863600 | 1.45508800  |
| H | 4.71759800  | -0.88458200 | -0.31956000 |
| H | 3.93845300  | 2.07346000  | -0.66202900 |
| C | 3.20878200  | 0.67477600  | -2.16648000 |
| H | 2.35410000  | -0.00130900 | -2.33955000 |
| H | 3.20706300  | 1.42122100  | -2.97724800 |
| H | 4.13583500  | 0.08438500  | -2.26517400 |
| H | -3.59602600 | -1.96128200 | -1.87405200 |
| C | -3.20825200 | -0.67456700 | 2.16680900  |
| H | -3.20663500 | -1.42094200 | 2.97764200  |
| H | -2.35335300 | 0.00128900  | 2.33970400  |
| H | -4.13512900 | -0.08390700 | 2.26556700  |
| H | -2.75952300 | -0.54954400 | -2.58571600 |



**T1-A2-Cat**

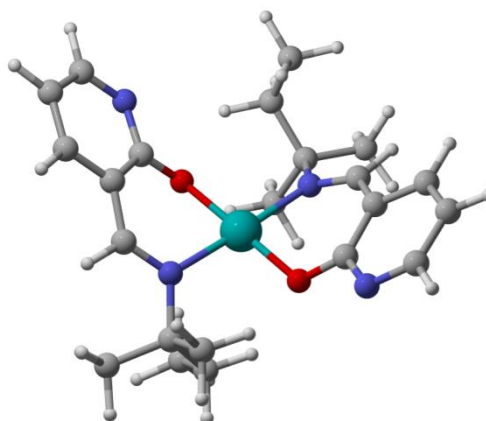
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.17461800 | 1.76470500  | -0.13364000 |
| C  | -0.98510100 | 2.67229800  | 0.07998100  |
| C  | 0.98568600  | -2.67255500 | -0.07951500 |
| C  | 2.17512700  | -1.76483900 | 0.13398000  |
| Pd | 0.00018100  | -0.00015900 | 0.00017100  |
| O  | 0.16619000  | 2.02250100  | 0.17903500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.12111000 | 3.89338000  | 0.15285300  |
| N | -1.96041000 | 0.49311500  | -0.21082000 |
| N | 1.96078500  | -0.49326700 | 0.21105200  |
| O | -0.16565200 | -2.02284800 | -0.17865900 |
| O | 1.12178800  | -3.89363800 | -0.15219200 |
| H | 3.18730200  | -2.18752000 | 0.21542000  |
| H | -3.18675000 | 2.18748700  | -0.21508300 |
| C | -3.06362400 | -0.47017400 | -0.39190200 |
| C | -3.12998200 | -1.40374800 | 0.83538000  |
| H | -2.21334300 | -2.01724900 | 0.85051700  |
| H | -3.97788700 | -2.09086700 | 0.66072000  |
| C | -2.85594500 | -1.23602000 | -1.70612600 |
| H | -1.93077000 | -1.83058900 | -1.65494900 |
| C | 3.06382900  | 0.47021700  | 0.39200200  |
| C | 3.12976500  | 1.40373300  | -0.83533000 |
| C | 2.85590500  | 1.23613700  | 1.70613200  |
| H | 2.21281300  | 2.01677500  | -0.85054100 |
| H | 2.79878000  | 0.54399300  | 2.56181700  |
| H | 3.70666100  | 1.91867000  | 1.86539300  |
| H | 1.93042900  | 1.83024800  | 1.65495700  |
| H | 3.97732800  | 2.09127800  | -0.66068500 |
| C | 3.31165600  | 0.65815900  | -2.16235100 |
| H | 2.43830400  | 0.02225400  | -2.38643300 |
| H | 3.42674500  | 1.36892600  | -2.99643500 |
| H | 4.20695900  | 0.01057600  | -2.14747400 |
| H | -3.70700800 | -1.91813100 | -1.86556200 |
| C | -3.31147600 | -0.65817500 | 2.16246000  |
| H | -3.42687400 | -1.36894200 | 2.99650100  |
| H | -2.43781300 | -0.02270200 | 2.38655700  |
| H | -4.20647100 | -0.01016300 | 2.14766200  |
| H | -2.79841800 | -0.54379300 | -2.56172000 |
| H | 3.99988500  | -0.12461300 | 0.44429800  |
| H | -3.99950400 | 0.12492700  | -0.44419500 |



### T1-A1-Cat

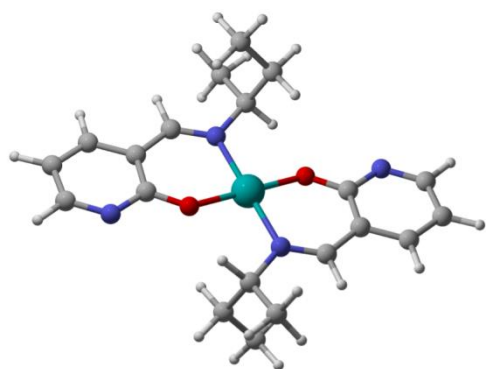
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.17185000 | 1.75525400  | -0.05929200 |
| C  | -0.97905600 | 2.65879400  | 0.18208000  |
| C  | 0.97942500  | -2.65894000 | -0.18218500 |
| C  | 2.17218600  | -1.75540700 | 0.05938800  |
| Pd | 0.00014300  | -0.00010100 | 0.00019900  |
| O  | 0.17246600  | 2.00890100  | 0.27552000  |
| O  | -1.12206400 | 3.87730400  | 0.28320000  |
| N  | -1.94751900 | 0.48803200  | -0.17488000 |
| N  | 1.94783300  | -0.48819800 | 0.17505900  |
| O  | -0.17218900 | -2.00912100 | -0.27500600 |
| O  | 1.12234500  | -3.87752200 | -0.28256800 |
| H  | 3.18692500  | -2.17516600 | 0.12481400  |
| H  | -3.18657500 | 2.17503500  | -0.12479600 |
| C  | -3.01319300 | -0.50203700 | -0.34376600 |
| C  | -3.12549000 | -1.39711500 | 0.90633100  |
| H  | -2.18365000 | -1.96227000 | 1.00637400  |
| H  | -3.92144600 | -2.13402800 | 0.69655500  |
| C  | 3.01349300  | 0.50189100  | 0.34392900  |
| C  | 3.12565600  | 1.39709400  | -0.90609300 |
| H  | 2.18378600  | 1.96222000  | -1.00601400 |
| H  | 3.92159600  | 2.13402400  | -0.69631200 |
| C  | 3.43972200  | 0.61401800  | -2.18553000 |
| H  | 2.62391800  | -0.08427300 | -2.43867000 |
| H  | 3.56579900  | 1.29859900  | -3.03969800 |
| H  | 4.37032000  | 0.02662900  | -2.08652900 |
| C  | -3.43961700 | -0.61390600 | 2.18567100  |
| H  | -3.56578200 | -1.29840200 | 3.03989500  |
| H  | -2.62380600 | 0.08437800  | 2.43880600  |
| H  | -4.37018600 | -0.02649200 | 2.08654700  |
| H  | 3.96585200  | -0.02649000 | 0.54435000  |
| H  | -3.96551700 | 0.02635800  | -0.54431600 |
| H  | 2.74668000  | 1.11857200  | 1.21823600  |
| H  | -2.74632600 | -1.11881100 | -1.21799000 |



### T2-A3-Cat

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.04971300  | 2.44459600  | -1.12671400 |
| C  | 1.89276500  | 1.34976000  | -2.98826700 |
| C  | 0.72087700  | 1.54393400  | -3.74769800 |
| C  | -0.34214300 | 2.19929100  | -3.12767500 |
| C  | -0.19997800 | 2.68349300  | -1.80980400 |
| C  | -1.34904400 | 3.22948800  | -1.12657600 |
| N  | -1.34998000 | 3.92557100  | -0.02451400 |
| H  | 2.74797700  | 0.82154200  | -3.43252500 |
| H  | 0.65121100  | 1.17634500  | -4.77433400 |
| H  | -1.29467300 | 2.34699700  | -3.65066000 |
| H  | -2.31913800 | 2.98084000  | -1.58201300 |
| O  | 1.25573200  | 2.80279900  | 0.11558900  |
| Pd | 0.47029700  | 4.56630000  | 0.72937600  |
| C  | 0.24365600  | 7.46006200  | 0.98678000  |
| C  | -0.01538700 | 9.72324400  | 0.55571500  |
| C  | 1.37293500  | 9.95962600  | 0.46842400  |
| C  | 2.21902000  | 8.87479000  | 0.68476300  |
| C  | 1.67960200  | 7.59280500  | 0.93541200  |
| C  | 2.57984200  | 6.51917100  | 1.27337600  |
| N  | 2.31444200  | 5.24337100  | 1.36036000  |
| H  | -0.71905100 | 10.55453800 | 0.40807400  |
| H  | 1.75929300  | 10.95909800 | 0.25466000  |
| H  | 3.30865300  | 8.99754000  | 0.66389200  |
| H  | 3.60156600  | 6.84590400  | 1.51134700  |
| O  | -0.35893100 | 6.33142900  | 1.25155500  |
| N  | 2.06689900  | 1.76409500  | -1.72582900 |
| N  | -0.57683400 | 8.53535800  | 0.81195300  |
| C  | 3.37878500  | 4.31053400  | 1.87817700  |
| C  | -2.66145900 | 4.24207500  | 0.64869800  |
| C  | -2.41981700 | 4.24441200  | 2.18207500  |
| C  | -3.74720400 | 3.19717400  | 0.30409400  |
| H  | -3.39307500 | 2.16363500  | 0.44901500  |

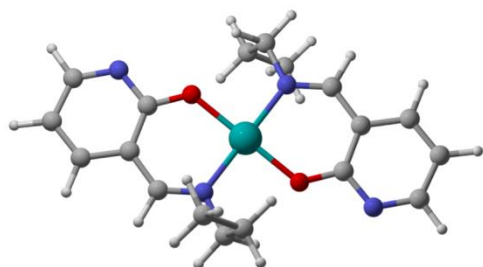
|   |             |            |             |    |             |             |             |
|---|-------------|------------|-------------|----|-------------|-------------|-------------|
| H | -4.60963700 | 3.36054500 | 0.97046000  | N  | -1.14056200 | 3.83758500  | -0.14515300 |
| H | -4.11978000 | 3.30044300 | -0.72907500 | H  | 2.46427100  | -1.05360600 | -1.37197200 |
| C | -3.12807000 | 5.63496600 | 0.17339900  | H  | 0.16812100  | -1.42379200 | -2.33563100 |
| H | -3.26563600 | 5.63536100 | -0.92179800 | H  | -1.56729400 | 0.38442200  | -1.98591700 |
| H | -4.09911000 | 5.87231300 | 0.64083500  | H  | -2.24252100 | 2.33635800  | -1.02092400 |
| H | -2.39803500 | 6.40911600 | 0.44654500  | O  | 1.57402500  | 2.82673000  | 0.28068700  |
| C | 4.09074400  | 3.61032700 | 0.68118600  | Pd | 0.65121400  | 4.60126400  | 0.47883200  |
| C | 4.42436200  | 5.05423700 | 2.74085400  | C  | 0.16273500  | 7.40294700  | 1.35515200  |
| H | 5.05522300  | 4.30021900 | 3.23752500  | C  | -0.38639800 | 9.48491300  | 2.21756700  |
| H | 5.10029100  | 5.69709100 | 2.15252700  | C  | 0.89780100  | 9.70050300  | 2.76389600  |
| H | 3.94460200  | 5.66620100 | 3.52358400  | C  | 1.84576600  | 8.70196200  | 2.56894900  |
| C | 2.68031700  | 3.26983900 | 2.77594800  | C  | 1.50839800  | 7.52074600  | 1.86496800  |
| H | 1.94567800  | 2.68662700 | 2.20501100  | C  | 2.54525800  | 6.54765800  | 1.64829500  |
| H | 3.43511100  | 2.57385100 | 3.17921300  | N  | 2.44292000  | 5.36500400  | 1.10313600  |
| H | 2.17588500  | 3.76453400 | 3.62305500  | H  | -1.16532900 | 10.25060400 | 2.34124100  |
| H | -1.71906600 | 5.06028600 | 2.41727900  | H  | 1.12968700  | 10.61907000 | 3.30825100  |
| H | -3.38354300 | 4.51289300 | 2.65324300  | H  | 2.86653900  | 8.81304100  | 2.95434700  |
| C | -1.90366400 | 2.91877800 | 2.75920600  | H  | 3.54414600  | 6.86511300  | 1.98179100  |
| H | -0.96120800 | 2.61546900 | 2.27132000  | O  | -0.27103300 | 6.37619500  | 0.67672400  |
| H | -1.70048400 | 3.02462200 | 3.83757200  | N  | 2.05779800  | 0.80441400  | -0.57391000 |
| H | -2.62980200 | 2.09704000 | 2.63757700  | N  | -0.75699200 | 8.39538200  | 1.53761200  |
| H | 4.96691300  | 3.08508300 | 1.10623600  | C  | 3.66798200  | 4.56528100  | 0.83881300  |
| H | 3.41771700  | 2.84773100 | 0.26448600  | C  | -2.36527000 | 4.63887800  | 0.11618100  |
| C | 4.53819000  | 4.54710400 | -0.44583000 | C  | -2.67913900 | 4.57475200  | 1.63317000  |
| H | 5.19477100  | 5.36388600 | -0.09384700 | C  | -3.56907800 | 4.27362200  | -0.76133200 |
| H | 5.09794500  | 3.97984900 | -1.20693900 | H  | -4.01185700 | 3.29275100  | -0.51686500 |
| H | 3.66835700  | 5.00300000 | -0.94678000 | H  | -4.35254400 | 5.03169200  | -0.60129800 |



### T2-A2-Cat

|   |             |             |             |   |             |            |             |
|---|-------------|-------------|-------------|---|-------------|------------|-------------|
| C | 1.13880700  | 1.79795800  | -0.39366500 | H | -3.80281900 | 2.67935500 | 1.67938900  |
| C | 1.68591800  | -0.28705100 | -1.25001400 | H | 4.85019200  | 3.97591300 | -0.86027700 |
| C | 0.40105700  | -0.50363300 | -1.79442300 | H | 3.12764500  | 4.17488600 | -1.21041100 |
| C | -0.54611300 | 0.49608200  | -1.60176700 | C | 4.24357400  | 6.04048700 | -1.22217200 |
| C | -0.20744500 | 1.67930500  | -0.90174600 | H | 5.09968000  | 6.52873500 | -0.72441500 |
| C | -1.24352900 | 2.65376200  | -0.68768400 | H | 4.47148800  | 6.00151900 | -2.30007400 |

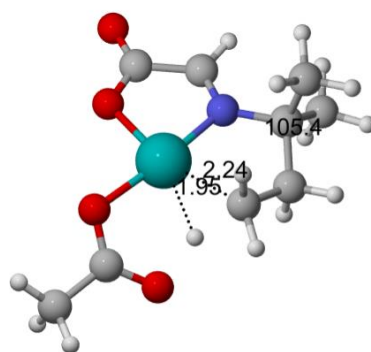
|   |             |            |             |
|---|-------------|------------|-------------|
| H | 3.36116000  | 6.68968300 | -1.09317600 |
| H | 3.38175900  | 3.52428400 | 1.05256600  |
| H | -2.07758700 | 5.67932200 | -0.09825800 |



### T2-A1-Cat

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.09169700  | 1.82136100  | -0.49432200 |
| C  | 1.57326400  | -0.27677900 | -1.35906000 |
| C  | 0.26147100  | -0.48247500 | -1.84157600 |
| C  | -0.66292700 | 0.53070500  | -1.61689400 |
| C  | -0.27876200 | 1.71469900  | -0.94038700 |
| C  | -1.28661500 | 2.71014900  | -0.70383700 |
| N  | -1.14703900 | 3.88612800  | -0.14950000 |
| H  | 2.33583700  | -1.05387800 | -1.51036700 |
| H  | -0.00678300 | -1.40424200 | -2.36326500 |
| H  | -1.70087500 | 0.43048400  | -1.95641200 |
| H  | -2.30545800 | 2.43380100  | -1.02580000 |
| O  | 1.57633400  | 2.84988300  | 0.14602100  |
| Pd | 0.65037100  | 4.60085900  | 0.47977500  |
| C  | 0.20896500  | 7.38037100  | 1.45370700  |
| C  | -0.27248600 | 9.47871800  | 2.31801500  |
| C  | 1.03935900  | 9.68452000  | 2.80033800  |
| C  | 1.96372600  | 8.67128300  | 2.57579000  |
| C  | 1.57948900  | 7.48713900  | 1.89958800  |
| C  | 2.58733200  | 6.49163800  | 1.66319500  |
| N  | 2.44777300  | 5.31558900  | 1.10900000  |
| H  | -1.03504100 | 10.25585000 | 2.46925000  |
| H  | 1.30766900  | 10.60641100 | 3.32177800  |
| H  | 3.00170800  | 8.77157400  | 2.91518200  |
| H  | 3.60616000  | 6.76802100  | 1.98517600  |
| O  | -0.27575400 | 6.35170700  | 0.81366900  |
| N  | 1.98903100  | 0.81523600  | -0.71121500 |
| N  | -0.68833900 | 8.38655300  | 1.67047900  |
| C  | 3.66118500  | 4.51617100  | 0.86698900  |
| C  | -2.36041500 | 4.68554700  | 0.09263800  |
| C  | -2.77281600 | 4.64371400  | 1.57531000  |
| C  | 4.07353400  | 4.55768800  | -0.61571000 |
| H  | -1.96326900 | 5.10270500  | 2.16673100  |

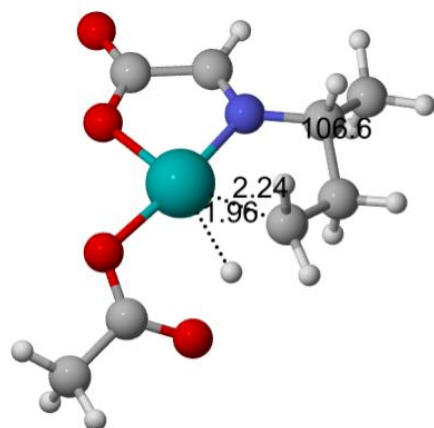
|   |             |            |             |
|---|-------------|------------|-------------|
| H | -3.65426100 | 5.30154400 | 1.68477200  |
| C | -3.08763400 | 3.23360100 | 2.08717700  |
| H | -2.20037400 | 2.58034000 | 2.03158500  |
| H | -3.41481200 | 3.25973400 | 3.13964400  |
| H | -3.89386100 | 2.75853700 | 1.49878500  |
| H | 4.95493500  | 3.89979000 | -0.72506400 |
| H | 3.26393700  | 4.09866200 | -1.20703500 |
| C | 4.38844800  | 5.96768300 | -1.12788000 |
| H | 5.19468000  | 6.44285000 | -0.53954700 |
| H | 4.71574500  | 5.94128400 | -2.18030000 |
| H | 3.50123700  | 6.62100200 | -1.07246000 |
| H | 4.47532600  | 4.91402300 | 1.50366400  |
| H | 3.44780700  | 3.47705700 | 1.15499400  |
| H | -2.14699800 | 5.72472500 | -0.19512700 |
| H | -3.17455700 | 4.28788000 | -0.54415000 |



### T1-A3-TS2-3'

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.42579900 | -1.81481500 | 1.44079900  |
| C  | 0.49846900  | -1.47874000 | 2.81306200  |
| H  | 1.02482700  | -0.94648500 | 3.61689100  |
| N  | 1.01982600  | -2.46953100 | 2.16887300  |
| Pd | -0.11637500 | -3.20977100 | 0.71966000  |
| C  | 2.35449300  | -3.08853000 | 2.41821100  |
| C  | 2.74117300  | -3.78023600 | 1.08963900  |
| H  | 3.05962300  | -3.00487800 | 0.37012400  |
| H  | 3.62594100  | -4.41599800 | 1.28196200  |
| O  | -1.41936500 | -3.78471900 | -0.75640100 |
| O  | 0.43375800  | -4.29701100 | -1.94791400 |
| C  | -0.82909200 | -4.16121500 | -1.83828300 |
| C  | -1.71244100 | -4.42202000 | -3.04019800 |
| H  | -2.73857200 | -4.65419200 | -2.72489800 |
| H  | -1.73609100 | -3.50987000 | -3.66057000 |
| H  | -1.29257000 | -5.23616300 | -3.64807300 |
| C  | 1.60638200  | -4.61546700 | 0.46919200  |
| H  | 1.15080100  | -5.33463500 | 1.17143100  |
| H  | 0.90524900  | -4.18908800 | -0.62766600 |

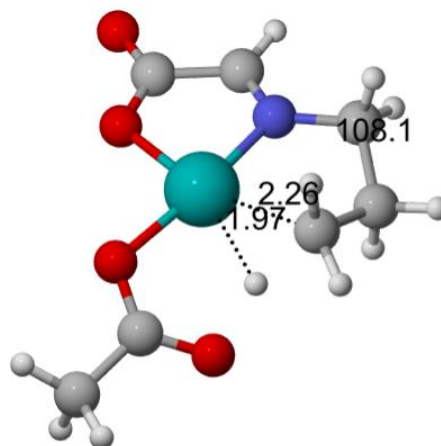
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.03240000  | -5.25520300 | -0.32775200 |
| C | -0.91819500 | -1.08682800 | 2.42034900  |
| O | -1.49400100 | -0.17157000 | 3.01052100  |
| C | 3.39860200  | -2.03196100 | 2.81211200  |
| H | 3.17560400  | -1.57351900 | 3.78947700  |
| H | 4.38925800  | -2.50767000 | 2.89117900  |
| H | 3.45600800  | -1.23586300 | 2.05179800  |
| C | 2.15290200  | -4.11703300 | 3.55241400  |
| H | 3.09131100  | -4.66866700 | 3.72516800  |
| H | 1.86672000  | -3.60770200 | 4.48699700  |
| H | 1.35992700  | -4.83894300 | 3.30240000  |



**T1-A2-TS2-3'**

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.49733800 | -1.92293700 | 1.50790200  |
| C  | 0.43602800  | -1.53654700 | 2.85634300  |
| H  | 0.95606700  | -0.99522000 | 3.65794100  |
| N  | 0.98376300  | -2.49403400 | 2.18415200  |
| Pd | -0.14167200 | -3.24018600 | 0.72800700  |
| C  | 2.34903600  | -3.04362300 | 2.36210900  |
| C  | 2.75839900  | -3.64927000 | 1.00852600  |
| H  | 3.00249100  | -2.83052700 | 0.30749400  |
| H  | 3.68778400  | -4.22977200 | 1.15824500  |
| O  | -1.43790200 | -3.82654600 | -0.74654600 |
| O  | 0.41541900  | -4.25580600 | -1.97037900 |
| C  | -0.84955400 | -4.16414400 | -1.84227300 |
| C  | -1.73986400 | -4.43308600 | -3.03719200 |
| H  | -1.80058500 | -3.51217100 | -3.64188300 |
| H  | -1.30229800 | -5.22328800 | -3.66388000 |
| H  | -2.75380200 | -4.70321700 | -2.71284600 |
| C  | 1.65494200  | -4.54522100 | 0.41599500  |
| H  | 1.25991700  | -5.27484400 | 1.14617800  |
| H  | 0.90376900  | -4.14929400 | -0.65777000 |
| H  | 2.08577700  | -5.17171300 | -0.38853100 |
| C  | -1.00415600 | -1.19904500 | 2.49767100  |

|   |             |             |            |
|---|-------------|-------------|------------|
| O | -1.60826700 | -0.32546200 | 3.12160900 |
| C | 3.34777300  | -2.02367300 | 2.91474400 |
| H | 3.07769100  | -1.67977500 | 3.92608800 |
| H | 4.34641100  | -2.48374500 | 2.97955700 |
| H | 3.41333800  | -1.14636100 | 2.24960000 |
| H | 2.22468600  | -3.87739200 | 3.08276300 |

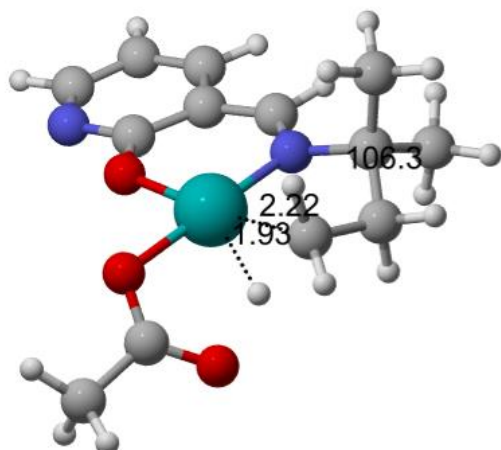


**T1-A1-TS2-3'**

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.49275000 | -1.90849600 | 1.52368300  |
| C  | 0.42684700  | -1.56760800 | 2.90223100  |
| H  | 0.95637400  | -1.05261800 | 3.71776500  |
| N  | 0.96519800  | -2.52037200 | 2.21607400  |
| Pd | -0.14495600 | -3.23545900 | 0.73249400  |
| C  | 2.31066200  | -3.08933700 | 2.39834100  |
| C  | 2.76354400  | -3.67962400 | 1.05604500  |
| H  | 3.03328300  | -2.86110200 | 0.36592700  |
| H  | 3.68313000  | -4.27144500 | 1.22463000  |
| O  | -1.43062600 | -3.78453300 | -0.76821500 |
| O  | 0.42465700  | -4.28274800 | -1.96251500 |
| C  | -0.83844900 | -4.15065200 | -1.85327000 |
| C  | -1.72024400 | -4.40514100 | -3.05964000 |
| H  | -1.71613900 | -3.50228000 | -3.69404500 |
| H  | -1.31490700 | -5.23711700 | -3.65368200 |
| H  | -2.75416500 | -4.61010800 | -2.75086000 |
| C  | 1.66237300  | -4.56203500 | 0.42880600  |
| H  | 1.25169200  | -5.30069100 | 1.14147400  |
| H  | 0.91174600  | -4.16533900 | -0.64762700 |
| H  | 2.10747700  | -5.17821800 | -0.37673800 |
| C  | -1.00600300 | -1.20617100 | 2.53310100  |
| O  | -1.61060600 | -0.33750800 | 3.16320600  |
| H  | 2.21566000  | -3.89612500 | 3.15008800  |



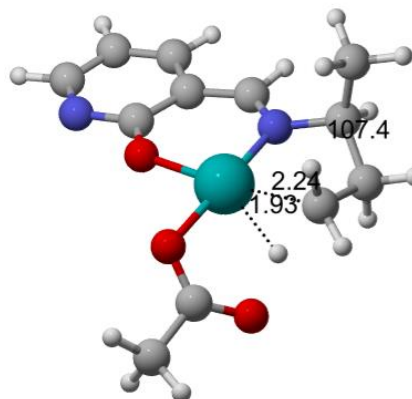
|   |            |             |            |
|---|------------|-------------|------------|
| H | 3.00371900 | -2.32682600 | 2.79734000 |
|---|------------|-------------|------------|



**T2-A3-TS2-3'**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.35420700 | -0.51148500 | 1.47063900  |
| C  | -0.26117800 | -0.24603300 | 2.38837100  |
| C  | -0.36282900 | 0.89253500  | 3.23067800  |
| C  | -1.47472600 | 1.71864800  | 3.16496800  |
| C  | -2.48309900 | 1.36929900  | 2.23454100  |
| N  | -2.44486200 | 0.31429000  | 1.42092900  |
| H  | 0.45364800  | 1.10337500  | 3.93210000  |
| H  | -1.57813800 | 2.60194500  | 3.79975200  |
| H  | -3.38227500 | 1.99642500  | 2.15053100  |
| O  | -1.39984700 | -1.52216800 | 0.65394100  |
| C  | 0.90566400  | -1.06421900 | 2.52239400  |
| H  | 1.60596300  | -0.74956900 | 3.31092500  |
| N  | 1.22837100  | -2.12744600 | 1.82739000  |
| Pd | 0.08737000  | -2.83431600 | 0.34823000  |
| C  | 2.44103800  | -2.93247700 | 2.19784900  |
| C  | 2.85807900  | -3.69652900 | 0.92603900  |
| H  | 3.33636400  | -2.98591900 | 0.22791300  |
| H  | 3.63038800  | -4.43735400 | 1.20710200  |
| O  | -1.10235400 | -3.49230300 | -1.21716600 |
| O  | 0.86149600  | -3.81568600 | -2.29215700 |
| C  | -0.41292500 | -3.76606100 | -2.26933500 |
| C  | -1.18981900 | -4.01203400 | -3.54741500 |
| C  | 1.68268900  | -4.38020800 | 0.22498100  |
| H  | 1.18685700  | -3.80830300 | -0.90129100 |
| H  | 2.05968200  | -5.07431000 | -0.54976400 |
| H  | 1.08366400  | -5.02774000 | 0.88859800  |
| C  | 3.61340900  | -2.04771200 | 2.66368900  |
| H  | 3.44170600  | -1.59518300 | 3.65422600  |
| H  | 4.52013500  | -2.66841400 | 2.74816900  |
| H  | 3.81153200  | -1.24465400 | 1.93471800  |

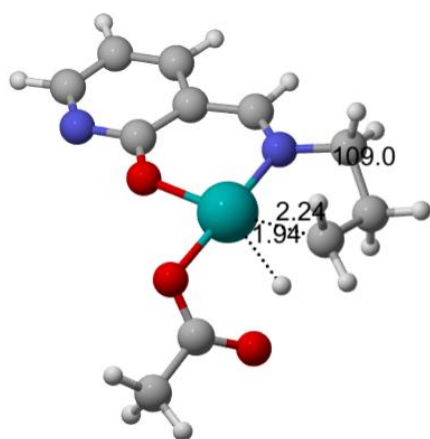
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.01865100  | -3.90276700 | 3.32201300  |
| H | 2.85738200  | -4.56609800 | 3.59196100  |
| H | 1.71636100  | -3.33829200 | 4.21965900  |
| H | 1.16283500  | -4.52326100 | 3.01284200  |
| H | -2.21319600 | -4.34168500 | -3.32242800 |
| H | -1.24625400 | -3.06358000 | -4.10838300 |
| H | -0.66665900 | -4.74876200 | -4.17370300 |



**T2-A2-TS2-3'**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.36754500 | -0.53784700 | 1.50172400  |
| C  | -0.25135700 | -0.24309200 | 2.38431100  |
| C  | -0.32988400 | 0.92169300  | 3.19199600  |
| C  | -1.44459500 | 1.74434500  | 3.13053300  |
| C  | -2.47992400 | 1.36210000  | 2.24363500  |
| N  | -2.46260600 | 0.28209000  | 1.46257900  |
| H  | 0.50494200  | 1.15410000  | 3.86426000  |
| H  | -1.53181800 | 2.64760400  | 3.73907800  |
| H  | -3.38427600 | 1.98283600  | 2.16861100  |
| O  | -1.43300000 | -1.56752200 | 0.70856100  |
| C  | 0.90893200  | -1.06930500 | 2.51641000  |
| H  | 1.64377600  | -0.75812800 | 3.27921300  |
| N  | 1.18968800  | -2.15580100 | 1.84073900  |
| Pd | 0.06283400  | -2.86343800 | 0.36209500  |
| C  | 2.37774000  | -2.96355200 | 2.20966500  |
| C  | 2.86602100  | -3.66908800 | 0.93807900  |
| H  | 3.32926400  | -2.92478300 | 0.26712000  |
| H  | 3.65515700  | -4.39457100 | 1.21149900  |
| O  | -1.11436200 | -3.51618400 | -1.21159200 |
| O  | 0.85424000  | -3.78390000 | -2.29315600 |
| C  | -0.42114600 | -3.76126400 | -2.26816200 |
| C  | -1.19360600 | -4.00675700 | -3.54879000 |
| C  | 1.71301900  | -4.36816700 | 0.20528100  |
| H  | 1.18985200  | -3.78825900 | -0.90921800 |
| H  | 2.11511200  | -5.02638200 | -0.58776800 |
| H  | 1.13172100  | -5.05266400 | 0.84706800  |

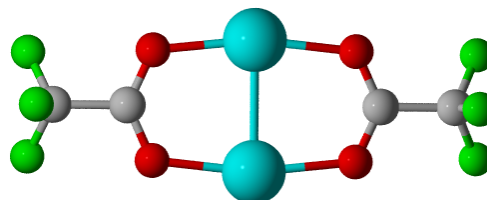
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.99322800  | -3.94014600 | 3.33494300  |
| H | 2.85661500  | -4.56872000 | 3.60947100  |
| H | 1.66315800  | -3.38823400 | 4.22993800  |
| H | 1.16443100  | -4.59553600 | 3.02190300  |
| H | -2.21631500 | -4.34085100 | -3.32776300 |
| H | -1.25051300 | -3.05768100 | -4.10861500 |
| H | -0.66570000 | -4.74024500 | -4.17505800 |
| H | 3.16227700  | -2.27638900 | 2.58339500  |



### T2-A1-TS2-3'

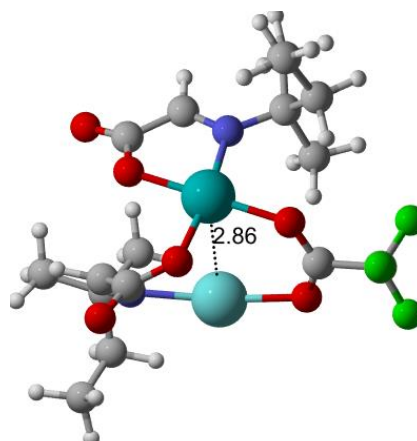
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.36133800 | -0.52493900 | 1.49377000  |
| C  | -0.25407700 | -0.24563200 | 2.39262700  |
| C  | -0.33894100 | 0.90840700  | 3.21533800  |
| C  | -1.45112600 | 1.73424400  | 3.15352500  |
| C  | -2.47738700 | 1.36728200  | 2.24973500  |
| N  | -2.45348300 | 0.29871700  | 1.45341100  |
| H  | 0.48908200  | 1.12984400  | 3.89957300  |
| H  | -1.54309100 | 2.62883900  | 3.77402900  |
| H  | -3.37948300 | 1.99112200  | 2.17352300  |
| O  | -1.42112100 | -1.54235700 | 0.68441500  |
| C  | 0.90682900  | -1.07132700 | 2.52267300  |
| H  | 1.63959500  | -0.76347900 | 3.28836400  |
| N  | 1.18874700  | -2.15252800 | 1.83898100  |
| Pd | 0.06462100  | -2.85168100 | 0.35206200  |
| C  | 2.38495200  | -2.94862600 | 2.17016400  |
| C  | 2.88019700  | -3.65027400 | 0.90795100  |
| H  | 3.32780300  | -2.91069000 | 0.22089300  |
| H  | 3.67728300  | -4.36588600 | 1.18348500  |
| O  | -1.11035200 | -3.49792200 | -1.22347100 |
| O  | 0.85798400  | -3.82668400 | -2.28859000 |
| C  | -0.41655600 | -3.77434900 | -2.27189000 |
| C  | -1.18720300 | -4.02081000 | -3.55338400 |
| C  | 1.71221400  | -4.36906400 | 0.21922200  |
| H  | 1.18606900  | -3.81501400 | -0.90484700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.08668200  | -5.07134100 | -0.54895800 |
| H | 1.13642100  | -5.00820600 | 0.91395400  |
| H | -2.21935100 | -4.32533400 | -3.33360200 |
| H | -1.21638200 | -3.07995400 | -4.12897400 |
| H | -0.67422600 | -4.77754400 | -4.16421200 |
| H | 3.15671600  | -2.30289500 | 2.62836800  |
| H | 2.08841700  | -3.70964600 | 2.91908000  |



### Ag<sub>2</sub>TFA<sub>2</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.66234400 | -0.00092700 | -0.03015300 |
| O  | -2.13461500 | -1.15615100 | -0.03128000 |
| O  | -2.13520300 | 1.15461900  | -0.03100000 |
| C  | -4.21929400 | -0.00040500 | 0.03685300  |
| C  | 2.66234300  | 0.00108400  | -0.03019700 |
| O  | 2.13518500  | -1.15446100 | -0.03131800 |
| O  | 2.13463200  | 1.15630900  | -0.03103100 |
| C  | 4.21929500  | 0.00025900  | 0.03676400  |
| Ag | -0.00042300 | 1.38094600  | -0.03134700 |
| Ag | 0.00042200  | -1.38080000 | -0.03168300 |
| F  | -4.59559200 | 0.01214600  | 1.34332200  |
| F  | -4.73818900 | -1.10152100 | -0.54769300 |
| F  | -4.73725800 | 1.09002500  | -0.56855500 |
| F  | 4.59563300  | -0.01625400 | 1.34317600  |
| F  | 4.73840000  | 1.10297800  | -0.54451300 |
| F  | 4.73701300  | -1.08849700 | -0.57191200 |

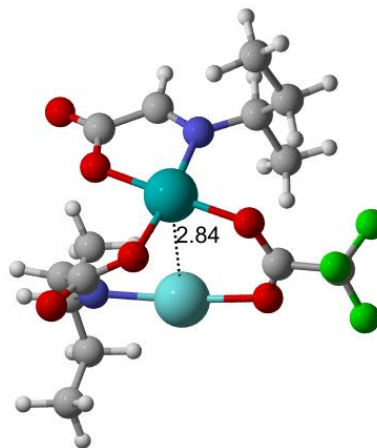


### T1-A3-Int1

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -1.72393800 | -0.84494000 | 2.27694100 |
| O | -0.41604600 | -0.81532100 | 2.12684200 |
| O | -2.30738500 | -1.47729200 | 3.16305400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 0.23084600  | 3.09990200  | -0.25047400 |
| C  | -1.04000200 | 2.92238500  | 0.54175100  |
| Pd | 0.45523000  | 0.58231800  | 0.93735300  |
| O  | -1.01013400 | 1.89370700  | 1.37188800  |
| O  | -2.00222000 | 3.68028200  | 0.38870400  |
| N  | 1.10057400  | 2.14093400  | -0.23717600 |
| H  | 0.36859800  | 4.01970200  | -0.82948000 |
| C  | 2.36751300  | 2.19577700  | -1.02703200 |
| C  | 3.53364900  | 1.81980300  | -0.07167200 |
| H  | 3.45029800  | 0.75201300  | 0.17824300  |
| H  | 4.46482000  | 1.93852600  | -0.65491700 |
| C  | 2.60367700  | 3.58422900  | -1.64976300 |
| H  | 1.82820000  | 3.84728800  | -2.38856600 |
| H  | 3.56777000  | 3.56330500  | -2.18153300 |
| H  | 2.65535400  | 4.38098300  | -0.89011500 |
| C  | 2.22369700  | 1.14909900  | -2.15201200 |
| H  | 1.96080400  | 0.16083400  | -1.75233000 |
| H  | 3.17760900  | 1.06141200  | -2.69652400 |
| C  | -2.65104500 | -0.14760700 | 1.29695800  |
| H  | -3.45417800 | 0.44063800  | 1.75814000  |
| N  | -2.61915700 | -0.37821100 | 0.02761000  |
| C  | -3.62945500 | 0.16308200  | -0.92223300 |
| C  | -2.84555600 | 0.96553400  | -1.98058100 |
| C  | -4.65528700 | 1.08795000  | -0.24708300 |
| C  | -4.29318500 | -1.06825600 | -1.59414300 |
| H  | -2.04523300 | 0.34584300  | -2.42803200 |
| H  | -2.39358000 | 1.86446500  | -1.53416600 |
| H  | -3.52346200 | 1.28274700  | -2.79002000 |
| H  | -5.24454100 | 0.56978100  | 0.52669900  |
| H  | -5.36072700 | 1.45707900  | -1.00865600 |
| H  | -4.15513800 | 1.96160400  | 0.20434400  |
| H  | -4.97270100 | -0.69440300 | -2.38178700 |
| H  | -3.49201000 | -1.63240000 | -2.11300100 |
| C  | -5.04188000 | -2.00459100 | -0.63877700 |
| H  | -4.37963200 | -2.36935900 | 0.16392200  |
| H  | -5.42681400 | -2.88266300 | -1.18222200 |
| H  | -5.90387000 | -1.50582200 | -0.16565100 |
| Ag | -0.85372500 | -1.33426600 | -0.72651900 |
| O  | 1.12057800  | -2.18271300 | -0.97186600 |
| C  | 2.00058400  | -1.77802000 | -0.15937800 |
| O  | 1.99584800  | -0.79919300 | 0.65682000  |
| C  | 3.36611100  | -2.52242500 | -0.18201600 |
| H  | 1.43836200  | 1.45261900  | -2.86417800 |
| C  | 3.60181600  | 2.64596200  | 1.21881100  |

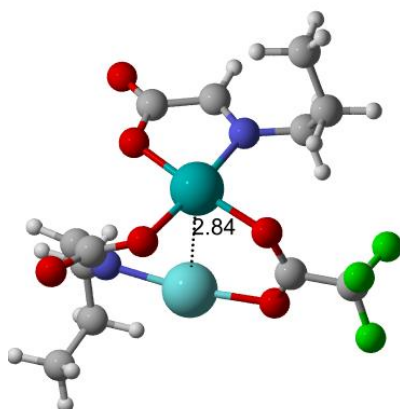
|   |            |             |             |
|---|------------|-------------|-------------|
| H | 3.70495900 | 3.72736300  | 1.02528100  |
| H | 4.46868100 | 2.33304100  | 1.82239100  |
| H | 2.69914700 | 2.49276600  | 1.83491400  |
| F | 4.30000200 | -1.69784200 | -0.74142200 |
| F | 3.31173200 | -3.65364000 | -0.91180900 |
| F | 3.77033300 | -2.83224000 | 1.06932800  |



### T1-A2-Int1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.82773300 | -0.68070900 | 2.37635400  |
| O  | -0.52574400 | -0.69417700 | 2.19404800  |
| O  | -2.40444800 | -1.20361700 | 3.33582000  |
| C  | 0.37845900  | 3.11765200  | -0.28962200 |
| C  | -0.91610600 | 3.07005600  | 0.48132100  |
| Pd | 0.39647900  | 0.61559400  | 0.94443600  |
| O  | -1.03575500 | 1.99795800  | 1.25101800  |
| O  | -1.76898100 | 3.95180600  | 0.36363400  |
| N  | 1.15220700  | 2.08094200  | -0.24654000 |
| H  | 0.63164500  | 4.00417500  | -0.88854900 |
| C  | 2.40809000  | 2.05291500  | -1.02715600 |
| C  | 3.60381800  | 1.73092000  | -0.11141800 |
| H  | 3.53988800  | 0.67903900  | 0.20605100  |
| H  | 4.50966600  | 1.82399800  | -0.73772400 |
| C  | 2.24744600  | 1.06910600  | -2.19510900 |
| H  | 2.03115800  | 0.05221600  | -1.83788600 |
| H  | 3.18084200  | 1.03829100  | -2.77980000 |
| C  | -2.77035300 | -0.09879900 | 1.33833600  |
| H  | -3.62103900 | 0.47251400  | 1.74056800  |
| N  | -2.71551100 | -0.40800800 | 0.08696500  |
| C  | -3.74632800 | 0.05950700  | -0.85782100 |
| C  | -3.15818300 | 1.21915000  | -1.67448300 |
| C  | -4.18466300 | -1.12257200 | -1.73847000 |
| H  | -2.21752200 | 0.90107500  | -2.16171100 |
| H  | -2.94401000 | 2.08901600  | -1.03501700 |
| H  | -3.86549600 | 1.52494000  | -2.46279100 |

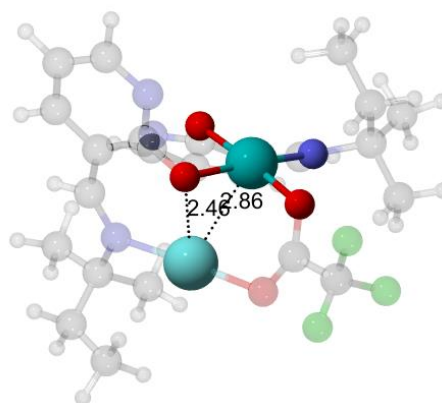
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -4.91344200 | -0.74570000 | -2.47846100 |
| H  | -3.29962900 | -1.46290400 | -2.31622400 |
| C  | -4.77868300 | -2.29040300 | -0.94203200 |
| H  | -4.04731800 | -2.69320900 | -0.22116300 |
| H  | -5.08413800 | -3.11191900 | -1.60976300 |
| H  | -5.66754500 | -1.97044500 | -0.37097800 |
| Ag | -0.92805500 | -1.33146600 | -0.64378500 |
| O  | 1.04645500  | -2.17632800 | -0.88748300 |
| C  | 1.92211500  | -1.78070300 | -0.06470600 |
| O  | 1.91939600  | -0.79988800 | 0.74817700  |
| C  | 3.27644100  | -2.54591600 | -0.07201700 |
| H  | 1.42684800  | 1.38197000  | -2.86097000 |
| C  | 3.69922800  | 2.65411800  | 1.10906700  |
| H  | 3.72866500  | 3.71858400  | 0.81444500  |
| H  | 4.61102400  | 2.43949000  | 1.68858800  |
| H  | 2.83662900  | 2.51201200  | 1.78235600  |
| F  | 4.21626300  | -1.75443500 | -0.66974200 |
| F  | 3.19874900  | -3.70069600 | -0.76147400 |
| F  | 3.68952300  | -2.81725300 | 1.18475100  |
| H  | 2.54232900  | 3.07636600  | -1.43526100 |
| H  | -4.61720700 | 0.42204200  | -0.27462100 |



### T1-A1-Int1

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.91331400 | -0.71714400 | 2.43764100  |
| O  | -0.61623000 | -0.76682900 | 2.24445700  |
| O  | -2.50331300 | -1.22679200 | 3.39684800  |
| C  | 0.50871000  | 2.99333500  | -0.25652700 |
| C  | -0.80026400 | 3.04385200  | 0.49935800  |
| Pd | 0.35375900  | 0.52278400  | 1.01123900  |
| O  | -1.01052300 | 1.98326600  | 1.27176800  |
| O  | -1.56912600 | 3.99787200  | 0.38959100  |
| N  | 1.21760700  | 1.91561800  | -0.15265900 |
| H  | 0.83606500  | 3.84786300  | -0.86549100 |
| C  | 2.53333500  | 1.77541500  | -0.78403100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.64930300  | 1.72958200  | 0.27775000  |
| H  | 3.50197000  | 0.83120700  | 0.89888100  |
| H  | 4.59756900  | 1.58650700  | -0.27017900 |
| C  | -2.84949800 | -0.10916200 | 1.40951800  |
| H  | -3.69297400 | 0.46482500  | 1.82352600  |
| N  | -2.80824700 | -0.40403100 | 0.15345700  |
| C  | -3.86634000 | 0.05158700  | -0.75691800 |
| C  | -4.36037700 | -1.10477800 | -1.63697300 |
| H  | -5.08464600 | -0.69706300 | -2.36467100 |
| H  | -3.50217300 | -1.48378800 | -2.22857300 |
| C  | -4.98782700 | -2.24619700 | -0.82720100 |
| H  | -4.26146900 | -2.67387300 | -0.11551300 |
| H  | -5.33416200 | -3.05813500 | -1.48662900 |
| H  | -5.85503100 | -1.88988200 | -0.24431600 |
| Ag | -1.04504100 | -1.34478400 | -0.60790000 |
| O  | 0.93126100  | -2.09065900 | -1.04978300 |
| C  | 1.85625500  | -1.72852000 | -0.26754900 |
| O  | 1.85790000  | -0.89346000 | 0.69543100  |
| C  | 3.26681700  | -2.30886700 | -0.56609800 |
| C  | 3.70895700  | 2.99078100  | 1.14586200  |
| H  | 3.83741200  | 3.90120300  | 0.53336200  |
| H  | 4.55528000  | 2.93840500  | 1.84919100  |
| H  | 2.78973200  | 3.11018200  | 1.74404400  |
| F  | 3.93342200  | -1.39511400 | -1.34120100 |
| F  | 3.20498700  | -3.46995500 | -1.24531300 |
| F  | 3.98246100  | -2.50065100 | 0.56109600  |
| H  | 2.68432900  | 2.62273800  | -1.48020800 |
| H  | -4.70074800 | 0.48930700  | -0.17528500 |
| H  | 2.53118900  | 0.83716400  | -1.36167400 |
| H  | -3.43145800 | 0.85157300  | -1.38428300 |

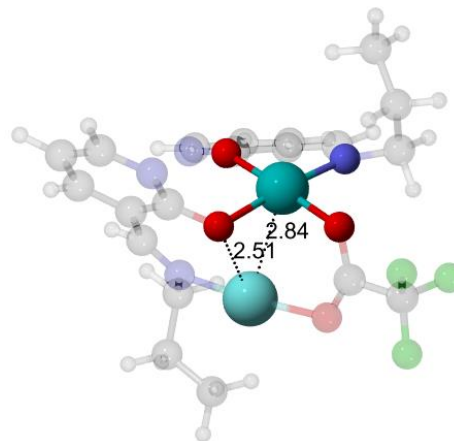


### T2-A3-Int1

|   |             |             |            |
|---|-------------|-------------|------------|
| C | -2.98560000 | -0.08746900 | 2.50429900 |
| C | -3.78239600 | 0.29524500  | 4.65611700 |



|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| O  | -2.84012300 | -1.03095500 | 1.75252900  | H  | 3.79586000  | -2.95604800 | 1.93491900  |
| Pd | -0.80331900 | -1.41422800 | 1.73038900  | H  | -1.51270500 | 3.33256300  | -0.64876300 |
| C  | 0.48648700  | 1.16218000  | 1.89832700  | C  | -0.37398000 | 1.81762200  | -1.67025900 |
| C  | 1.22809400  | 3.31631900  | 1.44373800  | H  | 0.04845100  | 2.49862400  | -2.42836100 |
| C  | 2.46044000  | 2.88175000  | 0.91409300  | H  | 0.34996300  | 1.71403600  | -0.84840700 |
| C  | 2.69620800  | 1.50871000  | 0.89377600  | H  | -0.50412100 | 0.82292400  | -2.13436000 |
| C  | 1.71292900  | 0.60918400  | 1.36391500  |    |             |             |             |
| C  | 2.01500800  | -0.80204300 | 1.36214800  |    |             |             |             |
| N  | 1.16874200  | -1.78057200 | 1.53024800  |    |             |             |             |
| H  | 0.99892800  | 4.39063000  | 1.47793500  |    |             |             |             |
| H  | 3.19562000  | 3.59853100  | 0.54093400  |    |             |             |             |
| H  | 3.63980100  | 1.10738000  | 0.50547500  |    |             |             |             |
| H  | 3.07166700  | -1.05947600 | 1.20110000  |    |             |             |             |
| O  | -0.46674400 | 0.43488700  | 2.41654600  |    |             |             |             |
| N  | -3.83612800 | -0.47026200 | 3.71025300  |    |             |             |             |
| N  | 0.27174700  | 2.51104300  | 1.92383000  |    |             |             |             |
| C  | 1.61523300  | -3.18933400 | 1.66285600  |    |             |             |             |
| C  | -1.71051500 | 2.36220200  | -1.14935800 |    |             |             |             |
| C  | -2.74582900 | 2.62363300  | -2.27142400 |    |             |             |             |
| H  | -3.64830800 | 3.05683200  | -1.80245000 |    |             |             |             |
| C  | 1.29636000  | -3.65652300 | 3.10721100  |    |             |             |             |
| H  | 0.20070800  | -3.62227600 | 3.23769500  |    |             |             |             |
| H  | 1.59043300  | -4.71965100 | 3.17745700  |    |             |             |             |
| C  | 1.97563200  | -2.83232500 | 4.20729400  |    |             |             |             |
| H  | 3.07610300  | -2.84512100 | 4.12208700  |    |             |             |             |
| H  | -2.32459700 | 3.40842200  | -2.92732000 |    |             |             |             |
| C  | -3.14360100 | 1.40677000  | -3.11893400 |    |             |             |             |
| H  | -2.27734900 | 0.96061300  | -3.63535900 |    |             |             |             |
| H  | -3.61270900 | 0.61890500  | -2.50254900 |    |             |             |             |
| H  | -3.87584900 | 1.69742100  | -3.89042000 |    |             |             |             |
| Ag | -2.19166800 | -0.65432000 | -0.63792900 | Pd | -0.87111100 | -1.42504300 | 1.70350800  |
| O  | -1.25122400 | -3.32555400 | 1.04742200  | C  | 0.49029500  | 1.12655600  | 1.79888800  |
| C  | -1.66454600 | -3.56209400 | -0.13851800 | C  | 1.27895800  | 3.26039900  | 1.33010700  |
| C  | -1.67518900 | -5.08505300 | -0.45127200 | C  | 2.48988000  | 2.79464800  | 0.77740300  |
| O  | -1.99016700 | -2.78786700 | -1.07616700 | C  | 2.68702000  | 1.41646600  | 0.74593800  |
| F  | -0.37849800 | -5.51095500 | -0.56670700 | C  | 1.68898000  | 0.54243500  | 1.23386700  |
| F  | -2.30975700 | -5.36434100 | -1.60745700 | C  | 1.94480000  | -0.87525900 | 1.21144500  |
| F  | -2.25931100 | -5.79268100 | 0.54217800  | N  | 1.07364800  | -1.82930000 | 1.40061500  |
| H  | 1.71805200  | -3.23351700 | 5.20076300  | H  | 1.07905900  | 4.34041000  | 1.36995400  |
| H  | 1.64142200  | -1.78172300 | 4.17672300  | H  | 3.23746900  | 3.49302200  | 0.39406000  |
| H  | 0.96098700  | -3.76621800 | 0.99003100  | H  | 3.61100400  | 0.99084500  | 0.33697500  |
| C  | 3.07175800  | -3.43868400 | 1.25693100  | H  | 2.98524800  | -1.18038500 | 1.00869500  |
| H  | 3.25879400  | -4.52367300 | 1.29272300  | O  | -0.46852200 | 0.42688500  | 2.34547900  |
| H  | 3.27137400  | -3.09936500 | 0.22648600  | N  | -3.82694500 | -0.45446800 | 3.81400600  |

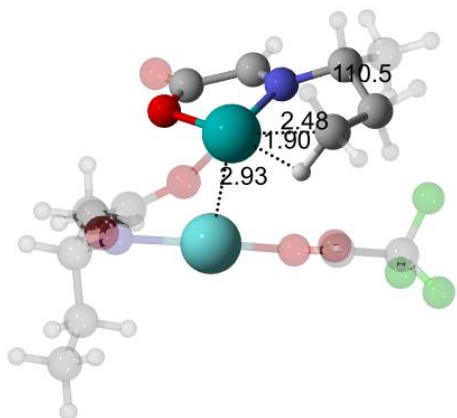


### T2-A1-Int1

|    |             |             |             |  |  |  |  |
|----|-------------|-------------|-------------|--|--|--|--|
| C  | -3.30656300 | -0.04845000 | 2.62616600  |  |  |  |  |
| C  | -4.30298600 | 0.46141000  | 4.66658800  |  |  |  |  |
| C  | -4.26747800 | 1.84971500  | 4.43809400  |  |  |  |  |
| C  | -3.71012200 | 2.28190500  | 3.23791200  |  |  |  |  |
| C  | -3.23290400 | 1.35513100  | 2.27980000  |  |  |  |  |
| C  | -2.66440600 | 1.96730400  | 1.08765500  |  |  |  |  |
| N  | -2.33879500 | 1.46782700  | -0.07026700 |  |  |  |  |
| H  | -4.72839500 | 0.06786900  | 5.60013400  |  |  |  |  |
| H  | -4.64757200 | 2.55456500  | 5.18207600  |  |  |  |  |
| H  | -3.63384800 | 3.35315400  | 3.01673600  |  |  |  |  |
| H  | -2.49097600 | 3.05260200  | 1.21253400  |  |  |  |  |
| O  | -2.89678600 | -1.01347100 | 1.82453500  |  |  |  |  |
| Pd | -0.87111100 | -1.42504300 | 1.70350800  |  |  |  |  |
| C  | 0.49029500  | 1.12655600  | 1.79888800  |  |  |  |  |
| C  | 1.27895800  | 3.26039900  | 1.33010700  |  |  |  |  |
| C  | 2.48988000  | 2.79464800  | 0.77740300  |  |  |  |  |
| C  | 2.68702000  | 1.41646600  | 0.74593800  |  |  |  |  |
| C  | 1.68898000  | 0.54243500  | 1.23386700  |  |  |  |  |
| C  | 1.94480000  | -0.87525900 | 1.21144500  |  |  |  |  |
| N  | 1.07364800  | -1.82930000 | 1.40061500  |  |  |  |  |
| H  | 1.07905900  | 4.34041000  | 1.36995400  |  |  |  |  |
| H  | 3.23746900  | 3.49302200  | 0.39406000  |  |  |  |  |
| H  | 3.61100400  | 0.99084500  | 0.33697500  |  |  |  |  |
| H  | 2.98524800  | -1.18038500 | 1.00869500  |  |  |  |  |
| O  | -0.46852200 | 0.42688500  | 2.34547900  |  |  |  |  |
| N  | -3.82694500 | -0.45446800 | 3.81400600  |  |  |  |  |



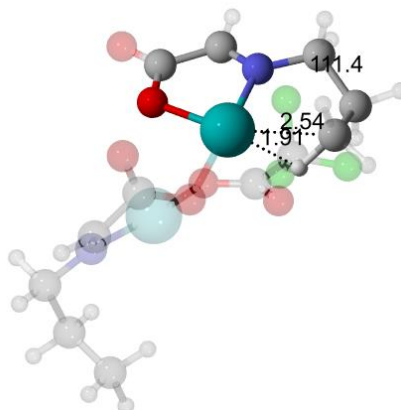
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.74230900 | -0.38388000 | 2.94733100  |
| H | -1.48755900 | -0.30363000 | 1.83379400  |
| F | -3.83044500 | 2.09493400  | -0.92105800 |
| F | -3.38556900 | 3.73236100  | 0.47743500  |
| F | -2.66573900 | 3.83736300  | -1.58879300 |
| H | -1.81246200 | -2.19644300 | -2.69365900 |
| H | 3.97793000  | -1.41556000 | 1.14624500  |



### T1-A2-Int2

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.28611300  | -1.14265200 | 2.29854300  |
| O  | 0.98306300  | -1.28174800 | 2.28150600  |
| O  | 2.95260200  | -1.14983800 | 3.34046100  |
| C  | -1.23534900 | -2.01681600 | -1.79830100 |
| C  | 0.26376400  | -2.18848500 | -1.89315700 |
| Pd | -0.32037000 | -1.50656100 | 0.77666100  |
| O  | 0.89964000  | -2.11743900 | -0.72375600 |
| O  | 0.83042600  | -2.41756200 | -2.96016500 |
| N  | -1.70948500 | -1.78331900 | -0.61841400 |
| C  | -3.15242700 | -1.78837400 | -0.24646000 |
| C  | -3.38936000 | -0.91890400 | 1.00276000  |
| H  | -3.39416200 | 0.14341800  | 0.71733400  |
| H  | -4.39791900 | -1.16529700 | 1.37808300  |
| C  | -4.06738900 | -1.39370400 | -1.41038200 |
| H  | -3.83514800 | -0.37141400 | -1.74675000 |
| H  | -5.11252800 | -1.40839700 | -1.06351100 |
| C  | 3.10693400  | -0.91465200 | 1.05171500  |
| N  | 2.84955100  | -0.04192700 | 0.14118500  |
| C  | 3.86536500  | 0.23979500  | -0.89604000 |
| C  | 3.29398600  | -0.11597800 | -2.27398600 |
| C  | 4.27144100  | 1.72343600  | -0.79666600 |
| H  | 2.42663800  | 0.52797100  | -2.51152400 |
| H  | 2.95809400  | -1.16264000 | -2.31994300 |
| H  | 4.06080000  | 0.05329600  | -3.04791500 |
| H  | 4.99060600  | 1.92506000  | -1.61127400 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.37478400  | 2.33952900  | -1.01072900 |
| C  | 4.87049400  | 2.11116600  | 0.56010400  |
| H  | 4.14308600  | 1.96469800  | 1.37569200  |
| H  | 5.17632300  | 3.16975300  | 0.56783300  |
| H  | 5.76142300  | 1.50171600  | 0.79273000  |
| Ag | 0.96753700  | 0.93427000  | -0.21130600 |
| O  | -0.68564500 | 2.00274800  | -1.08906400 |
| C  | -1.58060600 | 2.08241600  | -0.17358800 |
| O  | -1.55279400 | 1.61428800  | 0.98601100  |
| C  | -2.87846800 | 2.82542700  | -0.60395400 |
| H  | -3.99568100 | -2.08931300 | -2.26142800 |
| C  | -2.36196700 | -1.12127000 | 2.12338400  |
| H  | -2.15394200 | -2.17882200 | 2.36346100  |
| H  | -2.66843100 | -0.63750000 | 3.06656600  |
| H  | -1.44115000 | -0.47537300 | 1.91732800  |
| F  | -3.86762300 | 1.89288200  | -0.85357100 |
| F  | -3.33456000 | 3.63431700  | 0.37931400  |
| F  | -2.73274000 | 3.56096500  | -1.72613600 |
| H  | -1.86615000 | -2.15039300 | -2.68471600 |
| H  | 4.07645400  | -1.44053800 | 1.05731400  |
| H  | -3.33199100 | -2.84657100 | 0.03491000  |
| H  | 4.75481300  | -0.39074100 | -0.68866100 |

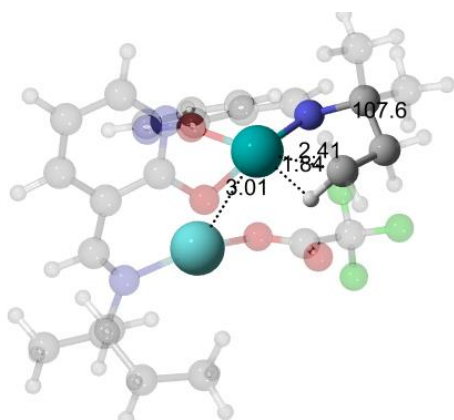


### T1-A1-Int2

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.23618900  | -1.76115800 | 1.39144000  |
| O  | 1.21572800  | -0.96127300 | 1.62694800  |
| O  | 2.29429200  | -2.98974400 | 1.45527100  |
| C  | -2.00976900 | -1.69964700 | -1.57760600 |
| C  | -0.57341500 | -1.89537400 | -2.00539900 |
| Pd | -0.56484700 | -1.38511900 | 0.76955700  |
| O  | 0.30104500  | -1.88042700 | -0.99281500 |
| O  | -0.25112700 | -2.07874700 | -3.17430700 |
| N  | -2.21282800 | -1.55208700 | -0.30963100 |
| C  | -3.53537000 | -1.41379200 | 0.32372700  |

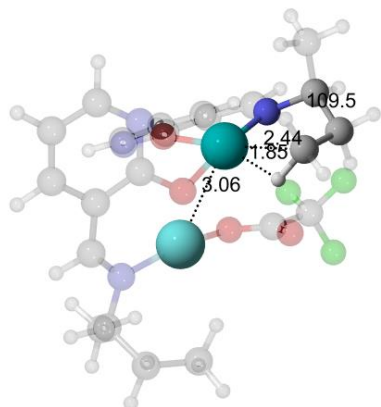


|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C  | -3.46373900 | -0.54324000 | 1.58624000  | C  | -4.23447500 | 2.02362100  | 3.08363900  |
| H  | -3.31263100 | 0.50854400  | 1.29973300  | C  | -4.11246800 | 2.47019700  | 1.76763500  |
| H  | -4.43833700 | -0.62334900 | 2.09882400  | C  | -3.30236000 | 1.77446300  | 0.84273800  |
| C  | 3.47504100  | -1.01751800 | 0.93501000  | C  | -3.15547100 | 2.37190200  | -0.47831200 |
| N  | 3.38601300  | -0.05742100 | 0.07983900  | N  | -2.29313400 | 2.09665400  | -1.41046200 |
| C  | 4.60171300  | 0.55490000  | -0.46971800 | H  | -3.55224000 | 0.49633000  | 4.47678800  |
| C  | 4.52469500  | 2.08594200  | -0.36084100 | H  | -4.84052300 | 2.55954900  | 3.81823700  |
| H  | 5.42172800  | 2.50590200  | -0.85020100 | H  | -4.61708500 | 3.38811500  | 1.44184500  |
| H  | 3.65147700  | 2.43336900  | -0.94800400 | H  | -3.88341700 | 3.18329200  | -0.65370500 |
| C  | 4.41341800  | 2.57773400  | 1.08769900  | O  | -2.06129000 | -0.22429700 | 0.44569100  |
| H  | 3.49605700  | 2.19397500  | 1.56565500  | Pd | -0.30974800 | -1.00628900 | 1.16597500  |
| H  | 4.37982500  | 3.67818100  | 1.13037400  | C  | 1.36987300  | 1.31211000  | 1.59265600  |
| H  | 5.27502300  | 2.24117100  | 1.69116800  | C  | 2.66078600  | 3.21954500  | 1.35009500  |
| Ag | 1.43224800  | 0.68202400  | -0.56832000 | C  | 3.87733800  | 2.50579700  | 1.34079600  |
| O  | -0.36417600 | 1.46073400  | -1.50161600 | C  | 3.80620900  | 1.12261300  | 1.46351200  |
| C  | -1.26910400 | 1.61179400  | -0.60687700 | C  | 2.55122400  | 0.48197100  | 1.58192200  |
| O  | -1.20425900 | 1.40899400  | 0.62618100  | C  | 2.53828800  | -0.95135900 | 1.69678800  |
| C  | -2.64161800 | 2.05018800  | -1.20162100 | N  | 1.49703400  | -1.73247300 | 1.60310700  |
| C  | -2.33805800 | -0.96333100 | 2.54567500  | H  | 2.66841600  | 4.31319100  | 1.24625100  |
| H  | -2.25216900 | -2.05415500 | 2.68703000  | H  | 4.83156100  | 3.02559600  | 1.22758500  |
| H  | -2.45330600 | -0.51339300 | 3.54666000  | H  | 4.71384000  | 0.50918900  | 1.44922800  |
| H  | -1.35259600 | -0.47333300 | 2.24594100  | H  | 3.51575200  | -1.42223700 | 1.86391200  |
| F  | -3.51263700 | 2.44616000  | -0.23621500 | O  | 0.14732300  | 0.85166300  | 1.75143900  |
| F  | -2.52533800 | 3.05386500  | -2.09702800 | N  | -2.78724500 | 0.13694300  | 2.58921900  |
| F  | -3.23084800 | 0.98465100  | -1.84934600 | N  | 1.44896400  | 2.66413700  | 1.47052400  |
| H  | -2.82575400 | -1.70400200 | -2.31062500 | C  | 1.56322300  | -3.20685600 | 1.86722800  |
| H  | 4.45331800  | -1.41615700 | 1.25420900  | C  | -2.35235600 | 2.81916100  | -2.71478800 |
| H  | -3.85245300 | -2.43977900 | 0.59024400  | C  | -2.80505000 | 1.78557200  | -3.79290300 |
| H  | 5.49883600  | 0.16639600  | 0.05307600  | H  | -3.84004500 | 1.48578800  | -3.54266500 |
| H  | 4.66518300  | 0.25639600  | -1.53206400 | C  | -0.93781200 | 3.35833000  | -3.01048400 |
| H  | -4.24731500 | -1.00302800 | -0.41235600 | H  | -0.18193800 | 2.55249900  | -2.99733900 |
|    |             |             |             | H  | -0.91202600 | 3.83455800  | -4.00509700 |
|    |             |             |             | H  | -0.64511600 | 4.10394300  | -2.25287800 |
|    |             |             |             | C  | -3.33794600 | 4.00459400  | -2.74829800 |
|    |             |             |             | H  | -3.09745200 | 4.75810200  | -1.97885800 |
|    |             |             |             | H  | -3.26927500 | 4.49785100  | -3.73089600 |
|    |             |             |             | H  | -4.38591600 | 3.68455100  | -2.61664700 |
|    |             |             |             | C  | 0.67993500  | -3.91178400 | 0.80644500  |
|    |             |             |             | H  | 1.18021400  | -3.83949100 | -0.17267200 |
|    |             |             |             | H  | 0.62081200  | -4.97989100 | 1.08103800  |
|    |             |             |             | C  | -0.72815600 | -3.32955100 | 0.66658400  |
|    |             |             |             | H  | -1.28805800 | -3.23387500 | 1.61188400  |
|    |             |             |             | H  | -2.86043100 | 2.33262700  | -4.75306200 |
|    |             |             |             | C  | -1.94340500 | 0.52897600  | -3.97168300 |



**T2-A3-Int2**

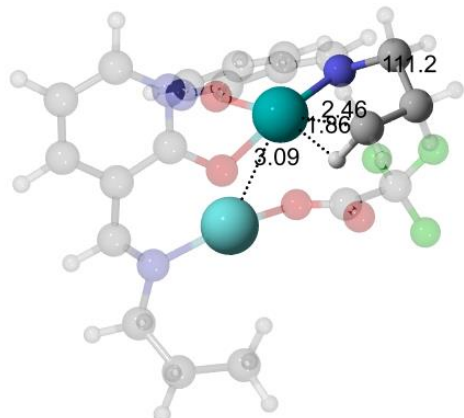
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H  | -0.89654600 | 0.77118000  | -4.22043900 | Pd | -0.30278700 | -0.94291600 | 1.18466400  |
| H  | -1.93839300 | -0.10255600 | -3.06785400 | C  | 1.48770800  | 1.32929100  | 1.50144700  |
| H  | -2.34105000 | -0.08477000 | -4.79774100 | C  | 2.85334400  | 3.18355400  | 1.25730400  |
| Ag | -0.43458300 | 0.89590700  | -1.16268600 | C  | 4.04293300  | 2.42457200  | 1.27180200  |
| O  | 0.55311700  | -1.84031500 | -1.75813400 | C  | 3.91874800  | 1.04748500  | 1.40865300  |
| C  | 1.55679300  | -1.10067900 | -1.66307700 | C  | 2.63856100  | 0.45531000  | 1.52143700  |
| C  | 2.95939800  | -1.75754900 | -1.84277500 | C  | 2.56634300  | -0.97258000 | 1.64953500  |
| O  | 1.62477900  | 0.16067500  | -1.45216900 | N  | 1.48621700  | -1.70370500 | 1.59007100  |
| F  | 2.91392200  | -3.11795000 | -1.71399500 | H  | 2.90346200  | 4.27501100  | 1.14294500  |
| F  | 3.86163900  | -1.31282000 | -0.91369600 | H  | 5.01714000  | 2.90734700  | 1.16551600  |
| F  | 3.47175800  | -1.48398700 | -3.07004700 | H  | 4.80224800  | 0.39995000  | 1.41169800  |
| C  | 1.01154400  | -3.41848300 | 3.29390700  | H  | 3.52048700  | -1.50341100 | 1.79815800  |
| H  | 0.95882200  | -4.49586700 | 3.52341200  | O  | 0.24237400  | 0.92571000  | 1.63879300  |
| H  | 1.66987100  | -2.93196300 | 4.03217800  | N  | -2.70777000 | 0.31358000  | 2.64570200  |
| H  | 0.00609800  | -2.98108900 | 3.40439000  | N  | 1.62069400  | 2.67533300  | 1.36606700  |
| C  | 2.99615400  | -3.75807700 | 1.75739500  | C  | 1.53537500  | -3.15977700 | 1.86321100  |
| H  | 3.64989100  | -3.38979500 | 2.56552100  | C  | -2.50112100 | 2.73265500  | -2.75234100 |
| H  | 2.95959400  | -4.85555700 | 1.84543200  | C  | -2.92354300 | 1.73092200  | -3.85702800 |
| H  | 3.44027300  | -3.50689900 | 0.78153200  | H  | -3.87719900 | 1.26889500  | -3.54252600 |
| H  | -0.67978300 | -2.38958500 | 0.00591800  | C  | -1.19629600 | 3.47741700  | -3.07059000 |
| H  | -1.36558500 | -3.92125300 | -0.01285800 | H  | -0.33761500 | 2.78274500  | -3.10650800 |



## T2-A2-Int2

|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -2.67204200 | 0.65643200  | 1.33174700  | H  | -2.30197100 | -0.00182100 | -5.02017000 |
| C | -3.42763400 | 1.07417100  | 3.48254400  | Ag | -0.49596000 | 0.89847000  | -1.24662500 |
| C | -4.17549700 | 2.19972900  | 3.08668900  | O  | 0.59767600  | -1.86474900 | -1.66199300 |
| C | -4.10752300 | 2.57780000  | 1.74564000  | C  | 1.56162200  | -1.06989600 | -1.60624000 |
| C | -3.31656900 | 1.84466100  | 0.83337800  | C  | 2.98942400  | -1.68996900 | -1.69686800 |
| C | -3.20699800 | 2.36303900  | -0.52012000 | O  | 1.56150100  | 0.20666900  | -1.50069500 |
| N | -2.37214600 | 2.03299500  | -1.46086400 | F  | 3.29986500  | -1.99331900 | -2.98417200 |
| H | -3.41508800 | 0.76448900  | 4.53590400  | F  | 3.07381000  | -2.85507900 | -0.97435300 |
| H | -4.76610800 | 2.76345100  | 3.81291900  | F  | 3.96314600  | -0.87052600 | -1.21693400 |
| H | -4.63922500 | 3.46828000  | 1.38877500  | C  | 1.15744100  | -3.39387700 | 3.33592800  |
| H | -3.93215800 | 3.17330200  | -0.74424400 | H  | 1.17337300  | -4.47208800 | 3.56590500  |
| O | -2.05668100 | -0.14903700 | 0.49562200  | H  | 1.86678600  | -2.88021600 | 4.00464000  |

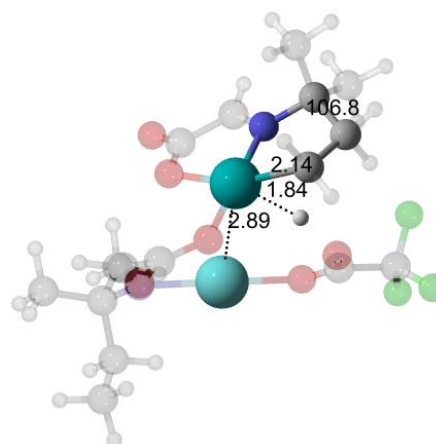
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.15013600  | -3.00097500 | 3.55250400  |
| H | -0.77699500 | -2.38720800 | 0.12626700  |
| H | -1.49289500 | -3.91263400 | 0.20804500  |
| H | 2.57686600  | -3.49331000 | 1.69439300  |
| H | -3.31591100 | 3.48436000  | -2.66731300 |



### T2-A1-Int2

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.67382300 | 0.59916200  | 1.31094300  |
| C  | -3.42181400 | 0.99794100  | 3.46768800  |
| C  | -4.19055800 | 2.11275500  | 3.08068900  |
| C  | -4.13847800 | 2.49599500  | 1.74054100  |
| C  | -3.34121300 | 1.77877900  | 0.82099500  |
| C  | -3.25178300 | 2.29709000  | -0.53301400 |
| N  | -2.40884200 | 1.98762300  | -1.47389800 |
| H  | -3.39729200 | 0.68500900  | 4.51986100  |
| H  | -4.78529900 | 2.66424300  | 3.81288100  |
| H  | -4.68781100 | 3.37814600  | 1.38987200  |
| H  | -4.00041600 | 3.08500900  | -0.76108500 |
| O  | -2.05238200 | -0.19308500 | 0.46711500  |
| Pd | -0.30013900 | -0.99591300 | 1.14574100  |
| C  | 1.49381900  | 1.26942000  | 1.50856400  |
| C  | 2.86636500  | 3.12518400  | 1.32431200  |
| C  | 4.05414700  | 2.36283000  | 1.33427300  |
| C  | 3.92523400  | 0.98376500  | 1.43981900  |
| C  | 2.64220100  | 0.39204200  | 1.52572000  |
| C  | 2.56799600  | -1.03773000 | 1.62263000  |
| N  | 1.48596700  | -1.76515500 | 1.55019100  |
| H  | 2.92031700  | 4.21891600  | 1.23678500  |
| H  | 5.03057000  | 2.84538400  | 1.24981100  |
| H  | 4.80726100  | 0.33418400  | 1.43938700  |
| H  | 3.52201300  | -1.57239300 | 1.75558200  |
| O  | 0.24513200  | 0.86771300  | 1.61587300  |
| N  | -2.69595500 | 0.25136100  | 2.62366400  |
| N  | 1.63166200  | 2.61775500  | 1.40670900  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.53213900  | -3.22505800 | 1.74632000  |
| C  | -2.58031900 | 2.65251900  | -2.77124000 |
| C  | -3.00358300 | 1.66067300  | -3.87373100 |
| H  | -3.96689200 | 1.20466300  | -3.57891300 |
| C  | 0.63602600  | -3.94870000 | 0.73453900  |
| H  | 1.06587800  | -3.84092100 | -0.27314200 |
| H  | 0.61510200  | -5.02059000 | 0.99849300  |
| C  | -0.78493700 | -3.37291200 | 0.72752200  |
| H  | -1.22674300 | -3.25360200 | 1.73297100  |
| H  | -3.20145000 | 2.25695400  | -4.78390400 |
| C  | -1.97494900 | 0.56491200  | -4.18607300 |
| H  | -0.98898000 | 0.99891400  | -4.43086600 |
| H  | -1.83430000 | -0.12423100 | -3.33587500 |
| H  | -2.29808400 | -0.04037500 | -5.04964800 |
| Ag | -0.51358200 | 0.90626600  | -1.27608600 |
| O  | 0.62084800  | -1.83221200 | -1.70862600 |
| C  | 1.57110700  | -1.02155400 | -1.64567400 |
| C  | 3.00845900  | -1.61723000 | -1.74511500 |
| O  | 1.54864300  | 0.25374100  | -1.52501200 |
| F  | 3.12049500  | -2.76680300 | -1.00046500 |
| F  | 3.97462500  | -0.77354400 | -1.29623600 |
| F  | 3.30448900  | -1.94233600 | -3.03042000 |
| H  | -0.79435300 | -2.43156700 | 0.07381200  |
| H  | -1.49761800 | -3.97004200 | 0.13354400  |
| H  | 1.17556100  | -3.42804600 | 2.77512100  |
| H  | -1.61297900 | 3.11438300  | -3.04530400 |
| H  | 2.57897500  | -3.56980400 | 1.67025400  |
| H  | -3.33542400 | 3.46348100  | -2.69341900 |

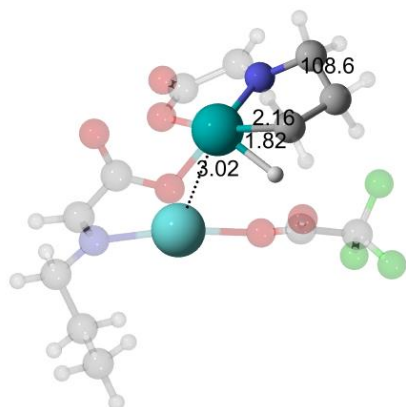


### T1-A3-TS2-3

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.01709600  | -0.74976100 | 2.32414600  |
| O | 0.71696100  | -0.61668900 | 2.24098900  |
| O | 2.64453900  | -0.77784100 | 3.39117600  |
| C | -1.28487400 | -2.18052600 | -1.77471900 |



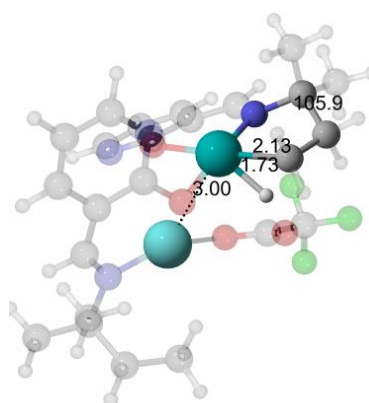
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 4.35541700  | 1.97062000  | 1.30559500  |
| H  | 5.53231900  | 3.01721800  | 0.47290400  |
| H  | 5.90415400  | 1.29580300  | 0.74206100  |
| Ag | 0.96856800  | 1.13919300  | -0.27896600 |
| O  | -0.82564600 | 2.19086400  | -0.80998900 |
| C  | -1.76649800 | 2.18874700  | 0.03285000  |
| O  | -1.85041000 | 1.60246400  | 1.16052300  |
| C  | -3.04193300 | 2.97871500  | -0.37881200 |
| H  | -4.08616000 | -2.21537200 | -2.26251300 |
| C  | -2.26195600 | -0.89393100 | 1.91181400  |
| H  | -2.04586200 | -1.86973200 | 2.38457600  |
| H  | -2.38256700 | -0.17411700 | 2.73784800  |
| H  | -1.50661600 | 0.27573900  | 1.32035900  |
| F  | -3.97824800 | 2.07609500  | -0.82592600 |
| F  | -3.57552400 | 3.64075800  | 0.66961800  |
| F  | -2.80797400 | 3.85623700  | -1.37325000 |
| H  | -1.90677200 | -2.57654400 | -2.58079100 |
| H  | 3.82335800  | -1.34011200 | 1.15832900  |
| H  | -3.38380500 | -2.89776700 | 0.05847100  |
| H  | 4.65588500  | -0.49596000 | -0.67892500 |



### T1-A1-TS2-3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.04035300  | -1.53105000 | 1.62733300  |
| O  | 1.02059500  | -0.69672800 | 1.67990300  |
| O  | 2.07501300  | -2.72931400 | 1.91470400  |
| C  | -1.79275100 | -2.16711900 | -1.74975600 |
| C  | -0.30379700 | -2.15501700 | -2.08225900 |
| Pd | -0.63288500 | -1.30243300 | 0.62394100  |
| O  | 0.48025700  | -1.90449800 | -1.04218200 |
| O  | 0.07142100  | -2.38173800 | -3.23201600 |
| N  | -2.12337600 | -1.82440800 | -0.54923300 |
| C  | -3.46858000 | -1.86092400 | 0.05905600  |
| C  | -3.52108200 | -0.82994700 | 1.19526500  |
| H  | -3.66497600 | 0.17443400  | 0.76741200  |
| H  | -4.39504100 | -1.04281900 | 1.83715800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 3.31342100  | -0.91345400 | 1.08027600  |
| N  | 3.26875900  | -0.05331100 | 0.12222000  |
| C  | 4.50120200  | 0.41608600  | -0.51838200 |
| C  | 4.50788500  | 1.94999000  | -0.60726600 |
| H  | 5.40982000  | 2.25435300  | -1.16777600 |
| H  | 3.63649500  | 2.26731900  | -1.21427600 |
| C  | 4.46657000  | 2.62927700  | 0.76734800  |
| H  | 3.54787200  | 2.35760700  | 1.31492100  |
| H  | 4.48745100  | 3.72643900  | 0.66831400  |
| H  | 5.32950700  | 2.32829500  | 1.38727100  |
| Ag | 1.30772000  | 0.72830100  | -0.47277600 |
| O  | -0.50260000 | 1.79863600  | -1.01724400 |
| C  | -1.42998800 | 1.96881700  | -0.17914700 |
| O  | -1.56234700 | 1.52647100  | 1.01020600  |
| C  | -2.64053200 | 2.81163700  | -0.67626900 |
| C  | -2.21614700 | -0.84949900 | 2.01961500  |
| H  | -2.03216700 | -1.81677100 | 2.52239500  |
| H  | -2.20440000 | -0.08491800 | 2.81464900  |
| H  | -1.42446700 | 0.18145700  | 1.31093900  |
| F  | -3.06913400 | 3.67273900  | 0.27421600  |
| F  | -2.36613600 | 3.50851900  | -1.79648400 |
| F  | -3.67367200 | 1.95142200  | -0.95933500 |
| H  | -2.53740900 | -2.47442500 | -2.49805900 |
| H  | 4.26979100  | -1.33562200 | 1.43329000  |
| H  | -3.58483300 | -2.88363900 | 0.46468500  |
| H  | 5.38846500  | 0.04829600  | 0.03518400  |
| H  | 4.52384400  | -0.01967000 | -1.53400400 |
| H  | -4.24285200 | -1.70193100 | -0.71206500 |

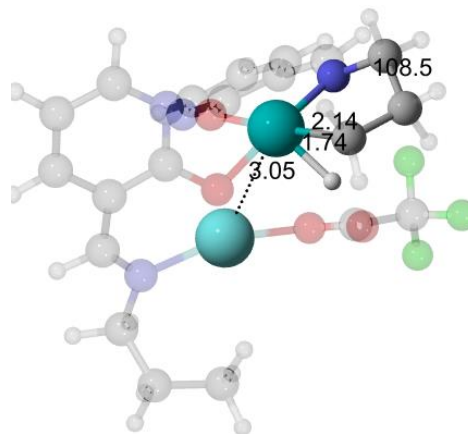


### T2-A3-TS2-3

|   |             |            |            |
|---|-------------|------------|------------|
| C | -1.60749400 | 6.22066600 | 0.31827100 |
| C | -2.45082500 | 6.41601400 | 2.47234000 |
| C | -3.24393000 | 7.53227300 | 2.14652900 |
| C | -3.13650100 | 8.03698500 | 0.85052500 |



|    |             |             |             |   |             |            |             |
|----|-------------|-------------|-------------|---|-------------|------------|-------------|
| O  | -0.92807700 | 5.46392900  | -0.54313400 | H | 2.78359800  | 3.25158200 | 3.44996300  |
| Pd | 0.85590600  | 4.79049300  | 0.26394400  | H | 1.11736300  | 3.06839800 | 2.84298500  |
| C  | 2.56582500  | 7.18703000  | 0.44725900  | H | 0.91565600  | 3.63025400 | -1.04336800 |
| C  | 3.94511200  | 9.01597300  | 0.04297000  | H | -0.09769000 | 2.26169800 | -0.79213400 |
| C  | 5.13719900  | 8.29000600  | 0.25789700  | H | 3.70487200  | 2.39430700 | 1.28607100  |
| C  | 5.01063600  | 6.94107800  | 0.56501500  | H | -2.03209600 | 9.52580000 | -3.30355100 |
| C  | 3.73045500  | 6.34023100  | 0.64988300  |   |             |            |             |
| C  | 3.67794800  | 4.93523900  | 0.95065100  |   |             |            |             |
| N  | 2.62560300  | 4.16539300  | 0.89442700  |   |             |            |             |
| H  | 3.99821500  | 10.08071500 | -0.22434900 |   |             |            |             |
| H  | 6.11305400  | 8.77343900  | 0.17100100  |   |             |            |             |
| H  | 5.89772200  | 6.31782100  | 0.72899000  |   |             |            |             |
| H  | 4.62718100  | 4.45804400  | 1.24765900  |   |             |            |             |
| O  | 1.32966900  | 6.77776400  | 0.55282600  |   |             |            |             |
| N  | -1.67252200 | 5.73260600  | 1.60682900  |   |             |            |             |
| N  | 2.71237600  | 8.50866300  | 0.13281500  |   |             |            |             |
| C  | 2.65599900  | 2.74753000  | 1.32589800  |   |             |            |             |
| C  | -1.26236100 | 8.74120000  | -3.47053500 |   |             |            |             |
| C  | -1.69305800 | 7.94406000  | -4.72784800 |   |             |            |             |
| H  | -2.70641700 | 7.54415900  | -4.54057200 |   |             |            |             |
| C  | 0.09913200  | 9.43449000  | -3.62519700 |   |             |            |             |
| H  | 0.91086700  | 8.69518800  | -3.75606900 |   |             |            |             |
| H  | 0.09456000  | 10.09786900 | -4.50651400 |   |             |            |             |
| H  | 0.33402800  | 10.03069900 | -2.72922000 |   |             |            |             |
| C  | 1.78604200  | 1.95574800  | 0.33194500  |   |             |            |             |
| H  | 2.34027800  | 1.84672600  | -0.61305700 |   |             |            |             |
| H  | 1.59903900  | 0.94330100  | 0.73471500  |   |             |            |             |
| C  | 0.46747800  | 2.69425200  | 0.05064000  |   |             |            |             |
| H  | -0.22664200 | 2.72411600  | 0.90793600  |   |             |            |             |
| H  | -1.78968800 | 8.67275000  | -5.55463700 |   |             |            |             |
| C  | -0.76407800 | 6.79856200  | -5.15487900 |   |             |            |             |
| H  | 0.26076000  | 7.14983900  | -5.36195200 |   |             |            |             |
| H  | -0.70380900 | 6.01595500  | -4.37899600 |   |             |            |             |
| H  | -1.14227900 | 6.32207600  | -6.07477400 |   |             |            |             |
| Ag | 0.59498100  | 6.63417300  | -2.12235400 |   |             |            |             |
| O  | 1.55979600  | 3.50071400  | -2.31212000 |   |             |            |             |
| C  | 2.49673200  | 4.32700800  | -2.57150000 |   |             |            |             |
| C  | 3.87508400  | 3.66152000  | -2.84672600 |   |             |            |             |
| O  | 2.48012800  | 5.58744100  | -2.59218000 |   |             |            |             |
| F  | 3.76718600  | 2.64635500  | -3.73708500 |   |             |            |             |
| F  | 4.35112100  | 3.13055000  | -1.67107200 |   |             |            |             |
| F  | 4.79968100  | 4.53254500  | -3.30247100 |   |             |            |             |
| C  | 2.14125700  | 2.66544700  | 2.77281600  |   |             |            |             |
| H  | 2.13424500  | 1.61647800  | 3.11268700  |   |             |            |             |
|    |             |             |             | H | 2.78359800  | 3.25158200 | 3.44996300  |
|    |             |             |             | H | 1.11736300  | 3.06839800 | 2.84298500  |
|    |             |             |             | H | 0.91565600  | 3.63025400 | -1.04336800 |
|    |             |             |             | H | -0.09769000 | 2.26169800 | -0.79213400 |
|    |             |             |             | H | 3.70487200  | 2.39430700 | 1.28607100  |
|    |             |             |             | H | -2.03209600 | 9.52580000 | -3.30355100 |



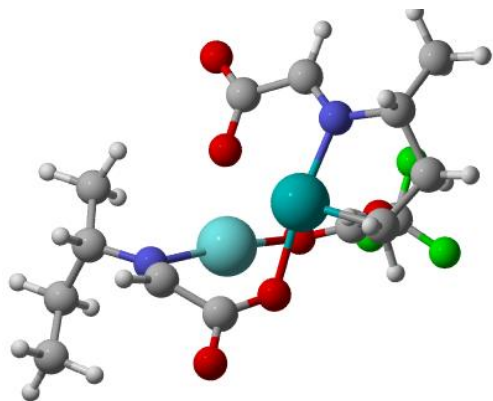
**T2-A1-TS2-3**

|    |             |             |             |  |  |  |  |
|----|-------------|-------------|-------------|--|--|--|--|
| C  | -1.60198700 | 6.21029300  | 0.34344700  |  |  |  |  |
| C  | -2.43074200 | 6.43356200  | 2.49967800  |  |  |  |  |
| C  | -3.25193600 | 7.52565700  | 2.15838000  |  |  |  |  |
| C  | -3.16601700 | 8.00812200  | 0.85293100  |  |  |  |  |
| C  | -2.30233200 | 7.39692600  | -0.08440200 |  |  |  |  |
| C  | -2.15024600 | 8.05493900  | -1.36840000 |  |  |  |  |
| N  | -1.25555500 | 7.86049400  | -2.29364200 |  |  |  |  |
| H  | -2.41614700 | 6.05735700  | 3.53123800  |  |  |  |  |
| H  | -3.90091200 | 7.99338200  | 2.90263600  |  |  |  |  |
| H  | -3.73817200 | 8.89223300  | 0.54605300  |  |  |  |  |
| H  | -2.88870300 | 8.86562900  | -1.54336900 |  |  |  |  |
| O  | -0.92409400 | 5.49444200  | -0.52246400 |  |  |  |  |
| Pd | 0.85860900  | 4.80377500  | 0.26810100  |  |  |  |  |
| C  | 2.56690600  | 7.20156200  | 0.52777500  |  |  |  |  |
| C  | 3.94839700  | 9.04927100  | 0.23269500  |  |  |  |  |
| C  | 5.13789700  | 8.31903700  | 0.45067300  |  |  |  |  |
| C  | 5.00889200  | 6.95933900  | 0.70152100  |  |  |  |  |
| C  | 3.72891000  | 6.35139700  | 0.73143300  |  |  |  |  |
| C  | 3.67947100  | 4.93633700  | 0.97408400  |  |  |  |  |
| N  | 2.63042400  | 4.16377200  | 0.88446400  |  |  |  |  |
| H  | 4.00400400  | 10.12409100 | 0.00982300  |  |  |  |  |
| H  | 6.11360800  | 8.80872700  | 0.40884500  |  |  |  |  |
| H  | 5.89393300  | 6.33293700  | 0.86403900  |  |  |  |  |
| H  | 4.63003600  | 4.45265200  | 1.25504400  |  |  |  |  |
| O  | 1.33027600  | 6.78575000  | 0.58141600  |  |  |  |  |
| N  | -1.63547000 | 5.78750000  | 1.63589900  |  |  |  |  |





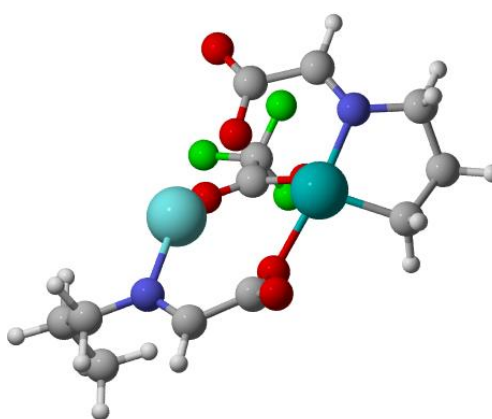
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.63348300 | 0.65080700  | 0.38243400  |
| F | -3.68500800 | 2.88610500  | -1.83835200 |
| F | -3.72505100 | 3.73187100  | 0.19372800  |
| F | -2.37592800 | 4.57459200  | -1.32122300 |
| H | -2.13602000 | -2.37987400 | -2.53179500 |
| H | 3.52620000  | -1.41526400 | 1.40093400  |



### T1-A2-Int3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.98240600  | -0.58110600 | 2.36882900  |
| O  | 0.71462700  | -0.31074900 | 2.18622800  |
| O  | 2.56771200  | -0.58592200 | 3.46000100  |
| C  | -1.52012600 | -2.06640600 | -1.73546900 |
| C  | -0.17348600 | -1.50849200 | -2.18748600 |
| Pd | -0.46508800 | -1.22137100 | 0.75160400  |
| O  | 0.61906900  | -1.14184700 | -1.20661900 |
| O  | 0.06262500  | -1.45748300 | -3.40099400 |
| N  | -1.79026600 | -2.05226800 | -0.47244000 |
| C  | -3.02285600 | -2.57577700 | 0.18772900  |
| C  | -3.20455400 | -1.71790800 | 1.45383200  |
| H  | -3.61165100 | -0.73544100 | 1.15452600  |
| H  | -3.96173200 | -2.19227400 | 2.10785100  |
| C  | -4.24324000 | -2.62401800 | -0.73195100 |
| H  | -4.47345400 | -1.61846000 | -1.12302200 |
| H  | -5.11742000 | -2.97991100 | -0.16418200 |
| C  | 2.92084400  | -0.78451600 | 1.19524200  |
| N  | 2.95096100  | 0.02935700  | 0.19610400  |
| C  | 4.07247000  | 0.00553100  | -0.75764200 |
| C  | 3.53318300  | 0.05763100  | -2.19072000 |
| C  | 4.99766300  | 1.20184700  | -0.44154100 |
| H  | 3.03721500  | 1.03005300  | -2.37582500 |
| H  | 2.79080800  | -0.73352900 | -2.37264200 |
| H  | 4.36391700  | -0.03661000 | -2.90950100 |
| H  | 5.77274500  | 1.23592100  | -1.22901800 |
| H  | 4.40131100  | 2.12900000  | -0.54573900 |

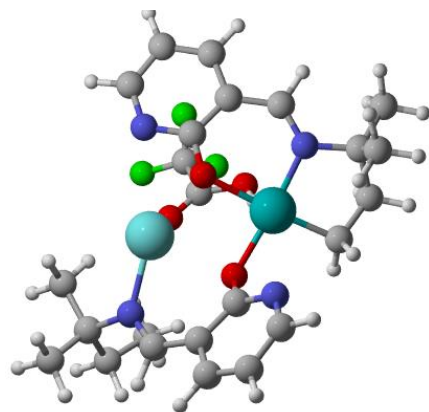
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 5.64839300  | 1.13964400  | 0.94525600  |
| H  | 4.89465800  | 1.13568000  | 1.74993000  |
| H  | 6.30787000  | 2.00760900  | 1.10866000  |
| H  | 6.26208600  | 0.22837100  | 1.05747600  |
| Ag | 1.15192000  | 1.13926500  | -0.28518100 |
| O  | -0.56268700 | 2.47846800  | -0.70643900 |
| C  | -1.74320800 | 2.24776000  | -0.41687400 |
| O  | -2.25056400 | 1.21254000  | 0.21002500  |
| C  | -2.85159500 | 3.25298900  | -0.83367200 |
| H  | -4.10151900 | -3.31014300 | -1.58272300 |
| C  | -1.86396300 | -1.54226700 | 2.18716200  |
| H  | -1.52813400 | -2.46945100 | 2.68771900  |
| H  | -1.85356400 | -0.71432700 | 2.91223800  |
| H  | -1.53563500 | 0.48552800  | 0.43353500  |
| F  | -3.62861200 | 2.68175100  | -1.78792200 |
| F  | -3.62803300 | 3.56379200  | 0.22905400  |
| F  | -2.30894000 | 4.37843500  | -1.32705900 |
| H  | -2.21750900 | -2.46874000 | -2.48274900 |
| H  | 3.71714100  | -1.53511400 | 1.33658000  |
| H  | -2.74605900 | -3.60172800 | 0.50502000  |
| H  | 4.64125000  | -0.93570400 | -0.60361400 |



### T1-A1-Int3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 2.02051000  | -1.39972500 | 1.85127400  |
| O  | 0.96238500  | -0.66506300 | 1.61188100  |
| O  | 2.09797400  | -2.56111600 | 2.26661000  |
| C  | -2.36024600 | -1.80439600 | -1.48109800 |
| C  | -1.12807800 | -1.16037000 | -2.11536600 |
| Pd | -0.71358700 | -1.52260100 | 0.78912100  |
| O  | -0.07254000 | -1.16229800 | -1.32612300 |
| O  | -1.22422000 | -0.68082700 | -3.24808800 |
| N  | -2.33085800 | -2.05111300 | -0.21251200 |
| C  | -3.43096900 | -2.56877700 | 0.62533000  |
| C  | -3.28567300 | -1.87020600 | 1.98786500  |

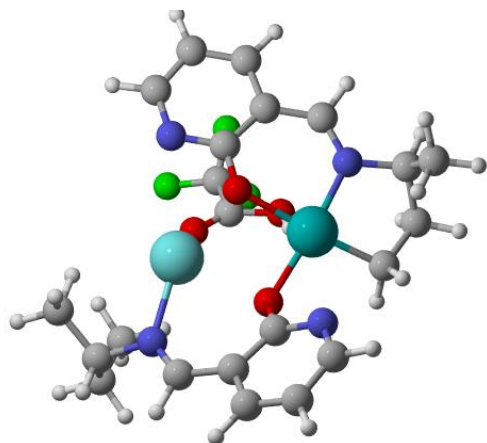
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H  | -3.61593100 | -0.82177600 | 1.88198700  | C  | -4.87411500 | 1.44457800  | 1.21514500  |
| H  | -3.95671800 | -2.35118400 | 2.72602600  | C  | -3.66485600 | 1.24371300  | 0.51482000  |
| C  | 3.32516800  | -0.70912600 | 1.49591000  | C  | -3.47042300 | 2.01522500  | -0.70298700 |
| N  | 3.44218100  | -0.04344800 | 0.39718600  | N  | -2.35008200 | 2.32914900  | -1.28613900 |
| C  | 4.74010000  | 0.50141300  | -0.01096100 | H  | -4.17019600 | -0.44931300 | 3.94442000  |
| C  | 4.59507300  | 1.98234300  | -0.39487600 | H  | -6.02004900 | 0.98508500  | 3.01159200  |
| H  | 5.56894100  | 2.33399100  | -0.78011300 | H  | -5.62031200 | 2.12803100  | 0.79111600  |
| H  | 3.87774500  | 2.05360600  | -1.23708200 | H  | -4.41620400 | 2.38633500  | -1.14379500 |
| C  | 4.12292800  | 2.85914200  | 0.77172200  | O  | -1.69866000 | -0.10402100 | 0.36628600  |
| H  | 3.13498800  | 2.53102900  | 1.13716900  | Pd | -0.10506800 | -0.98705600 | 1.34405100  |
| H  | 4.03543700  | 3.91377000  | 0.46505300  | C  | 2.12681300  | 1.03798300  | 0.98687100  |
| H  | 4.82951000  | 2.80930100  | 1.61900300  | C  | 3.84232500  | 2.32748900  | 0.08297500  |
| Ag | 1.58092500  | 0.34877300  | -0.74805800 | C  | 4.85094100  | 1.48300100  | 0.58641600  |
| O  | -0.05294300 | 2.06792400  | -0.99036500 | C  | 4.44823800  | 0.33403000  | 1.26455300  |
| C  | -1.25046800 | 2.06341800  | -0.71573900 | C  | 3.07610400  | 0.05233700  | 1.45947400  |
| O  | -1.92921800 | 1.21845200  | 0.04482700  | C  | 2.73307200  | -1.22247200 | 2.05669100  |
| C  | -2.19408400 | 3.17044500  | -1.26163100 | N  | 1.55415900  | -1.78106000 | 2.11569800  |
| C  | -1.81160200 | -1.91532100 | 2.44472600  | H  | 4.10685100  | 3.21240100  | -0.50998200 |
| H  | -1.49197200 | -2.92700900 | 2.75661700  | H  | 5.90577900  | 1.70562300  | 0.41037800  |
| H  | -1.58472700 | -1.19506200 | 3.24624200  | H  | 5.19156300  | -0.38413900 | 1.63088200  |
| H  | -1.35552500 | 0.43231600  | 0.37041000  | H  | 3.58754700  | -1.79094100 | 2.45419600  |
| F  | -2.65153900 | 3.92835100  | -0.23214300 | O  | 0.84439000  | 0.94435400  | 1.20356300  |
| F  | -1.53775100 | 3.96409900  | -2.12600800 | N  | -2.93030000 | -0.26529400 | 2.30120300  |
| F  | -3.25602700 | 2.61547500  | -1.89205800 | N  | 2.53096400  | 2.12421900  | 0.26723300  |
| H  | -3.25770200 | -1.98516700 | -2.09057300 | C  | 1.32530400  | -3.13539400 | 2.72554600  |
| H  | 4.19836500  | -0.91415700 | 2.13987900  | C  | -2.39537900 | 3.04797100  | -2.59795200 |
| H  | -3.25643600 | -3.65543400 | 0.73646000  | C  | -2.87863400 | 2.03588100  | -3.67605500 |
| H  | 5.48680600  | 0.37503200  | 0.79926100  | H  | -3.94174600 | 1.80712600  | -3.46729200 |
| H  | 5.08228100  | -0.08048600 | -0.88655300 | C  | -0.96663200 | 3.53400300  | -2.90062600 |
| H  | -4.41034000 | -2.41523000 | 0.13745700  | H  | -0.25234900 | 2.69377100  | -2.92417600 |
|    |             |             |             | H  | -0.92928900 | 4.04373900  | -3.87853900 |
|    |             |             |             | H  | -0.63532900 | 4.25124000  | -2.12879500 |
|    |             |             |             | C  | -3.33759000 | 4.26900200  | -2.55429800 |
|    |             |             |             | H  | -3.04872200 | 4.95027300  | -1.73628600 |
|    |             |             |             | H  | -3.27480400 | 4.82320000  | -3.50519500 |
|    |             |             |             | H  | -4.39344000 | 3.98345600  | -2.41337300 |
|    |             |             |             | C  | 0.30080300  | -3.79512100 | 1.77039900  |
|    |             |             |             | H  | 0.82864100  | -4.04504300 | 0.83141700  |
|    |             |             |             | H  | -0.03799500 | -4.75140300 | 2.21694000  |
|    |             |             |             | C  | -0.87357300 | -2.85359700 | 1.47575000  |
|    |             |             |             | H  | -1.60937100 | -2.79018700 | 2.29479000  |
|    |             |             |             | H  | -2.85928400 | 2.55148000  | -4.65479700 |
|    |             |             |             | C  | -2.07900500 | 0.72725500  | -3.74487000 |
|    |             |             |             | H  | -1.02389900 | 0.90121200  | -4.00889600 |



### T2-A3-Int3

|   |             |            |            |   |             |            |             |
|---|-------------|------------|------------|---|-------------|------------|-------------|
| C | -2.73152900 | 0.27786200 | 1.06668600 | H | -2.85928400 | 2.55148000 | -4.65479700 |
| C | -4.06931500 | 0.01034600 | 2.95163500 | C | -2.07900500 | 0.72725500 | -3.74487000 |
| C | -5.09944800 | 0.82475600 | 2.44534400 | H | -1.02389900 | 0.90121200 | -4.00889600 |

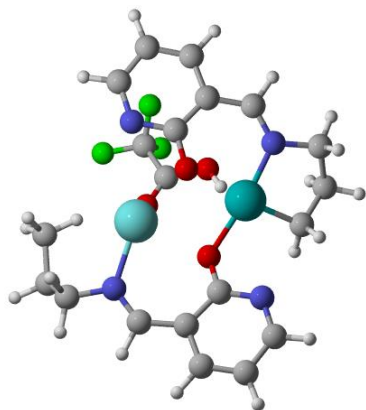
|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H  | -2.08958200 | 0.20560500  | -2.77448500 | Pd | -0.20353000 | -0.95658600 | 1.45140300  |
| H  | -2.51016800 | 0.05576100  | -4.50603100 | C  | 2.08184100  | 0.96772700  | 0.83272200  |
| Ag | -0.38822000 | 1.96342200  | -0.37068800 | C  | 3.81262200  | 2.14491600  | -0.18882800 |
| O  | 1.60524500  | -1.50631400 | -1.12809000 | C  | 4.81112200  | 1.30361200  | 0.34292800  |
| C  | 1.65586000  | -0.48847900 | -1.97913200 | C  | 4.39494900  | 0.22295200  | 1.11608600  |
| C  | 2.93570200  | -0.58284300 | -2.85202800 | C  | 3.02017000  | 0.00048500  | 1.36809400  |
| O  | 0.87138300  | 0.44343700  | -2.10019000 | C  | 2.65679800  | -1.20311400 | 2.08337600  |
| F  | 3.08297600  | -1.82040400 | -3.38618000 | N  | 1.45987400  | -1.70110800 | 2.24140800  |
| F  | 4.02683600  | -0.31760200 | -2.08444400 | H  | 4.08849400  | 2.98268100  | -0.84246300 |
| F  | 2.89121800  | 0.31682800  | -3.85535600 | H  | 5.86658300  | 1.48079800  | 0.12415800  |
| C  | 0.71268600  | -2.89534900 | 4.12120500  | H  | 5.12664600  | -0.48751600 | 1.51880100  |
| H  | 0.42544200  | -3.85794000 | 4.57692500  | H  | 3.49738500  | -1.78557300 | 2.50025300  |
| H  | 1.44252500  | -2.39728800 | 4.78113700  | O  | 0.79912300  | 0.91167500  | 1.05542300  |
| H  | -0.17985900 | -2.25434400 | 4.04929300  | N  | -3.04885700 | -0.21143900 | 2.36628800  |
| C  | 2.60159500  | -3.98252500 | 2.83456900  | N  | 2.50204000  | 1.99356600  | 0.03580600  |
| H  | 3.31744000  | -3.57767700 | 3.57021900  | C  | 1.24080900  | -2.97748100 | 2.96833900  |
| H  | 2.32956500  | -4.99492200 | 3.17353100  | C  | -2.57400300 | 3.04472300  | -2.58410900 |
| H  | 3.10565900  | -4.07511900 | 1.85749700  | C  | -2.59238500 | 2.14607900  | -3.84622500 |
| H  | 0.85817500  | -1.36073300 | -0.42811900 | H  | -3.50604200 | 1.52492600  | -3.80062500 |
| H  | -1.39875600 | -3.10295100 | 0.53933100  | C  | -1.43371200 | 4.07153100  | -2.59025600 |



### T2-A2-Int3

|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C | -2.84184000 | 0.29126000  | 1.11568800  | H  | -1.45625100 | 0.65800300  | -4.96080000 |
| C | -4.18301600 | 0.09654900  | 3.00831300  | Ag | -0.45090300 | 1.71002800  | -0.65985300 |
| C | -5.19834400 | 0.91845200  | 2.48324400  | O  | 1.38601500  | -1.91830700 | -0.96297200 |
| C | -4.96039000 | 1.50426000  | 1.24063300  | C  | 1.62579800  | -0.96702600 | -1.85624200 |
| C | -3.76093200 | 1.25402600  | 0.53493200  | C  | 2.88445000  | -1.32156900 | -2.69316200 |
| C | -3.55919400 | 2.02072600  | -0.68121600 | O  | 1.01921900  | 0.08046800  | -2.04104100 |
| N | -2.47308600 | 2.20671300  | -1.37660300 | F  | 2.81964400  | -2.58820600 | -3.17217900 |
| H | -4.29193500 | -0.33810300 | 4.01150900  | F  | 3.99105200  | -1.21842800 | -1.90872600 |
| H | -6.11450000 | 1.11173300  | 3.04632100  | F  | 3.01719100  | -0.47357200 | -3.73197400 |
| H | -5.69076000 | 2.19663800  | 0.80380600  | C  | 0.78010100  | -2.66263600 | 4.40001800  |
| H | -4.47363200 | 2.54977900  | -1.02377300 | H  | 0.56496900  | -3.59854800 | 4.94221400  |
| O | -1.80572800 | -0.12055600 | 0.43854100  | H  | 1.55923200  | -2.10892400 | 4.94900200  |

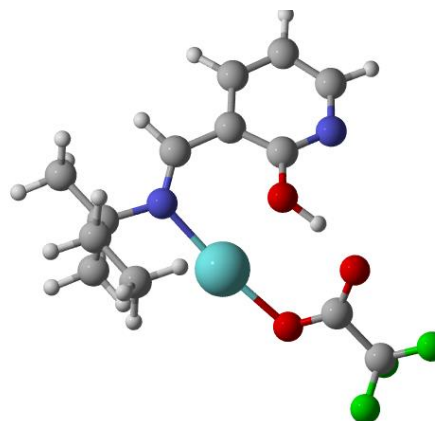
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.13206700 | -2.04450500 | 4.38151000  |
| H | 0.67410700  | -1.60784100 | -0.28029300 |
| H | -1.58497100 | -3.11628700 | 0.94984500  |
| H | 2.19512800  | -3.54104900 | 3.00164500  |
| H | -3.53931600 | 3.59604000  | -2.55940700 |



### T2-A1-Int3

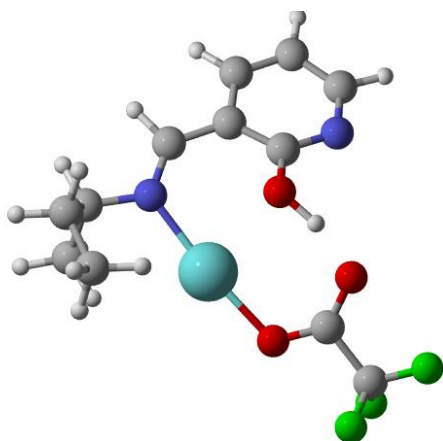
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.95774600 | 0.18769200  | 1.24413400  |
| C  | -4.51494000 | -0.21928800 | 2.92583600  |
| C  | -5.55245500 | 0.45515700  | 2.25471400  |
| C  | -5.22651200 | 1.07672700  | 1.05106000  |
| C  | -3.91681900 | 1.00637400  | 0.51809700  |
| C  | -3.69216700 | 1.80257900  | -0.67648300 |
| N  | -2.59662700 | 2.13831400  | -1.29959400 |
| H  | -4.70210800 | -0.67786300 | 3.90685900  |
| H  | -6.55753000 | 0.51119100  | 2.67946700  |
| H  | -5.98143900 | 1.65748900  | 0.50668600  |
| H  | -4.63461200 | 2.22469900  | -1.08534100 |
| O  | -1.78624100 | -0.05365200 | 0.73070500  |
| Pd | -0.14803800 | -0.79783700 | 1.74174300  |
| C  | 2.10641000  | 0.93381100  | 0.60456400  |
| C  | 3.76267900  | 1.88567200  | -0.72449100 |
| C  | 4.79626500  | 1.16475900  | -0.09484500 |
| C  | 4.43311200  | 0.24177400  | 0.88351100  |
| C  | 3.07695600  | 0.07078100  | 1.24773200  |
| C  | 2.75940700  | -0.99194000 | 2.17515900  |
| N  | 1.57460100  | -1.43473200 | 2.50551000  |
| H  | 3.99269200  | 2.57991900  | -1.54290700 |
| H  | 5.83678200  | 1.29921000  | -0.39891800 |
| H  | 5.19271800  | -0.38366500 | 1.36734100  |
| H  | 3.62627200  | -1.51672100 | 2.61351900  |
| O  | 0.84608100  | 0.94452300  | 0.93543800  |
| N  | -3.26942700 | -0.35322900 | 2.45526000  |
| N  | 2.46691300  | 1.78244500  | -0.39994100 |
| C  | 1.41077200  | -2.59493200 | 3.40499700  |

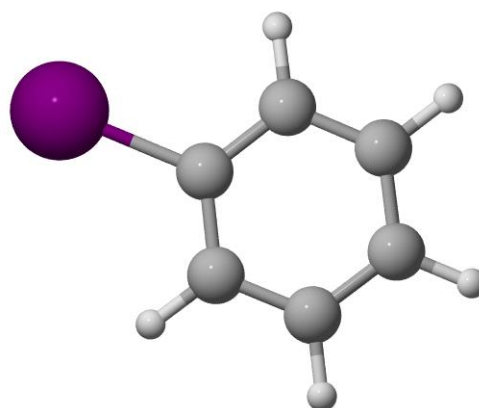
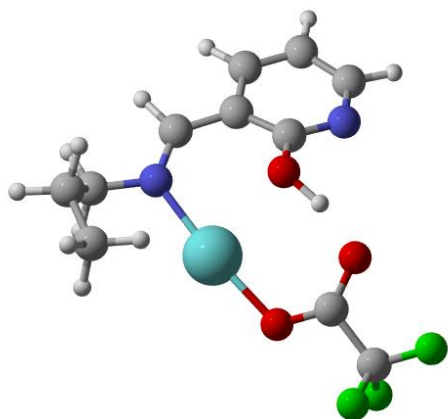
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.73987400 | 3.02743200  | -2.45917200 |
| C  | -2.12871300 | 2.45045800  | -3.75065000 |
| H  | -2.54798100 | 1.44182400  | -3.91972300 |
| C  | 0.27379900  | -3.43769900 | 2.81400600  |
| H  | 0.63570500  | -3.91978100 | 1.88763100  |
| H  | 0.00093900  | -4.24581900 | 3.52101200  |
| C  | -0.91625400 | -2.51358900 | 2.51076200  |
| H  | -1.45102400 | -2.18436400 | 3.41834800  |
| H  | -2.48938600 | 3.08576100  | -4.58111000 |
| C  | -0.59452900 | 2.40116200  | -3.77908400 |
| H  | -0.15948000 | 3.38396400  | -3.52335200 |
| H  | -0.18610500 | 1.64778600  | -3.08391900 |
| H  | -0.23271800 | 2.12574900  | -4.78415100 |
| Ag | -0.58391300 | 1.69655500  | -0.59968000 |
| O  | 1.29058700  | -1.99947000 | -0.67461300 |
| C  | 1.13722100  | -1.22065000 | -1.74318000 |
| C  | 2.32814400  | -1.40802900 | -2.71987000 |
| O  | 0.22269000  | -0.44390000 | -1.97877300 |
| F  | 2.39952600  | -2.69425200 | -3.14902300 |
| F  | 3.49779600  | -1.10185600 | -2.10039200 |
| F  | 2.18859700  | -0.60356600 | -3.79213200 |
| H  | 0.60038100  | -1.73232200 | 0.03832900  |
| H  | -1.64215200 | -2.94640900 | 1.80449300  |
| H  | 1.10957200  | -2.20909400 | 4.39779400  |
| H  | -2.23117300 | 3.98118700  | -2.21597700 |
| H  | 2.36488400  | -3.14450800 | 3.51605100  |
| H  | -3.81351200 | 3.25682100  | -2.62756100 |



|   |            |             |             |
|---|------------|-------------|-------------|
| C | 0.53986800 | -2.16510100 | 0.56304500  |
| C | 0.47613800 | -4.39030700 | -0.04671100 |
| C | 1.82801400 | -4.40338100 | -0.43415000 |
| C | 2.52563400 | -3.19583300 | -0.37405500 |
| C | 1.88393400 | -2.01826400 | 0.07175600  |

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C  | 2.64043700  | -0.77449000 | -0.03177000 |    |             |             |             |
| N  | 2.17915700  | 0.43852000  | -0.11136700 | C  | 0.94878500  | -2.09606500 | 0.51281300  |
| H  | -0.13502400 | -5.29773300 | -0.13516400 | C  | 1.19719800  | -4.32056400 | -0.04835400 |
| H  | 2.30010600  | -5.32062200 | -0.79412400 | C  | 2.54959300  | -4.16144500 | -0.40230900 |
| H  | 3.56795900  | -3.13680500 | -0.70929300 | C  | 3.07907500  | -2.87160600 | -0.35459100 |
| H  | 3.73121900  | -0.92978300 | -0.09578800 | C  | 2.27646600  | -1.78106700 | 0.05354500  |
| O  | -0.03842200 | -1.13780600 | 1.18509500  | C  | 2.85888100  | -0.45269500 | -0.07137100 |
| N  | -0.15250600 | -3.31445700 | 0.45493600  | N  | 2.26145900  | 0.70307300  | -0.11799100 |
| C  | 3.10455000  | 1.60552600  | -0.18410100 | H  | 0.71503000  | -5.30319100 | -0.13074700 |
| C  | 3.10071600  | 2.28728800  | 1.21891600  | H  | 3.14802200  | -5.01486400 | -0.72979500 |
| H  | 3.58927500  | 1.58945700  | 1.92419500  | H  | 4.11223200  | -2.68084000 | -0.66821400 |
| C  | 2.55458600  | 2.55070700  | -1.26986700 | H  | 3.96116700  | -0.45640600 | -0.19183400 |
| H  | 1.50383800  | 2.82944500  | -1.06918900 | O  | 0.22467100  | -1.14338700 | 1.09368500  |
| H  | 3.15059100  | 3.47732300  | -1.30973300 | N  | 0.41682100  | -3.32884900 | 0.41096100  |
| H  | 2.59123500  | 2.06645600  | -2.25968700 | C  | 3.09510400  | 1.90976400  | -0.27029600 |
| C  | 4.55654700  | 1.23485300  | -0.54281800 | C  | 3.07276400  | 2.73906200  | 1.03864900  |
| H  | 4.60970300  | 0.68262500  | -1.49655000 | H  | 3.46167900  | 2.09761100  | 1.85006900  |
| H  | 5.14470800  | 2.15917400  | -0.65636700 | C  | 2.62657800  | 2.69909600  | -1.50022800 |
| H  | 5.04572400  | 0.63532900  | 0.24365800  | H  | 1.56170500  | 2.98100900  | -1.41034200 |
| H  | 3.75969800  | 3.17244400  | 1.14466100  | H  | 3.21710400  | 3.62361400  | -1.61091500 |
| C  | 1.73757600  | 2.70355100  | 1.78652400  | H  | 2.73914100  | 2.09688200  | -2.41598300 |
| H  | 1.19492100  | 3.38902600  | 1.11338100  | H  | 3.80194400  | 3.56044900  | 0.90924700  |
| H  | 1.09545900  | 1.82790100  | 1.98001600  | C  | 1.71206000  | 3.31869900  | 1.44938400  |
| H  | 1.87278700  | 3.23013200  | 2.74581500  | H  | 1.29210100  | 3.98400300  | 0.67674700  |
| Ag | 0.05799900  | 0.84983800  | -0.33202500 | H  | 0.97426000  | 2.52213200  | 1.65252400  |
| O  | -2.48867800 | -0.78145200 | 0.86845000  | H  | 1.81227400  | 3.91000300  | 2.37429400  |
| C  | -2.79633700 | 0.18997900  | 0.12757800  | Ag | 0.12089300  | 0.93653100  | -0.26931700 |
| C  | -4.31563500 | 0.42540600  | -0.11982800 | O  | -2.24052700 | -1.05257200 | 0.76816300  |
| O  | -2.06038200 | 1.03749800  | -0.48573000 | C  | -2.64979400 | -0.04311900 | 0.13356700  |
| F  | -5.08853500 | -0.40277200 | 0.61528500  | C  | -4.18668400 | 0.06060100  | -0.09423200 |
| F  | -4.60638700 | 0.21996200  | -1.43388300 | O  | -2.00774400 | 0.93525200  | -0.38172700 |
| F  | -4.65486700 | 1.70517100  | 0.18914600  | F  | -4.86584300 | -0.91784000 | 0.54189500  |
| H  | -1.10292700 | -1.13196500 | 1.10981300  | F  | -4.46226700 | -0.02891000 | -1.42444700 |
|    |             |             |             | F  | -4.65279200 | 1.25736800  | 0.35084000  |
|    |             |             |             | H  | -0.83579700 | -1.26181500 | 1.00449100  |
|    |             |             |             | H  | 4.14596100  | 1.59104100  | -0.43745700 |

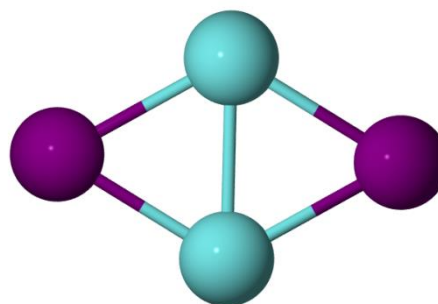




|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.28542400  | -1.82623800 | 0.52597800  |
| C  | 1.77268600  | -4.03578500 | 0.07255700  |
| C  | 3.08990800  | -3.74503400 | -0.32774000 |
| C  | 3.46987700  | -2.40324000 | -0.36251500 |
| C  | 2.55715900  | -1.38925700 | 0.01088500  |
| C  | 2.98157000  | -0.01334700 | -0.20023500 |
| N  | 2.25664300  | 1.06365200  | -0.30383000 |
| H  | 1.40361600  | -5.06935600 | 0.05415300  |
| H  | 3.77399500  | -4.54226800 | -0.62789200 |
| H  | 4.46694900  | -2.11491400 | -0.71580700 |
| H  | 4.07556200  | 0.10260500  | -0.34182900 |
| O  | 0.47257000  | -0.93146100 | 1.08047700  |
| N  | 0.89543300  | -3.11480400 | 0.50326700  |
| C  | 2.95403700  | 2.33708100  | -0.52384300 |
| C  | 2.83095200  | 3.28598300  | 0.68483800  |
| H  | 3.28173900  | 2.79187400  | 1.56489900  |
| H  | 3.45716300  | 4.16958700  | 0.46284800  |
| C  | 1.39960500  | 3.73553600  | 1.00704300  |
| H  | 0.90857900  | 4.18007900  | 0.12289200  |
| H  | 0.77570900  | 2.89346000  | 1.35569000  |
| H  | 1.39655900  | 4.49345700  | 1.80757500  |
| Ag | 0.10577800  | 1.04604600  | -0.38954400 |
| O  | -1.99312800 | -1.13205500 | 0.81637400  |
| C  | -2.52605300 | -0.21081000 | 0.14082200  |
| C  | -4.07000500 | -0.28733400 | -0.04660400 |
| O  | -2.00866000 | 0.80220000  | -0.44346900 |
| F  | -4.61919100 | -1.31022100 | 0.64274100  |
| F  | -4.36752100 | -0.45652400 | -1.36395200 |
| F  | -4.65487700 | 0.86668800  | 0.37069000  |
| H  | -0.56976600 | -1.17114100 | 1.02641000  |
| H  | 2.50494100  | 2.81532900  | -1.41441300 |
| H  | 4.02596200  | 2.15088200  | -0.74152900 |

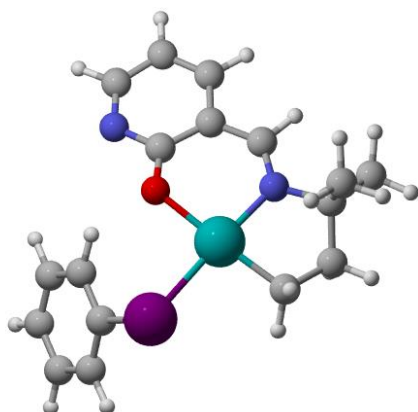
### PhI

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -0.81798500 | 1.07051600 | -0.00142900 |
| C | 0.58531900  | 1.06589000 | 0.01178600  |
| C | 1.28640500  | 2.28159800 | 0.01855200  |
| C | 0.59482000  | 3.50377600 | 0.01220900  |
| C | -0.80857600 | 3.48801800 | -0.00100700 |
| C | -1.52732800 | 2.28256200 | -0.00794300 |
| H | -1.37272800 | 0.12673500 | -0.00678400 |
| H | 1.13096100  | 0.11746400 | 0.01680800  |
| H | 1.13902800  | 4.45134700 | 0.01747800  |
| H | -2.61999800 | 2.28799300 | -0.01825900 |
| I | -1.86939900 | 5.33190100 | -0.01068900 |
| H | 2.38113800  | 2.28718900 | 0.02886300  |



### Ag<sub>2</sub>I<sub>2</sub>

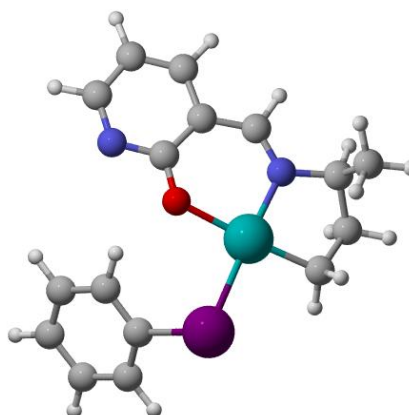
|    |             |             |             |
|----|-------------|-------------|-------------|
| Ag | -1.71786800 | 1.32293000  | -0.04064800 |
| Ag | -1.57555900 | -1.50109400 | -0.04585000 |
| I  | 0.77029600  | 0.03256100  | 0.07687100  |
| I  | -4.06373900 | -0.21060700 | -0.16328300 |



### T2-A3-Int4

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.68726100 | 0.43637700  | -3.71817200 |
| C  | -3.10035100 | 1.51036000  | -3.06197100 |
| C  | -2.20320300 | 1.29850300  | -1.98397100 |
| C  | -1.95061300 | -0.07615700 | -1.56882200 |
| C  | -3.33783900 | -0.85946900 | -3.27169100 |
| H  | -4.37737100 | 0.57585500  | -4.55388700 |
| H  | -3.31464800 | 2.54048100  | -3.37350100 |
| H  | -3.75728700 | -1.73826100 | -3.78343100 |
| O  | -1.21390000 | -0.39995200 | -0.55936600 |
| C  | -1.61341900 | 2.46787000  | -1.39174300 |
| H  | -1.97341700 | 3.42352400  | -1.80468600 |
| N  | -0.70034000 | 2.53388500  | -0.45559900 |
| Pd | 0.12255700  | 0.91891400  | 0.39468800  |
| C  | -0.21202300 | 3.84824300  | 0.08689100  |
| C  | -0.30305000 | 4.99596800  | -0.93349200 |
| H  | -1.34232400 | 5.30061900  | -1.14272300 |
| H  | 0.21398900  | 5.87937500  | -0.52521200 |
| H  | 0.18591500  | 4.72129700  | -1.88334000 |
| C  | -1.06237500 | 4.16769700  | 1.33383300  |
| H  | -1.03389500 | 3.33116200  | 2.04934500  |
| H  | -0.68422100 | 5.07659900  | 1.83171200  |
| H  | -2.11419800 | 4.33616300  | 1.04812400  |
| C  | 1.25722000  | 3.56820100  | 0.46077100  |
| H  | 1.83409900  | 3.47907300  | -0.47802700 |
| H  | 1.66687700  | 4.43925400  | 1.01152800  |
| C  | 1.38559100  | 2.27115300  | 1.26744700  |
| H  | 2.42231400  | 1.89481100  | 1.27278100  |
| H  | 1.05121000  | 2.39342300  | 2.31495700  |
| N  | -2.51551500 | -1.12484200 | -2.25613700 |
| C  | 1.72270400  | -2.42371200 | -0.10588300 |
| C  | 0.69099800  | -2.69169300 | -1.01245600 |
| C  | 3.01178700  | -2.95814400 | -0.23070000 |

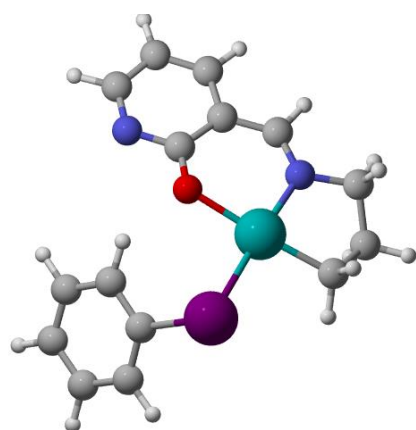
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.98396900  | -3.53332800 | -2.09935400 |
| H | -0.29599100 | -2.22882600 | -0.90105800 |
| C | 3.27241200  | -3.80472300 | -1.32175500 |
| H | 3.79653700  | -2.72227900 | 0.49297600  |
| C | 2.26275000  | -4.09106500 | -2.25413800 |
| H | 0.19165400  | -3.74417900 | -2.82435900 |
| H | 2.47562300  | -4.74805300 | -3.10327100 |
| I | 1.32015700  | -1.14667300 | 1.57525700  |
| H | 4.27311600  | -4.23277500 | -1.43917400 |



### T2-A2-Int4

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.72658000 | 0.62506600  | -3.74704500 |
| C  | -3.18407500 | 1.68226400  | -3.02859200 |
| C  | -2.30797400 | 1.44208700  | -1.93955900 |
| C  | -2.02471200 | 0.05577200  | -1.58220300 |
| C  | -3.35422000 | -0.68096200 | -3.35108300 |
| H  | -4.40072000 | 0.78518400  | -4.59201800 |
| H  | -3.41844200 | 2.72006500  | -3.29687500 |
| H  | -3.74010100 | -1.54527400 | -3.91153700 |
| O  | -1.29763100 | -0.29757100 | -0.57521700 |
| C  | -1.76237400 | 2.59003600  | -1.27189200 |
| H  | -2.12018400 | 3.57122300  | -1.63366000 |
| N  | -0.88087200 | 2.61555100  | -0.30457100 |
| Pd | -0.00410200 | 1.00045100  | 0.47168300  |
| C  | -0.44976200 | 3.90089800  | 0.30150500  |
| C  | -1.33707400 | 4.20709800  | 1.51864300  |
| H  | -1.28941600 | 3.38091400  | 2.24639600  |
| H  | -1.00350200 | 5.13567200  | 2.01153300  |
| H  | -2.38900800 | 4.33038100  | 1.21313900  |
| C  | 1.02848300  | 3.69615500  | 0.66167400  |
| H  | 1.61305400  | 3.66896500  | -0.27488200 |
| H  | 1.39662800  | 4.55865600  | 1.25291800  |
| C  | 1.20271700  | 2.36672200  | 1.41424600  |
| H  | 2.25283400  | 2.03017200  | 1.41194300  |

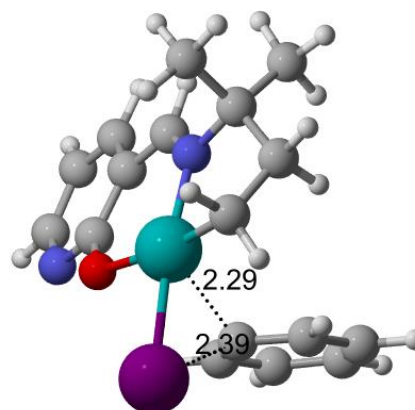
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.85465100  | 2.42919800  | 2.46241800  |
| N | -2.54804400 | -0.97298800 | -2.32986600 |
| C | 1.70171500  | -2.26396400 | -0.18101300 |
| C | 0.67690300  | -2.51399500 | -1.10037400 |
| C | 3.00230600  | -2.76412000 | -0.32657500 |
| C | 0.98931600  | -3.30011700 | -2.22287600 |
| H | -0.32021100 | -2.07810900 | -0.97141500 |
| C | 3.28228600  | -3.55594300 | -1.45335500 |
| H | 3.78116700  | -2.54331500 | 0.40813000  |
| C | 2.28005300  | -3.82263200 | -2.39951100 |
| H | 0.20240100  | -3.49535100 | -2.95803600 |
| H | 2.50811400  | -4.43662400 | -3.27641900 |
| I | 1.27031100  | -1.07111200 | 1.55430100  |
| H | 4.29219800  | -3.95655100 | -1.58754500 |
| H | -0.57065600 | 4.70766300  | -0.44985500 |



**T2-A1-Int4**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.80948300 | 0.76222500  | -3.67719600 |
| C  | -3.31266900 | 1.80090000  | -2.90139700 |
| C  | -2.43204900 | 1.53938400  | -1.82051700 |
| C  | -2.09297300 | 0.14853800  | -1.53605300 |
| C  | -3.38602600 | -0.54694700 | -3.34813100 |
| H  | -4.48676100 | 0.93940300  | -4.51622300 |
| H  | -3.58769400 | 2.84108000  | -3.11656100 |
| H  | -3.73517200 | -1.39545300 | -3.95492300 |
| O  | -1.35302600 | -0.22854800 | -0.54731800 |
| C  | -1.93378300 | 2.67364300  | -1.09527300 |
| H  | -2.31784200 | 3.65729100  | -1.42103900 |
| N  | -1.06758100 | 2.68390400  | -0.11371200 |
| Pd | -0.13841500 | 1.06435200  | 0.59547500  |
| C  | -0.65291300 | 3.94585400  | 0.53042700  |
| C  | 0.81731100  | 3.77435000  | 0.91243700  |
| H  | 1.42796300  | 3.77733000  | -0.00821600 |
| H  | 1.15244700  | 4.62849100  | 1.53439900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.97416900  | 2.43308900  | 1.64510500  |
| H | 2.02900000  | 2.12262500  | 1.72773200  |
| H | 0.52868800  | 2.47171200  | 2.65887700  |
| N | -2.57148900 | -0.85942400 | -2.33994000 |
| C | 1.71360600  | -2.10201600 | -0.16957100 |
| C | 0.72196200  | -2.33868200 | -1.12799000 |
| C | 3.03137800  | -2.55979100 | -0.29920500 |
| C | 1.08734300  | -3.06595600 | -2.27398000 |
| H | -0.29060400 | -1.93691500 | -1.00767500 |
| C | 3.36461900  | -3.29315700 | -1.45076000 |
| H | 3.78318200  | -2.35076000 | 0.46648900  |
| C | 2.39674600  | -3.54499700 | -2.43593900 |
| H | 0.32685900  | -3.25071800 | -3.03908000 |
| H | 2.66605200  | -4.11355100 | -3.33158100 |
| I | 1.20071900  | -1.00244300 | 1.60470700  |
| H | 4.38878200  | -3.65994400 | -1.57311900 |
| H | -0.84277900 | 4.80693000  | -0.13891200 |
| H | -1.26347200 | 4.07775400  | 1.44538200  |

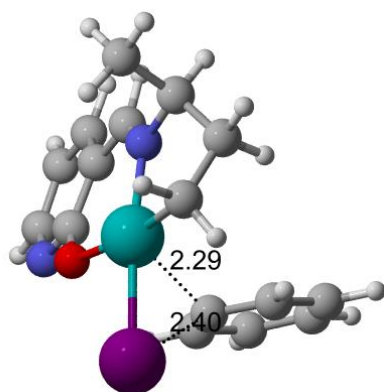


**T2-A3-TS4-5**

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | -2.94490400 | 5.03112100 | -0.57513800 |
| C  | -2.02326600 | 5.98066200 | -0.16027800 |
| C  | -1.20286200 | 5.74789800 | 0.97535600  |
| C  | -1.37949700 | 4.49434100 | 1.70451600  |
| C  | -3.01574800 | 3.83367900 | 0.17747000  |
| H  | -3.58414700 | 5.18597900 | -1.44774500 |
| H  | -1.90868500 | 6.92554400 | -0.70636300 |
| H  | -3.71892700 | 3.04537800 | -0.12990700 |
| O  | -0.73697000 | 4.18074800 | 2.77664900  |
| C  | -0.26655900 | 6.78175400 | 1.30892800  |
| H  | -0.32803100 | 7.67801900 | 0.67015100  |
| N  | 0.64816400  | 6.78722000 | 2.24593700  |
| Pd | 0.97833900  | 5.21281600 | 3.48230700  |
| C  | 1.52849700  | 7.98340400 | 2.47574900  |
| C  | 1.89149700  | 8.71184700 | 1.16904500  |



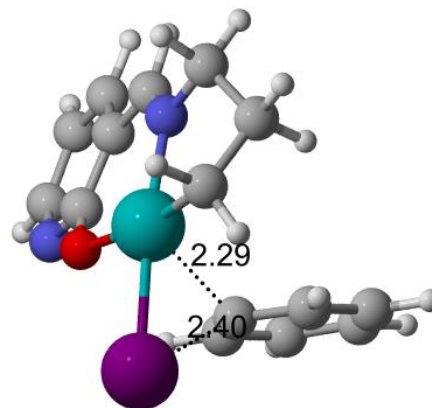
|   |             |            |             |
|---|-------------|------------|-------------|
| H | 1.03555000  | 9.24721900 | 0.72546700  |
| H | 2.66710100  | 9.46590900 | 1.38005800  |
| H | 2.29203800  | 8.00316500 | 0.42514200  |
| C | 0.77817300  | 8.93098300 | 3.43446300  |
| H | 0.47759200  | 8.40634300 | 4.35491500  |
| H | 1.41794700  | 9.78688400 | 3.70785000  |
| H | -0.13531600 | 9.31784800 | 2.95261000  |
| C | 2.79758600  | 7.39906900 | 3.12963200  |
| H | 3.37080900  | 6.86153800 | 2.35131700  |
| H | 3.43922700  | 8.22738400 | 3.49325800  |
| C | 2.44015200  | 6.43005500 | 4.25146800  |
| H | 3.30677600  | 5.86345800 | 4.62532800  |
| H | 1.95120700  | 6.92195100 | 5.11172100  |
| N | -2.28375800 | 3.55836200 | 1.25542700  |
| C | 2.34949700  | 3.53351900 | 2.73830200  |
| C | 1.64449700  | 2.77624900 | 1.78726800  |
| C | 3.68027000  | 3.93314400 | 2.53620400  |
| C | 2.27523300  | 2.49592400 | 0.56511700  |
| H | 0.61817100  | 2.46152300 | 1.98395900  |
| C | 4.28617100  | 3.63822800 | 1.30381400  |
| H | 4.23043800  | 4.47162200 | 3.30965500  |
| C | 3.58846800  | 2.92688700 | 0.31514700  |
| H | 1.72276500  | 1.93152500 | -0.19319700 |
| H | 4.07054200  | 2.69766500 | -0.63992900 |
| I | 1.69903400  | 3.16184900 | 5.00967600  |
| H | 5.31624400  | 3.96618400 | 1.12860000  |



**T2-A2-TS4-5**

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -2.82009400 | 4.97608700 | -0.63714100 |
| C | -1.92190700 | 5.94297800 | -0.21064600 |
| C | -1.15159300 | 5.74581000 | 0.96536400  |
| C | -1.35221300 | 4.51176400 | 1.72351900  |
| C | -2.91940200 | 3.80096500 | 0.14683300  |
| H | -3.42156500 | 5.10177700 | -1.54071600 |
| H | -1.78830900 | 6.87308100 | -0.77723000 |

|    |             |            |             |
|----|-------------|------------|-------------|
| H  | -3.60589900 | 3.00086200 | -0.16761700 |
| O  | -0.75244400 | 4.23012700 | 2.82913700  |
| C  | -0.23865100 | 6.79056900 | 1.32300600  |
| H  | -0.26374500 | 7.68918600 | 0.67938200  |
| N  | 0.62879300  | 6.80358700 | 2.30307800  |
| Pd | 0.99103600  | 5.23118200 | 3.52441000  |
| C  | 1.47829600  | 7.99422800 | 2.55369800  |
| C  | 0.74707300  | 8.94803200 | 3.51256700  |
| H  | 0.48628800  | 8.43402600 | 4.45183400  |
| H  | 1.38341400  | 9.81690700 | 3.74989200  |
| H  | -0.18813200 | 9.31330200 | 3.05769300  |
| C  | 2.79261200  | 7.44027400 | 3.12540100  |
| H  | 3.33939800  | 6.92284600 | 2.31653100  |
| H  | 3.43443300  | 8.27276800 | 3.47789600  |
| C  | 2.48775400  | 6.44660600 | 4.24766300  |
| H  | 3.37078900  | 5.87628600 | 4.57348200  |
| H  | 2.03499400  | 6.92245800 | 5.13609100  |
| N  | -2.23412800 | 3.56001200 | 1.26336300  |
| C  | 2.31919800  | 3.54203400 | 2.73524900  |
| C  | 1.58109200  | 2.77480600 | 1.81815800  |
| C  | 3.64381900  | 3.93411500 | 2.48517600  |
| C  | 2.17061800  | 2.47656100 | 0.57981100  |
| H  | 0.56123400  | 2.46422300 | 2.05146400  |
| C  | 4.20833000  | 3.62073300 | 1.23763700  |
| H  | 4.22093300  | 4.48053500 | 3.23288200  |
| C  | 3.47641300  | 2.89928100 | 0.28168500  |
| H  | 1.59159900  | 1.90431900 | -0.15231900 |
| H  | 3.92629400  | 2.65604500 | -0.68554400 |
| I  | 1.74263900  | 3.18292800 | 5.03558700  |
| H  | 5.23302800  | 3.94300700 | 1.02457000  |
| H  | 1.65578300  | 8.51447000 | 1.59096200  |



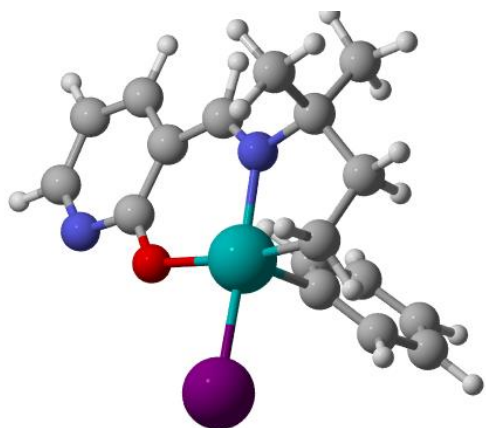
**T2-A1-TS4-5**

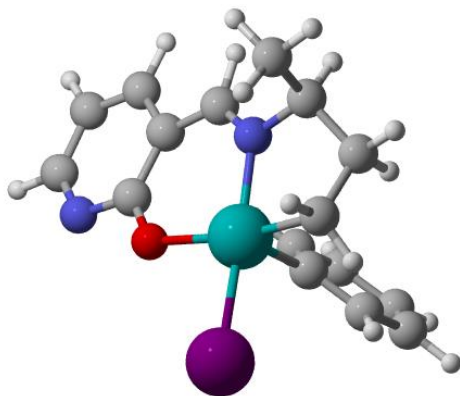
|   |             |            |             |
|---|-------------|------------|-------------|
| C | -2.87175900 | 5.00688800 | -0.61194700 |
| C | -1.96551100 | 5.96651100 | -0.18686600 |

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | -1.17710000 | 5.75345000 | 0.97476400  |
| C  | -1.36582500 | 4.50795800 | 1.71775500  |
| C  | -2.96083600 | 3.82162000 | 0.15806500  |
| H  | -3.48761700 | 5.14579100 | -1.50380600 |
| H  | -1.83981100 | 6.90396600 | -0.74302300 |
| H  | -3.65481100 | 3.02746300 | -0.15505300 |
| O  | -0.74636700 | 4.20691500 | 2.80727500  |
| C  | -0.25682500 | 6.79328100 | 1.32771400  |
| H  | -0.28348700 | 7.69302400 | 0.68614200  |
| N  | 0.61732000  | 6.79928100 | 2.30204500  |
| Pd | 0.98637400  | 5.21736600 | 3.51271600  |
| C  | 1.49733900  | 7.95922800 | 2.53895900  |
| C  | 2.80868600  | 7.40703700 | 3.10032500  |
| H  | 3.34942800  | 6.86782600 | 2.30124300  |
| H  | 3.45898100  | 8.23720100 | 3.44185300  |
| C  | 2.46924200  | 6.44673300 | 4.24093300  |
| H  | 3.33606400  | 5.88625900 | 4.62308600  |
| H  | 1.97693300  | 6.96328100 | 5.08722300  |
| N  | -2.25727300 | 3.56432700 | 1.25920600  |
| C  | 2.33640600  | 3.53960100 | 2.73757600  |
| C  | 1.61318400  | 2.77608700 | 1.80562700  |
| C  | 3.66411700  | 3.93490800 | 2.50938800  |
| C  | 2.22212100  | 2.48399300 | 0.57519300  |
| H  | 0.59001900  | 2.46421800 | 2.02250500  |
| C  | 4.24812000  | 3.62794100 | 1.26933000  |
| H  | 4.22848100  | 4.47861400 | 3.26882500  |
| C  | 3.53190100  | 2.90949700 | 0.29921700  |
| H  | 1.65533200  | 1.91455200 | -0.16860800 |
| H  | 3.99699100  | 2.67082900 | -0.66193100 |
| I  | 1.73419000  | 3.17058900 | 5.02746100  |
| H  | 5.27566100  | 3.95205200 | 1.07342700  |
| H  | 1.62513800  | 8.54810400 | 1.61108300  |
| H  | 1.01586800  | 8.61051000 | 3.29537800  |

### T2-A3-Int5

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.17440600 | 0.25085700  | -3.26194500 |
| C  | -3.15917100 | 1.14099700  | -2.95964900 |
| C  | -2.27238100 | 0.88604300  | -1.87547000 |
| C  | -2.46838800 | -0.33842000 | -1.09756600 |
| C  | -4.28995400 | -0.90144800 | -2.44041600 |
| H  | -4.86731000 | 0.42136200  | -4.08943000 |
| H  | -3.02181900 | 2.05748100  | -3.54687200 |
| H  | -5.09057100 | -1.62761600 | -2.64379200 |
| O  | -1.73337500 | -0.69154000 | -0.10156600 |
| C  | -1.28081900 | 1.88702500  | -1.61737800 |
| H  | -1.34587200 | 2.77554000  | -2.26669100 |
| N  | -0.32072500 | 1.87883300  | -0.72655400 |
| Pd | 0.05480900  | 0.28836700  | 0.50085800  |
| C  | 0.60310600  | 3.05271500  | -0.55988700 |
| C  | 0.98151500  | 3.68750800  | -1.91043100 |
| H  | 0.14128300  | 4.22457300  | -2.38120000 |
| H  | 1.78540500  | 4.42437200  | -1.75126400 |
| H  | 1.35018600  | 2.91723000  | -2.60770400 |
| C  | -0.11564900 | 4.07343200  | 0.34721100  |
| H  | -0.39304600 | 3.62173900  | 1.31293100  |
| H  | 0.53909900  | 4.93949300  | 0.54011900  |
| H  | -1.03890900 | 4.43569500  | -0.13496400 |
| C  | 1.86720400  | 2.48615200  | 0.12213100  |
| H  | 2.47395900  | 1.96187000  | -0.63645600 |
| H  | 2.47834600  | 3.32819800  | 0.50315100  |
| C  | 1.52397300  | 1.51681700  | 1.24621900  |
| H  | 2.38616700  | 0.94837300  | 1.61803300  |
| H  | 1.00899500  | 1.98859900  | 2.10230200  |
| N  | -3.49733500 | -1.19701300 | -1.41552100 |
| C  | 1.35615300  | -0.53697100 | -0.80542200 |
| C  | 0.85194600  | -0.73126700 | -2.09351800 |
| C  | 2.66521700  | -0.88644800 | -0.45752100 |
| C  | 1.70209200  | -1.27913800 | -3.07321300 |
| H  | -0.17586500 | -0.47161200 | -2.35589800 |
| C  | 3.49816700  | -1.43159200 | -1.45216500 |
| H  | 3.03306500  | -0.77112600 | 0.56256200  |
| C  | 3.02318400  | -1.62505400 | -2.75729700 |
| H  | 1.31304800  | -1.43086400 | -4.08547600 |
| H  | 3.67760700  | -2.05260000 | -3.52314400 |
| I  | 0.50214100  | -1.52314200 | 2.35430800  |
| H  | 4.52102900  | -1.71750500 | -1.18552500 |

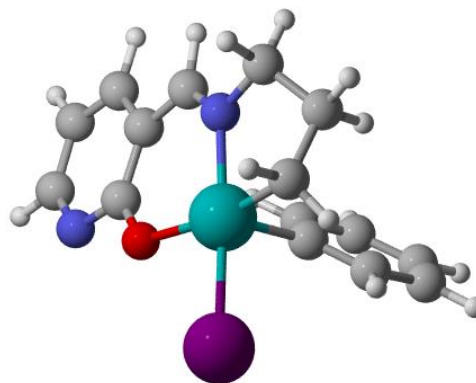




### T2-A2-Int5

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.12742400 | 0.22129600  | -3.34626400 |
| C  | -3.11977200 | 1.12599800  | -3.06298800 |
| C  | -2.26769500 | 0.92835200  | -1.94003100 |
| C  | -2.48516200 | -0.25599400 | -1.10469300 |
| C  | -4.27406600 | -0.88188100 | -2.46383400 |
| H  | -4.79510100 | 0.34675500  | -4.20205900 |
| H  | -2.96355000 | 2.01036900  | -3.69300900 |
| H  | -5.07458900 | -1.61321600 | -2.64809700 |
| O  | -1.77097400 | -0.56508000 | -0.07941600 |
| C  | -1.29251500 | 1.94433900  | -1.68598600 |
| H  | -1.32744600 | 2.82052700  | -2.35900500 |
| N  | -0.37252600 | 1.96393600  | -0.75429000 |
| Pd | 0.03657700  | 0.40672300  | 0.49981500  |
| C  | 0.50391100  | 3.14830000  | -0.57158200 |
| C  | -0.21282500 | 4.16815600  | 0.32992800  |
| H  | -0.45297300 | 3.72644800  | 1.31074500  |
| H  | 0.42706500  | 5.05154200  | 0.49044700  |
| H  | -1.15733300 | 4.50059800  | -0.13072300 |
| C  | 1.81702000  | 2.62441000  | 0.03206900  |
| H  | 2.39202100  | 2.10093800  | -0.75025500 |
| H  | 2.43261500  | 3.47616400  | 0.38212500  |
| C  | 1.52852800  | 1.65702800  | 1.17940300  |
| H  | 2.40946200  | 1.09774000  | 1.51842900  |
| H  | 1.04630900  | 2.13207300  | 2.05205600  |
| N  | -3.51288400 | -1.12374500 | -1.40177600 |
| C  | 1.32994100  | -0.47022000 | -0.78492400 |
| C  | 0.81229400  | -0.71520700 | -2.05846900 |
| C  | 2.64149300  | -0.81089000 | -0.43682600 |
| C  | 1.65003100  | -1.30566900 | -3.02404900 |
| H  | -0.21679400 | -0.46253200 | -2.32212000 |
| C  | 3.46233000  | -1.39829900 | -1.41728100 |
| H  | 3.02096800  | -0.65917000 | 0.57410400  |

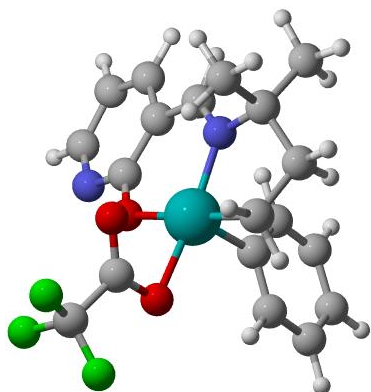
|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.97314700 | -1.64333900 | -2.70830500 |
| H | 1.24932700 | -1.49668000 | -4.02500800 |
| H | 3.61796800 | -2.10435300 | -3.46278900 |
| I | 0.50376600 | -1.35257100 | 2.39489400  |
| H | 4.48689900 | -1.67682500 | -1.14945500 |
| H | 0.68958100 | 3.60684500  | -1.56284500 |



### T2-A1-Int5

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.11280500 | 0.46655100  | -3.35437900 |
| C  | -3.09080700 | 1.35265000  | -3.06403100 |
| C  | -2.23298500 | 1.12541400  | -1.95096600 |
| C  | -2.45999500 | -0.07026900 | -1.13413200 |
| C  | -4.26804300 | -0.64882000 | -2.48907100 |
| H  | -4.78521900 | 0.61554700  | -4.20263300 |
| H  | -2.92763800 | 2.24510100  | -3.68071400 |
| H  | -5.08014100 | -1.36586200 | -2.67854100 |
| O  | -1.74150100 | -0.40804500 | -0.12076100 |
| C  | -1.24167000 | 2.12430000  | -1.69091600 |
| H  | -1.26781800 | 3.00860200  | -2.35319500 |
| N  | -0.31748800 | 2.11733900  | -0.76324200 |
| Pd | 0.08129500  | 0.53101700  | 0.46146200  |
| C  | 0.59728100  | 3.26015500  | -0.57499700 |
| C  | 1.90652400  | 2.71950800  | 0.00453200  |
| H  | 2.47047500  | 2.18898400  | -0.78120100 |
| H  | 2.53530900  | 3.55975000  | 0.35817200  |
| C  | 1.58645700  | 1.76115400  | 1.15097000  |
| H  | 2.44952300  | 1.19240200  | 1.51960900  |
| H  | 1.08486800  | 2.26085100  | 2.00117800  |
| N  | -3.50183800 | -0.91860900 | -1.43742800 |
| C  | 1.35456600  | -0.34286300 | -0.84417500 |
| C  | 0.82224800  | -0.57301500 | -2.11436600 |
| C  | 2.66825900  | -0.69191700 | -0.51322100 |
| C  | 1.64716200  | -1.15809900 | -3.09421500 |
| H  | -0.20811100 | -0.31220200 | -2.36464000 |
| C  | 3.47612800  | -1.27366800 | -1.50765400 |

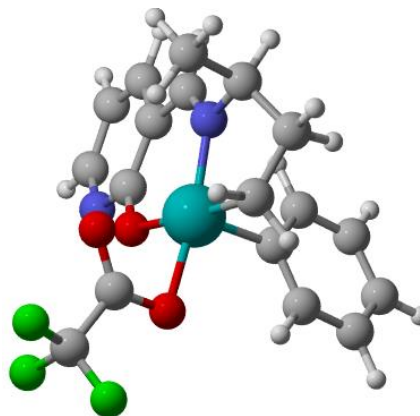
|   |            |             |             |
|---|------------|-------------|-------------|
| H | 3.05929600 | -0.54903400 | 0.49462400  |
| C | 2.97189400 | -1.50484200 | -2.79553600 |
| H | 1.23514200 | -1.33781200 | -4.09266400 |
| H | 3.60656000 | -1.96180900 | -3.56100200 |
| I | 0.54371000 | -1.26751800 | 2.31980800  |
| H | 4.50250900 | -1.55847400 | -1.25368300 |
| H | 0.73721700 | 3.80497400  | -1.52695800 |
| H | 0.12759200 | 3.95336700  | 0.15024300  |



### T2-A3-Int6

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.94966500 | -0.44801000 | -3.50604500 |
| C  | -3.02354800 | 0.55736500  | -3.29137500 |
| C  | -2.12017400 | 0.48686500  | -2.19328900 |
| C  | -2.22385200 | -0.65956900 | -1.28759300 |
| C  | -3.94984100 | -1.53156700 | -2.58938000 |
| H  | -4.65070200 | -0.42132400 | -4.34362000 |
| H  | -2.96633100 | 1.42098400  | -3.96546100 |
| H  | -4.66185200 | -2.35723400 | -2.73438600 |
| O  | -1.51498600 | -0.80919700 | -0.22381000 |
| C  | -1.19592900 | 1.57030600  | -2.06230800 |
| H  | -1.33187600 | 2.39036500  | -2.78405300 |
| N  | -0.19404900 | 1.70024800  | -1.22749200 |
| Pd | 0.20471800  | 0.35897500  | 0.19267800  |
| C  | 0.67248400  | 2.92906800  | -1.17271000 |
| C  | 0.86485700  | 3.56421000  | -2.55990600 |
| H  | -0.05599300 | 4.03224400  | -2.94564400 |
| H  | 1.62248600  | 4.36079300  | -2.48608300 |
| H  | 1.22074600  | 2.81637100  | -3.28793700 |
| C  | -0.00618100 | 3.91567100  | -0.19890100 |
| H  | -0.20095800 | 3.44128500  | 0.77555100  |
| H  | 0.63476300  | 4.79977800  | -0.04458800 |
| H  | -0.97267300 | 4.25256400  | -0.60913400 |
| C  | 2.02342100  | 2.42460500  | -0.62269400 |
| H  | 2.52188000  | 1.83416700  | -1.41170000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.67102000  | 3.29453100  | -0.39906800 |
| C | 1.82307200  | 1.55480800  | 0.61197200  |
| H | 2.68602700  | 0.91671000  | 0.84859600  |
| H | 1.49683600  | 2.10911700  | 1.50650900  |
| N | -3.14486400 | -1.65042700 | -1.53820000 |
| C | 1.36384800  | -0.73746900 | -1.02073900 |
| C | 2.31638000  | -1.53015300 | -0.37153100 |
| C | 1.18380100  | -0.78127000 | -2.40634300 |
| C | 3.12287100  | -2.38527800 | -1.14427100 |
| H | 2.41288200  | -1.50856000 | 0.71713000  |
| C | 1.99786300  | -1.64561500 | -3.16275000 |
| H | 0.41564000  | -0.18880200 | -2.90529300 |
| C | 2.96924700  | -2.44019400 | -2.53765200 |
| H | 3.59890900  | -3.10818200 | -3.13348400 |
| H | 1.85731000  | -1.69417500 | -4.24778800 |
| O | 0.52836400  | -0.76152700 | 1.94186800  |
| C | -0.23194600 | -0.02924400 | 2.68940100  |
| C | -0.44646100 | -0.52919600 | 4.13670300  |
| F | 0.67788100  | -1.11181300 | 4.62148100  |
| F | -0.78251000 | 0.49609300  | 4.95221200  |
| F | -1.44722100 | -1.44425000 | 4.16224100  |
| O | -0.80457700 | 1.01455400  | 2.28466700  |
| H | 3.86714900  | -3.01260700 | -0.64274400 |



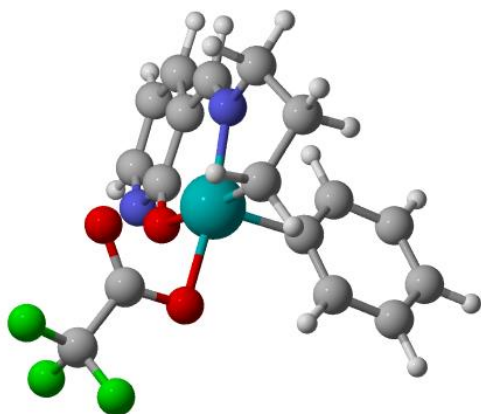
### T2-A2-Int6

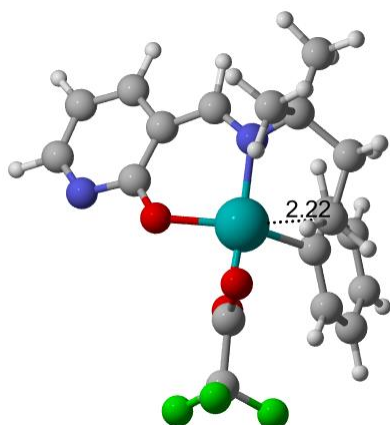
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.90064300 | -0.36726200 | -3.51605100 |
| C | -2.98921200 | 0.64567700  | -3.27666200 |
| C | -2.06247300 | 0.54371000  | -2.20093600 |
| C | -2.12226000 | -0.64522800 | -1.34507600 |
| C | -3.86285300 | -1.48894700 | -2.64672000 |
| H | -4.62001300 | -0.31783500 | -4.33686800 |
| H | -2.96259700 | 1.53957700  | -3.91192400 |
| H | -4.56465600 | -2.31952000 | -2.81201200 |
| O | -1.38367700 | -0.83308800 | -0.30773500 |
| C | -1.15915100 | 1.63690700  | -2.02759200 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -1.31189000 | 2.50406400  | -2.69363600 |
| N  | -0.15025900 | 1.73229200  | -1.19710500 |
| Pd | 0.34513900  | 0.32566500  | 0.12010400  |
| C  | 0.66979000  | 2.96722500  | -1.08332800 |
| C  | 0.01227000  | 3.91021700  | -0.06148700 |
| H  | -0.11378900 | 3.40721500  | 0.91062800  |
| H  | 0.63236900  | 4.81099800  | 0.07960000  |
| H  | -0.98517800 | 4.22399800  | -0.40974100 |
| C  | 2.07139600  | 2.49433000  | -0.66628600 |
| H  | 2.53769800  | 1.96906300  | -1.51734700 |
| H  | 2.70505100  | 3.36880900  | -0.42289900 |
| C  | 1.96206000  | 1.54057500  | 0.52255600  |
| H  | 2.85165300  | 0.91281300  | 0.67086600  |
| H  | 1.67151100  | 2.02890800  | 1.46641000  |
| N  | -3.03351000 | -1.63919400 | -1.61888200 |
| C  | 1.47223500  | -0.68366700 | -1.19592600 |
| C  | 2.46806500  | -1.48593700 | -0.62856300 |
| C  | 1.23034600  | -0.66435400 | -2.57214900 |
| C  | 3.25380600  | -2.28674100 | -1.47709300 |
| H  | 2.61395100  | -1.51413800 | 0.45435800  |
| C  | 2.02451900  | -1.47532800 | -3.40509400 |
| H  | 0.43027900  | -0.06426700 | -3.00799200 |
| C  | 3.03740800  | -2.27895800 | -2.86314700 |
| H  | 3.65110500  | -2.90510600 | -3.51813400 |
| H  | 1.83556500  | -1.47472000 | -4.48381400 |
| O  | 0.77387800  | -0.88161400 | 1.78426800  |
| C  | 0.04014300  | -0.20894700 | 2.61090300  |
| C  | -0.08504300 | -0.79433200 | 4.03659800  |
| F  | 1.08197100  | -1.36012300 | 4.43286300  |
| F  | -0.41500600 | 0.17164100  | 4.92345400  |
| F  | -1.05077800 | -1.74636700 | 4.05865200  |
| O  | -0.57300800 | 0.84245300  | 2.29650000  |
| H  | 4.03173500  | -2.92147500 | -1.04013900 |
| H  | 0.69980300  | 3.45638900  | -2.07677100 |

## T2-A1-Int6

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.92679500 | -0.18274900 | -3.49553600 |
| C  | -3.00364900 | 0.81920800  | -3.25675400 |
| C  | -2.06712700 | 0.70027300  | -2.19053500 |
| C  | -2.12735300 | -0.49787900 | -1.34686300 |
| C  | -3.89043500 | -1.31287800 | -2.63676400 |
| H  | -4.65453900 | -0.11888200 | -4.30790900 |
| H  | -2.97562200 | 1.71847000  | -3.88433000 |
| H  | -4.60262800 | -2.13468700 | -2.80134700 |
| O  | -1.37621800 | -0.70646800 | -0.32317000 |
| C  | -1.15079500 | 1.78334700  | -2.02371800 |
| H  | -1.29208700 | 2.64489600  | -2.69906000 |
| N  | -0.14354700 | 1.87424600  | -1.18984800 |
| Pd | 0.34145400  | 0.45914100  | 0.12642700  |
| C  | 0.72065400  | 3.07113900  | -1.11539700 |
| C  | 2.10453000  | 2.60128500  | -0.66199800 |
| H  | 2.58736700  | 2.04091500  | -1.48072900 |
| H  | 2.74183200  | 3.47543400  | -0.42772400 |
| C  | 1.93134700  | 1.69810200  | 0.55803500  |
| H  | 2.81227400  | 1.08640000  | 0.79760000  |
| H  | 1.57000500  | 2.23584300  | 1.45134800  |
| N  | -3.05064000 | -1.48099900 | -1.62061200 |
| C  | 1.49076800  | -0.53107200 | -1.18413600 |
| C  | 2.52113900  | -1.29141300 | -0.62121100 |
| C  | 1.22718200  | -0.53943500 | -2.55649700 |
| C  | 3.32219500  | -2.07518600 | -1.47141600 |
| H  | 2.68166900  | -1.30292300 | 0.45983100  |
| C  | 2.03667900  | -1.33336700 | -3.39096400 |
| H  | 0.39918500  | 0.02595700  | -2.98733800 |
| C  | 3.08552600  | -2.09320100 | -2.85403700 |
| H  | 3.71115900  | -2.70623500 | -3.51011400 |
| H  | 1.83117200  | -1.35484700 | -4.46642200 |
| O  | 0.77047600  | -0.77234900 | 1.76658400  |
| C  | 0.01726400  | -0.13215400 | 2.60313500  |
| C  | -0.10778900 | -0.75909800 | 4.01115200  |
| F  | 1.08324100  | -1.26215100 | 4.42276600  |
| F  | -0.51749400 | 0.16139300  | 4.91200800  |
| F  | -1.01213200 | -1.76950700 | 3.98630000  |
| O  | -0.60788700 | 0.91689100  | 2.31016200  |
| H  | 4.12785700  | -2.67710100 | -1.03829100 |
| H  | 0.73173400  | 3.59238100  | -2.09005500 |
| H  | 0.28930000  | 3.75559900  | -0.35953100 |

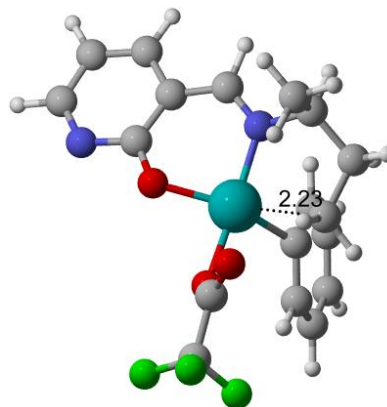




### T2-A3-TS6-7

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.96119300 | -0.28105500 | -3.26562100 |
| C  | -2.86576500 | 0.56991500  | -3.25362600 |
| C  | -2.04184700 | 0.65740900  | -2.10198200 |
| C  | -2.40138000 | -0.13745700 | -0.93831300 |
| C  | -4.22671400 | -1.00784500 | -2.08035700 |
| H  | -4.60465600 | -0.38383500 | -4.14255300 |
| H  | -2.61815100 | 1.18211000  | -4.12904500 |
| H  | -5.09121500 | -1.68558300 | -2.04324900 |
| O  | -1.76052200 | -0.11261000 | 0.19756100  |
| C  | -0.99603000 | 1.63715500  | -2.08935100 |
| H  | -1.04690100 | 2.40903700  | -2.87236000 |
| N  | -0.02322900 | 1.72520500  | -1.21918600 |
| Pd | 0.19847300  | 0.39916600  | 0.28032000  |
| C  | 0.78566400  | 2.97763500  | -1.05082900 |
| C  | 0.95542600  | 3.75401800  | -2.36756300 |
| H  | 0.01280100  | 4.20715400  | -2.71558300 |
| H  | 1.66813400  | 4.57826200  | -2.20522700 |
| H  | 1.35884100  | 3.10635300  | -3.16432800 |
| C  | 0.03614100  | 3.83646800  | -0.00559800 |
| H  | -0.10602500 | 3.28740000  | 0.93920100  |
| H  | 0.60593700  | 4.75748400  | 0.20307000  |
| H  | -0.95902500 | 4.11634700  | -0.38836400 |
| C  | 2.16970800  | 2.55189900  | -0.51317900 |
| H  | 2.79036600  | 2.16945000  | -1.34178300 |
| H  | 2.68018100  | 3.45294400  | -0.12377000 |
| C  | 2.09289600  | 1.52016700  | 0.59707900  |
| H  | 3.07696700  | 1.19357700  | 0.94746400  |
| H  | 1.52407500  | 1.84312100  | 1.49188500  |
| N  | -3.50354800 | -0.94466300 | -0.96116100 |
| C  | 2.07925700  | -0.32441900 | -0.29218400 |
| C  | 2.68760800  | -1.30463700 | 0.51793800  |
| C  | 2.29497900  | -0.32032500 | -1.68350400 |

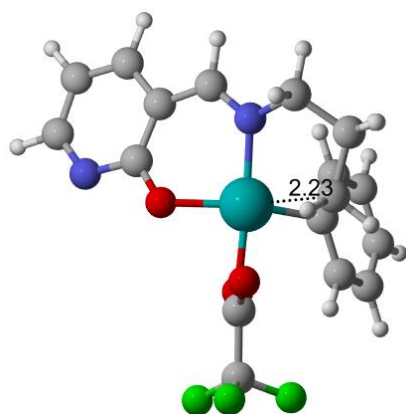
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.49286600  | -2.28466500 | -0.07719500 |
| H | 2.50802900  | -1.31592300 | 1.59470700  |
| C | 3.10390200  | -1.31250400 | -2.26467000 |
| H | 1.81037100  | 0.42320100  | -2.31977500 |
| C | 3.70787700  | -2.29333600 | -1.46637300 |
| H | 4.33896300  | -3.06264400 | -1.92156000 |
| H | 3.24672900  | -1.31604400 | -3.35026500 |
| O | 0.30300800  | -0.78690200 | 1.95833200  |
| C | 0.26443200  | -0.05438100 | 3.03630200  |
| C | 0.46210300  | -0.94037200 | 4.30088300  |
| F | 1.75851500  | -1.38654900 | 4.32198900  |
| F | 0.24655700  | -0.24182400 | 5.43510400  |
| F | -0.34934600 | -2.02394300 | 4.30437500  |
| O | 0.17254900  | 1.17523900  | 3.14236400  |
| H | 3.95615800  | -3.04738400 | 0.55694800  |



### T2-A2-TS6-7

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.02352900 | -0.19958900 | -3.24711500 |
| C  | -2.92545000 | 0.64702900  | -3.22589200 |
| C  | -2.07777300 | 0.68801300  | -2.08847600 |
| C  | -2.41508800 | -0.15071400 | -0.94764700 |
| C  | -4.26490000 | -0.97362100 | -2.08631400 |
| H  | -4.68632300 | -0.26617400 | -4.11304900 |
| H  | -2.69354700 | 1.29153400  | -4.08210100 |
| H  | -5.12944800 | -1.65172400 | -2.05845200 |
| O  | -1.75449200 | -0.17279700 | 0.17679600  |
| C  | -1.02338000 | 1.65504100  | -2.05873500 |
| H  | -1.06246700 | 2.46172700  | -2.81167700 |
| N  | -0.04233200 | 1.70417000  | -1.19405800 |
| Pd | 0.19704500  | 0.36950500  | 0.28625100  |
| C  | 0.75323400  | 2.94592400  | -1.02421300 |
| C  | 0.00142500  | 3.87018000  | -0.04754500 |
| H  | -0.14205400 | 3.37732000  | 0.92829200  |
| H  | 0.57081400  | 4.80171000  | 0.10681500  |

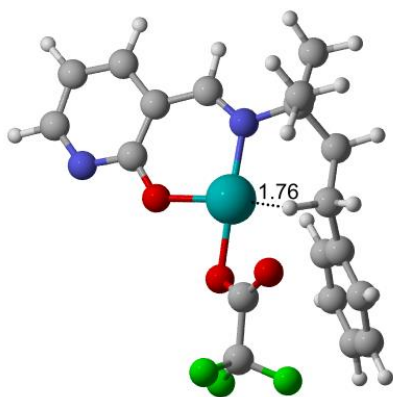
|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| H | -0.99299300 | 4.12705300  | -0.44665900 | H  | -4.73215500 | -0.23018200 | -4.09254400 |
| C | 2.14853300  | 2.56102800  | -0.50643200 | H  | -2.72753600 | 1.31158700  | -4.06929700 |
| H | 2.77137800  | 2.17536200  | -1.33038700 | H  | -5.17044400 | -1.62264500 | -2.04145900 |
| H | 2.65009300  | 3.46930200  | -0.12302200 | O  | -1.76297600 | -0.18857600 | 0.17155500  |
| C | 2.07355500  | 1.53460500  | 0.61377300  | C  | -1.03701100 | 1.65010500  | -2.06329900 |
| H | 3.05591700  | 1.22042200  | 0.97927300  | H  | -1.06834100 | 2.44601600  | -2.82766200 |
| H | 1.48601400  | 1.85459300  | 1.49742400  | N  | -0.05479600 | 1.69955000  | -1.19941900 |
| N | -3.51837300 | -0.95631400 | -0.98126600 | Pd | 0.18351500  | 0.36684200  | 0.28683300  |
| C | 2.09508800  | -0.31925900 | -0.27484400 | C  | 0.77800200  | 2.91155700  | -1.07016100 |
| C | 2.72377600  | -1.28171500 | 0.54055600  | C  | 2.16082400  | 2.55216000  | -0.51998100 |
| C | 2.31229200  | -0.31555800 | -1.66573600 | H  | 2.80884100  | 2.15094200  | -1.31642100 |
| C | 3.55181100  | -2.24586100 | -0.04941900 | H  | 2.64393800  | 3.47231500  | -0.14213100 |
| H | 2.54317500  | -1.29360900 | 1.61704800  | C  | 2.04562300  | 1.55262700  | 0.62176500  |
| C | 3.14376700  | -1.29218000 | -2.24164300 | H  | 3.00920800  | 1.25133300  | 1.04364900  |
| H | 1.81282000  | 0.41463100  | -2.30614300 | H  | 1.41467400  | 1.90168600  | 1.46626300  |
| C | 3.76855500  | -2.25562900 | -1.43825000 | N  | -3.54435600 | -0.94731900 | -0.97439900 |
| H | 4.41752600  | -3.01236900 | -1.88932100 | C  | 2.09853300  | -0.30384500 | -0.25165900 |
| H | 3.28805500  | -1.29705300 | -3.32700100 | C  | 2.74217500  | -1.24743900 | 0.57398600  |
| O | 0.31141800  | -0.82954800 | 1.95212700  | C  | 2.31267900  | -0.31726500 | -1.64328700 |
| C | 0.26664000  | -0.10693700 | 3.03698400  | C  | 3.58256500  | -2.20761800 | -0.00482700 |
| C | 0.47985100  | -1.00129800 | 4.29305500  | H  | 2.56558800  | -1.25022200 | 1.65097000  |
| F | 1.78683400  | -1.41647100 | 4.31395800  | C  | 3.15581500  | -1.29012700 | -2.20850800 |
| F | 0.24424600  | -0.31965900 | 5.43344600  | H  | 1.80228700  | 0.39670300  | -2.29330100 |
| F | -0.30510600 | -2.10398700 | 4.28281800  | C  | 3.79604300  | -2.23357600 | -1.39383400 |
| O | 0.16060100  | 1.12023400  | 3.15393800  | H  | 4.45448700  | -2.98724900 | -1.83621000 |
| H | 4.03145700  | -2.99506600 | 0.58863300  | H  | 3.29678900  | -1.30789000 | -3.29413100 |
| H | 0.83386100  | 3.44268200  | -2.01138900 | O  | 0.29518000  | -0.85406100 | 1.93259300  |



|    |             |             |             |   |             |             |             |
|----|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H  | -4.73215500 | -0.23018200 | -4.09254400 | H | 0.29518000  | -0.85406100 | 1.93259300  |
| H  | -2.72753600 | 1.31158700  | -4.06929700 | C | 0.27077500  | -0.15487500 | 3.03434000  |
| H  | -5.17044400 | -1.62264500 | -2.04145900 | C | 0.49463500  | -1.07995000 | 4.26636700  |
| O  | -1.76297600 | -0.18857600 | 0.17155500  | F | 1.80903700  | -1.47425800 | 4.27773400  |
| C  | -1.03701100 | 1.65010500  | -2.06329900 | F | 0.24798500  | -0.43240800 | 5.42400400  |
| H  | -1.06834100 | 2.44601600  | -2.82766200 | F | -0.27145200 | -2.19481700 | 4.22708400  |
| N  | -0.05479600 | 1.69955000  | -1.19941900 | O | 0.17890100  | 1.06887500  | 3.18146400  |
| Pd | 0.18351500  | 0.36684200  | 0.28683300  | H | 4.07425900  | -2.94099900 | 0.64230200  |
| C  | 0.77800200  | 2.91155700  | -1.07016100 | H | 0.83151800  | 3.43943100  | -2.04063500 |
| C  | 2.16082400  | 2.55216000  | -0.51998100 | H | 0.26370400  | 3.57663900  | -0.35035900 |
| H  | 2.80884100  | 2.15094200  | -1.31642100 |   |             |             |             |
| H  | 2.64393800  | 3.47231500  | -0.14213100 |   |             |             |             |
| C  | 2.04562300  | 1.55262700  | 0.62176500  |   |             |             |             |
| H  | 3.00920800  | 1.25133300  | 1.04364900  |   |             |             |             |
| H  | 1.41467400  | 1.90168600  | 1.46626300  |   |             |             |             |
| N  | -3.54435600 | -0.94731900 | -0.97439900 |   |             |             |             |
| C  | 2.09853300  | -0.30384500 | -0.25165900 |   |             |             |             |
| C  | 2.74217500  | -1.24743900 | 0.57398600  |   |             |             |             |
| C  | 2.31267900  | -0.31726500 | -1.64328700 |   |             |             |             |
| C  | 3.58256500  | -2.20761800 | -0.00482700 |   |             |             |             |
| H  | 2.56558800  | -1.25022200 | 1.65097000  |   |             |             |             |
| C  | 3.15581500  | -1.29012700 | -2.20850800 |   |             |             |             |
| H  | 1.80228700  | 0.39670300  | -2.29330100 |   |             |             |             |
| C  | 3.79604300  | -2.23357600 | -1.39383400 |   |             |             |             |
| H  | 4.45448700  | -2.98724900 | -1.83621000 |   |             |             |             |
| H  | 3.29678900  | -1.30789000 | -3.29413100 |   |             |             |             |
| O  | 0.29518000  | -0.85406100 | 1.93259300  |   |             |             |             |
| C  | 0.27077500  | -0.15487500 | 3.03434000  |   |             |             |             |
| C  | 0.49463500  | -1.07995000 | 4.26636700  |   |             |             |             |
| F  | 1.80903700  | -1.47425800 | 4.27773400  |   |             |             |             |
| F  | 0.24798500  | -0.43240800 | 5.42400400  |   |             |             |             |
| F  | -0.27145200 | -2.19481700 | 4.22708400  |   |             |             |             |
| O  | 0.17890100  | 1.06887500  | 3.18146400  |   |             |             |             |
| H  | 4.07425900  | -2.94099900 | 0.64230200  |   |             |             |             |
| H  | 0.83151800  | 3.43943100  | -2.04063500 |   |             |             |             |
| H  | 0.26370400  | 3.57663900  | -0.35035900 |   |             |             |             |

### T2-A1-TS6-7

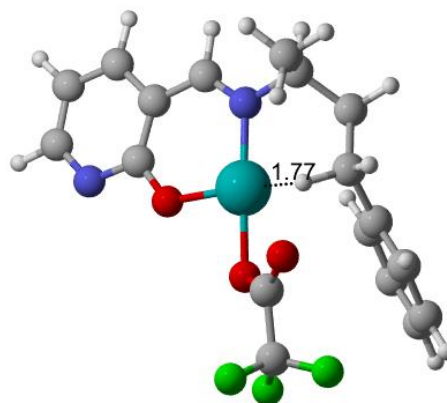
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.06180600 | -0.17369100 | -3.23174700 |
| C | -2.95742000 | 0.66427800  | -3.21464800 |
| C | -2.10051000 | 0.69356700  | -2.08319700 |
| C | -2.43433000 | -0.15056700 | -0.94537800 |
| C | -4.30019800 | -0.95203200 | -2.07293700 |



### T2-A3-Int7

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.82865100 | 0.28925500  | -3.64362900 |
| C  | -3.72656500 | 1.12051400  | -3.50987500 |
| C  | -2.73018700 | 0.84671300  | -2.53592100 |
| C  | -2.91260900 | -0.32102200 | -1.69701300 |
| C  | -4.90297100 | -0.82636800 | -2.77716900 |
| H  | -5.60929100 | 0.47838100  | -4.38411600 |
| H  | -3.60594100 | 2.00107900  | -4.15213300 |
| H  | -5.75622400 | -1.51512400 | -2.84827400 |
| O  | -2.09509600 | -0.70639500 | -0.74947100 |
| C  | -1.61590400 | 1.74618700  | -2.46203900 |
| H  | -1.64022400 | 2.58585900  | -3.17146100 |
| N  | -0.59220900 | 1.66057300  | -1.65349000 |
| Pd | -0.40334700 | 0.22010300  | -0.29288400 |
| C  | 0.50403600  | 2.68885100  | -1.62997500 |
| C  | 0.60886200  | 3.46855100  | -2.95270600 |
| H  | -0.26088900 | 4.12414000  | -3.12232700 |
| H  | 1.49720000  | 4.11858600  | -2.91511200 |
| H  | 0.71794200  | 2.78764700  | -3.81348800 |
| C  | 0.21497700  | 3.65621000  | -0.46287300 |
| H  | 0.08845600  | 3.11721000  | 0.48970800  |
| H  | 1.04169700  | 4.37803300  | -0.35370700 |
| H  | -0.71468500 | 4.21590400  | -0.65593100 |
| C  | 1.81054600  | 1.89106500  | -1.41310400 |
| H  | 1.91430500  | 1.18919900  | -2.25668700 |
| H  | 2.66624300  | 2.58677500  | -1.47406400 |
| C  | 1.89239500  | 1.13114400  | -0.07579900 |
| H  | 2.30805400  | 1.80087400  | 0.70179600  |
| H  | 0.89429600  | 1.04871500  | 0.55896000  |
| N  | -3.99851100 | -1.13250700 | -1.84577400 |
| C  | 2.65981900  | -0.16885800 | -0.04826700 |
| C  | 3.38207100  | -0.50906200 | 1.11191500  |
| C  | 2.60460700  | -1.09222200 | -1.11163200 |
| C  | 4.03377500  | -1.74617600 | 1.21040200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.39186900  | 0.18341700  | 1.95913700  |
| C | 3.26580800  | -2.32321700 | -1.01923700 |
| H | 2.01371000  | -0.86578900 | -2.00543800 |
| C | 3.98185800  | -2.65461800 | 0.14286500  |
| H | 4.48597500  | -3.62295800 | 0.21930500  |
| H | 3.20693700  | -3.03353000 | -1.84969200 |
| O | -0.13951000 | -1.26714800 | 1.09295700  |
| C | 0.35473400  | -0.82720600 | 2.20871500  |
| C | 0.64937600  | -1.95501400 | 3.23844600  |
| F | 1.89094900  | -1.77681400 | 3.76871700  |
| F | -0.24976500 | -1.89391600 | 4.25674800  |
| F | 0.59997200  | -3.19637800 | 2.70596600  |
| O | 0.61365700  | 0.34375200  | 2.53481600  |
| H | 4.57226900  | -2.00252100 | 2.12733700  |

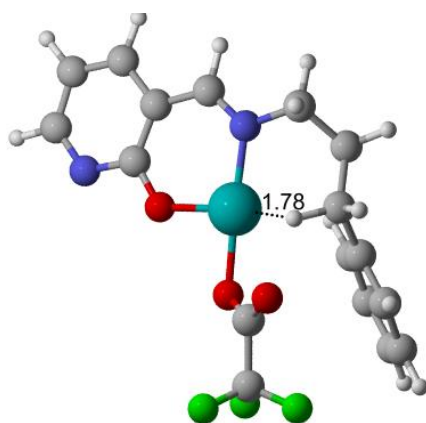


### T2-A2-Int7

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -4.81189400 | 0.37831400  | -3.75418900 |
| C  | -3.70653600 | 1.20575500  | -3.62490200 |
| C  | -2.72616300 | 0.94785900  | -2.63077600 |
| C  | -2.92522200 | -0.20161200 | -1.76818500 |
| C  | -4.90666000 | -0.71513500 | -2.86168500 |
| H  | -5.58118900 | 0.55488000  | -4.50946400 |
| H  | -3.57151400 | 2.07104000  | -4.28463100 |
| H  | -5.76497500 | -1.39810800 | -2.92657600 |
| O  | -2.12172200 | -0.57913000 | -0.80379700 |
| C  | -1.60816300 | 1.83995100  | -2.55045900 |
| H  | -1.59241700 | 2.67823300  | -3.26787700 |
| N  | -0.60821300 | 1.75304600  | -1.71343300 |
| Pd | -0.41628600 | 0.32806900  | -0.34975400 |
| C  | 0.47025900  | 2.77296400  | -1.70133200 |
| C  | 0.19438400  | 3.80906800  | -0.60033200 |
| H  | 0.11784900  | 3.32769800  | 0.38870900  |
| H  | 1.00548400  | 4.55540800  | -0.56784100 |
| H  | -0.75593700 | 4.33207200  | -0.79233000 |



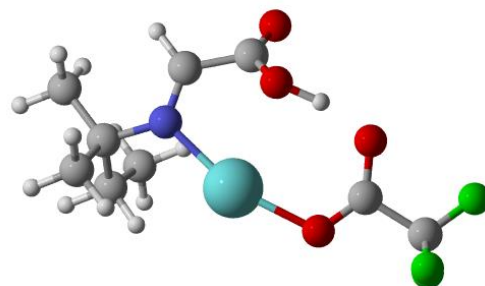
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.80267700  | 2.02493600  | -1.52887300 |
| H | 1.90745200  | 1.32094400  | -2.36972700 |
| H | 2.63670800  | 2.74444000  | -1.61030400 |
| C | 1.91944500  | 1.27052400  | -0.18747400 |
| H | 2.34565500  | 1.94107000  | 0.58300800  |
| H | 0.92457200  | 1.17730600  | 0.44409200  |
| N | -4.01652300 | -1.00606900 | -1.91175200 |
| C | 2.68190700  | -0.03237300 | -0.16960300 |
| C | 3.41803400  | -0.37426300 | 0.98141400  |
| C | 2.60424000  | -0.95901500 | -1.22867200 |
| C | 4.06264700  | -1.61549800 | 1.07446800  |
| H | 3.44463200  | 0.32055500  | 1.82634000  |
| C | 3.25816100  | -2.19435000 | -1.14182300 |
| H | 2.00204300  | -0.73191000 | -2.11471200 |
| C | 3.98885500  | -2.52693000 | 0.01077900  |
| H | 4.48710400  | -3.49859600 | 0.08317200  |
| H | 3.18207700  | -2.90698000 | -1.96886900 |
| O | -0.13246900 | -1.16034900 | 1.02563400  |
| C | 0.39644000  | -0.71972200 | 2.12592100  |
| C | 0.72318500  | -1.84707500 | 3.14610900  |
| F | 1.96628500  | -1.64923000 | 3.66487800  |
| F | -0.16663200 | -1.80931700 | 4.17385000  |
| F | 0.69125000  | -3.08580500 | 2.60565400  |
| O | 0.66148700  | 0.45243400  | 2.44135600  |
| H | 4.61228900  | -1.87280500 | 1.98445100  |
| H | 0.46955200  | 3.27877500  | -2.68689300 |



### T2-A1-Int7

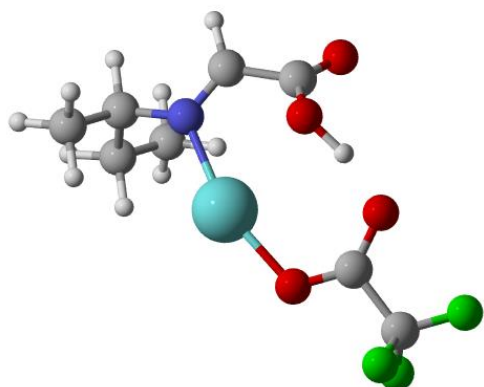
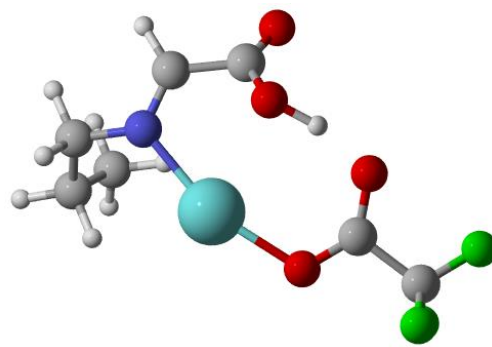
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.89146000 | 0.63206100  | -3.62353200 |
| C | -3.74929700 | 1.41475500  | -3.54835800 |
| C | -2.74711700 | 1.13599900  | -2.58162900 |
| C | -2.96312000 | 0.01120300  | -1.69082100 |
| C | -5.00074900 | -0.43913800 | -2.70595200 |
| H | -5.67840600 | 0.82647800  | -4.35586700 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | -3.60160900 | 2.26072800  | -4.23000400 |
| H  | -5.88859000 | -1.08614400 | -2.72743100 |
| O  | -2.14149200 | -0.38535700 | -0.74949400 |
| C  | -1.59014400 | 1.98021500  | -2.56160500 |
| H  | -1.55716700 | 2.79039200  | -3.30971400 |
| N  | -0.57358400 | 1.87741900  | -1.74609400 |
| Pd | -0.39889700 | 0.47678600  | -0.35309400 |
| C  | 0.56581500  | 2.81208800  | -1.81984200 |
| C  | 1.86593000  | 2.02140900  | -1.64246000 |
| H  | 1.91116000  | 1.24994100  | -2.42833100 |
| H  | 2.73024500  | 2.69041900  | -1.80086300 |
| C  | 1.98203200  | 1.37724700  | -0.24457800 |
| H  | 2.40603500  | 2.11465700  | 0.46438500  |
| H  | 0.98549600  | 1.31932500  | 0.38389700  |
| N  | -4.09080900 | -0.74936700 | -1.78133600 |
| C  | 2.74484900  | 0.08125200  | -0.12308700 |
| C  | 3.52609600  | -0.14926300 | 1.02553200  |
| C  | 2.62264300  | -0.94483400 | -1.08157300 |
| C  | 4.17398300  | -1.37801200 | 1.21356100  |
| H  | 3.58922200  | 0.62609800  | 1.79521000  |
| C  | 3.27791300  | -2.16886500 | -0.90027100 |
| H  | 1.98178100  | -0.80290000 | -1.95840000 |
| C  | 4.05490900  | -2.38944700 | 0.24896600  |
| H  | 4.55361000  | -3.35219200 | 0.39733300  |
| H  | 3.16549000  | -2.96000000 | -1.64788400 |
| O  | -0.11931200 | -1.00010600 | 1.02879000  |
| C  | 0.44321800  | -0.56091600 | 2.11460400  |
| C  | 0.77244100  | -1.69295800 | 3.12919200  |
| F  | 1.97714600  | -1.45472800 | 3.71243900  |
| F  | -0.16854600 | -1.71823700 | 4.11145200  |
| F  | 0.82107100  | -2.91935500 | 2.56023700  |
| O  | 0.72865800  | 0.60877800  | 2.41605900  |
| H  | 4.76095100  | -1.54759800 | 2.12082000  |
| H  | 0.54830000  | 3.34787400  | -2.78672700 |
| H  | 0.45475800  | 3.56025100  | -1.01179500 |



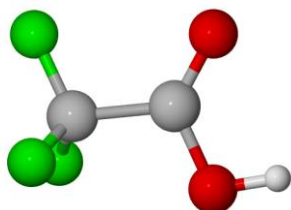
|   |            |            |            |
|---|------------|------------|------------|
| O | 0.71801300 | 3.17915000 | 0.79421900 |
|---|------------|------------|------------|

|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| C  | 0.82229700  | 2.32846400  | -0.08368900 | H  | 3.25771800  | 2.20700600  | -0.17813500 |
| O  | -0.10630600 | 1.87291200  | -0.91841100 | N  | 2.36505500  | 0.32209200  | -0.32767900 |
| C  | 2.15064900  | 1.60555700  | -0.21221700 | C  | 3.62973800  | -0.41984200 | -0.20904800 |
| H  | 3.06025500  | 2.20869700  | -0.08038900 | C  | 3.78872000  | -1.30759500 | -1.44985200 |
| N  | 2.17431600  | 0.31744400  | -0.28400100 | C  | 3.59238500  | -1.24335400 | 1.09446800  |
| C  | 3.41863200  | -0.48926200 | -0.20307300 | H  | 2.95204200  | -2.02583900 | -1.51606100 |
| C  | 3.45477600  | -1.33241700 | -1.49429700 | H  | 3.80077000  | -0.70578900 | -2.37229000 |
| C  | 4.69428800  | 0.35976500  | -0.08873900 | H  | 4.72927900  | -1.87855900 | -1.38826400 |
| C  | 3.24306500  | -1.43102600 | 1.02085800  | H  | 4.51560500  | -1.84946200 | 1.13003100  |
| H  | 2.53283700  | -1.93281800 | -1.58980200 | H  | 2.74865400  | -1.95902300 | 1.02232400  |
| H  | 3.54071100  | -0.68751300 | -2.38379200 | C  | 3.45921300  | -0.39041700 | 2.36128900  |
| H  | 4.31524900  | -2.02070500 | -1.47180500 | H  | 3.47541800  | -1.02294400 | 3.26305800  |
| H  | 5.56889300  | -0.30717500 | -0.03020700 | H  | 4.28752500  | 0.33477800  | 2.44473600  |
| H  | 4.82662700  | 1.00684100  | -0.97223400 | H  | 2.51367000  | 0.17707900  | 2.36874100  |
| H  | 4.10865400  | -2.11800100 | 1.03541500  | Ag | 0.42254800  | -0.64436800 | -0.32823300 |
| H  | 2.34937100  | -2.05850400 | 0.82878500  | O  | -1.67274400 | -0.97641300 | -0.08968100 |
| H  | 4.69732400  | 0.99302600  | 0.81311100  | C  | -2.43253400 | 0.04848100  | -0.01993500 |
| C  | 3.09172200  | -0.72683200 | 2.37405200  | O  | -2.17335900 | 1.27961900  | -0.13435900 |
| H  | 2.91944700  | -1.46632700 | 3.17233500  | C  | -3.92164000 | -0.32205000 | 0.24681100  |
| H  | 3.99261800  | -0.15241500 | 2.64604400  | H  | -0.92566900 | 1.74959300  | -0.57055000 |
| H  | 2.23385100  | -0.03346000 | 2.37291100  | F  | -4.70257800 | 0.76947400  | 0.38368400  |
| Ag | 0.21604700  | -0.63012400 | -0.33045500 | F  | -4.02336700 | -1.06335200 | 1.38082600  |
| O  | -1.88457300 | -0.95647700 | -0.12355000 | F  | -4.40230800 | -1.06303700 | -0.78702800 |
| C  | -2.63863000 | 0.07114400  | -0.03299400 | H  | 4.46680600  | 0.30685700  | -0.15379800 |
| O  | -2.37078800 | 1.30296700  | -0.11110600 |    |             |             |             |
| C  | -4.13221100 | -0.29742100 | 0.21048500  |    |             |             |             |
| H  | -1.11014100 | 1.77746500  | -0.51994500 |    |             |             |             |
| F  | -4.91007200 | 0.79488100  | 0.35946500  |    |             |             |             |
| F  | -4.24951500 | -1.05912100 | 1.32965400  |    |             |             |             |
| F  | -4.60579000 | -1.01705200 | -0.84162500 |    |             |             |             |



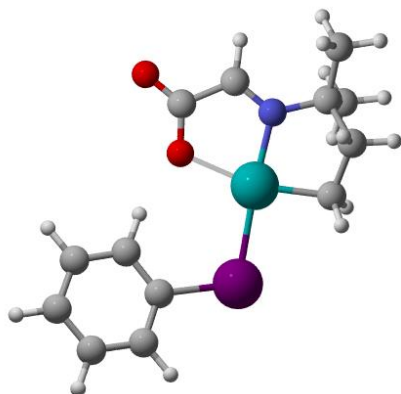
|   |            |            |             |   |            |             |             |
|---|------------|------------|-------------|---|------------|-------------|-------------|
| O | 0.91414000 | 3.22986500 | 0.65647000  | O | 1.22654100 | 3.01184800  | 1.04282800  |
| C | 1.01007800 | 2.34037900 | -0.18306700 | C | 1.26501000 | 2.26930100  | 0.06684100  |
| O | 0.07453600 | 1.84214800 | -0.98410700 | O | 0.28736800 | 1.93465100  | -0.76771900 |
| C | 2.33682800 | 1.61230500 | -0.29283100 | C | 2.56411100 | 1.53421700  | -0.20675200 |
|   |            |            |             | H | 3.50401300 | 2.07380900  | -0.00486000 |
|   |            |            |             | N | 2.55546700 | 0.27185300  | -0.47930100 |
|   |            |            |             | C | 3.80315100 | -0.49836700 | -0.51333500 |
|   |            |            |             | C | 3.73324500 | -1.67281600 | 0.47713300  |
|   |            |            |             | H | 4.64898100 | -2.27677700 | 0.34842900  |
|   |            |            |             | H | 2.88422100 | -2.32353700 | 0.18738700  |
|   |            |            |             | C | 3.58123100 | -1.22201300 | 1.93509500  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 3.56026500  | -2.08834700 | 2.61510800  |
| H  | 4.41893300  | -0.57152600 | 2.24181200  |
| H  | 2.64556500  | -0.65684300 | 2.08497800  |
| Ag | 0.57672700  | -0.62972800 | -0.53493600 |
| O  | -1.51450400 | -0.94013200 | -0.24347300 |
| C  | -2.23786800 | 0.08073000  | 0.01545100  |
| O  | -1.94484500 | 1.30814600  | 0.07629500  |
| C  | -3.72596300 | -0.28847300 | 0.28982700  |
| H  | -0.70121600 | 1.80475800  | -0.33360300 |
| F  | -4.46272400 | 0.78698000  | 0.63684300  |
| F  | -3.80473900 | -1.20075100 | 1.29327200  |
| F  | -4.27422400 | -0.83895100 | -0.82609100 |
| H  | 4.66644600  | 0.15715300  | -0.28423500 |
| H  | 3.91953200  | -0.88153000 | -1.54316200 |



### HTFA

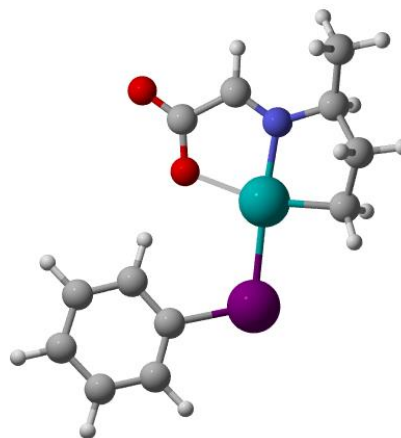
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.51599800  | 1.22779600  | -0.00024800 |
| C | 0.94006200  | 0.15852700  | -0.00001800 |
| O | 1.52330800  | -1.06220600 | 0.00002300  |
| H | 2.49233700  | -0.89798300 | -0.00002900 |
| C | -0.60361200 | 0.00088400  | 0.00001000  |
| F | -1.19054700 | 1.21082500  | -0.00076200 |
| F | -1.00624600 | -0.68168300 | 1.10077500  |
| F | -1.00624000 | -0.68308300 | -1.09987600 |



### T1-A3-Int4

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.14943400 | -1.65061000 | -1.79932400 |
| C | -3.76757000 | -1.36554600 | -0.41115500 |
| N | -2.91483500 | -0.25979600 | 0.12794300  |
| C | -3.26651300 | 0.68381600  | 0.93370200  |

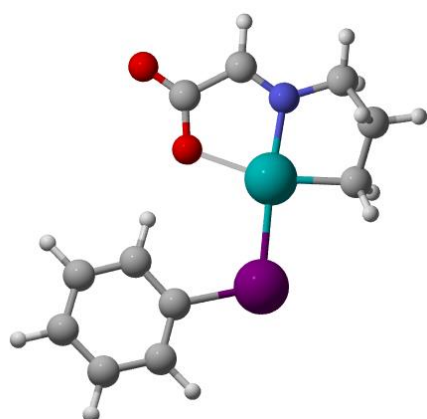
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.18932200 | 1.67187600  | 1.38897500  |
| O  | -2.51677000 | 2.57578900  | 2.16683800  |
| O  | -0.99984200 | 1.43404400  | 0.89578100  |
| C  | -1.61430200 | -1.75507600 | -1.73527900 |
| H  | -1.27335600 | -2.69214800 | -1.25880700 |
| H  | -1.17181400 | -1.68972400 | -2.74357100 |
| Pd | -1.02667800 | -0.20327500 | -0.51875700 |
| H  | -3.60124500 | -2.57340200 | -2.21552200 |
| H  | -3.43325900 | -0.82257600 | -2.47390400 |
| H  | -4.29573800 | 0.78761800  | 1.30547500  |
| C  | -3.58091500 | -2.56051500 | 0.54688700  |
| H  | -4.00154700 | -2.32919700 | 1.53920600  |
| H  | -4.09824100 | -3.44597700 | 0.14215300  |
| H  | -2.51353600 | -2.79925100 | 0.67362000  |
| C  | -5.24465200 | -0.95993100 | -0.50823400 |
| H  | -5.81705300 | -1.76790000 | -0.99143500 |
| H  | -5.69253100 | -0.78928800 | 0.48492300  |
| H  | -5.36261900 | -0.04455200 | -1.11171900 |
| C  | 2.30261100  | 1.64856700  | -1.05034800 |
| C  | 1.67409300  | 2.51776400  | -0.15278400 |
| C  | 3.49439300  | 1.95910700  | -1.71869200 |
| C  | 2.28859400  | 3.76277000  | 0.07438100  |
| H  | 0.73766500  | 2.25282000  | 0.35443200  |
| C  | 4.08485700  | 3.20879200  | -1.46733100 |
| H  | 3.95632000  | 1.25706100  | -2.41844700 |
| C  | 3.48401800  | 4.10907900  | -0.57370600 |
| H  | 1.81386900  | 4.46066200  | 0.77124500  |
| H  | 5.01616400  | 3.47217600  | -1.97873100 |
| H  | 3.94865500  | 5.08158500  | -0.38419100 |
| I  | 1.42912100  | -0.27705600 | -1.44857400 |



### T1-A2-Int4

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.13804000 | -1.89746600 | -1.54977000 |
| C | -3.75980400 | -1.56678000 | -0.18186200 |

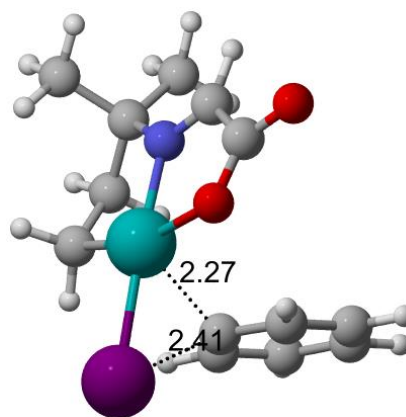
|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | -2.92841300 | -0.45387700 | 0.34674200  |
| C  | -3.30251000 | 0.52625300  | 1.09730400  |
| C  | -2.24268600 | 1.55099800  | 1.51285200  |
| O  | -2.59168200 | 2.48506500  | 2.24448700  |
| O  | -1.04630400 | 1.31053200  | 1.03880000  |
| C  | -1.60751400 | -2.01315800 | -1.43171700 |
| H  | -1.30743900 | -2.91135800 | -0.85918800 |
| H  | -1.12619200 | -2.04032200 | -2.42354100 |
| Pd | -1.03901300 | -0.39131800 | -0.30089900 |
| H  | -3.58571500 | -2.83230900 | -1.94191000 |
| H  | -3.40524200 | -1.09005700 | -2.25643800 |
| H  | -4.33815100 | 0.63812400  | 1.44831500  |
| C  | -5.25851600 | -1.26390900 | -0.20898100 |
| H  | -5.80145800 | -2.11939700 | -0.64110600 |
| H  | -5.66641100 | -1.08956700 | 0.80011700  |
| H  | -5.46481600 | -0.37549300 | -0.82979900 |
| C  | 2.20062300  | 1.54022900  | -0.99664600 |
| C  | 1.55392200  | 2.43971100  | -0.14289300 |
| C  | 3.35479800  | 1.86054800  | -1.72371700 |
| C  | 2.10897700  | 3.72701400  | -0.02468100 |
| H  | 0.64713200  | 2.16593200  | 0.41134400  |
| C  | 3.88662300  | 3.15294800  | -1.58061000 |
| H  | 3.83183700  | 1.13366700  | -2.38700000 |
| C  | 3.26572100  | 4.08452700  | -0.73402800 |
| H  | 1.61876300  | 4.44911400  | 0.63584000  |
| H  | 4.78780100  | 3.42471600  | -2.13940100 |
| H  | 3.68438600  | 5.09014600  | -0.62907200 |
| I  | 1.41762000  | -0.45070700 | -1.22792600 |
| H  | -3.55751500 | -2.41679400 | 0.50103900  |



**T1-A1-Int4**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.16811700 | -2.43533500 | -1.07114800 |
| C | -3.68198900 | -2.04499900 | 0.31969100  |
| N | -2.96556100 | -0.80873500 | 0.68241800  |

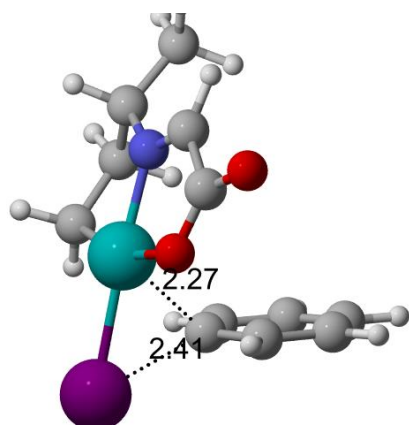
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -3.39759900 | 0.16674100  | 1.40608100  |
| C  | -2.44511900 | 1.34131500  | 1.64686300  |
| O  | -2.83202300 | 2.27177800  | 2.36335800  |
| O  | -1.28455900 | 1.21799600  | 1.05305000  |
| C  | -1.62796900 | -2.35801500 | -1.09330800 |
| H  | -1.16818500 | -3.15212100 | -0.47489300 |
| H  | -1.23662300 | -2.43099700 | -2.12200600 |
| Pd | -1.16988700 | -0.57743100 | -0.15735200 |
| H  | -3.52780100 | -3.44958600 | -1.33549700 |
| H  | -3.59066400 | -1.73679600 | -1.81478500 |
| H  | -4.40541100 | 0.16174100  | 1.84920600  |
| C  | 1.88261500  | 1.57368000  | -1.10979000 |
| C  | 1.21854100  | 2.44474000  | -0.24029200 |
| C  | 3.01416400  | 1.93787700  | -1.85172000 |
| C  | 1.73142900  | 3.74943900  | -0.12118400 |
| H  | 0.33155200  | 2.13741800  | 0.32774900  |
| C  | 3.50302700  | 3.24702800  | -1.70833100 |
| H  | 3.50701900  | 1.23170200  | -2.52577800 |
| C  | 2.86375400  | 4.15125000  | -0.84588300 |
| H  | 1.22730700  | 4.44969100  | 0.55223500  |
| H  | 4.38591100  | 3.55296700  | -2.27852000 |
| H  | 3.24927900  | 5.16994800  | -0.74028700 |
| I  | 1.16500600  | -0.44112900 | -1.34767200 |
| H  | -3.38853100 | -2.81161200 | 1.06148800  |
| H  | -4.77639300 | -1.90111600 | 0.37742900  |



**T1-A3-TS4-5**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.86788400 | -0.79545500 | -2.00536400 |
| C | -2.94097100 | -0.54443600 | -0.91715400 |
| N | -2.14912400 | -0.07808600 | 0.26411400  |
| C | -2.53919600 | 0.67578800  | 1.23378400  |
| C | -1.52763300 | 1.02242100  | 2.33503300  |
| O | -1.89840100 | 1.80292400  | 3.22194400  |
| O | -0.35981000 | 0.45048700  | 2.20793100  |

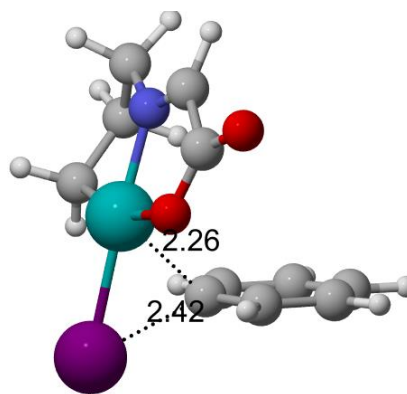
|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -0.66238100 | -1.56601300 | -1.45341600 |
| H  | -0.90870200 | -2.59447400 | -1.13411700 |
| H  | 0.17732900  | -1.61144700 | -2.16342600 |
| Pd | -0.19501600 | -0.59451100 | 0.29434700  |
| H  | -2.33154000 | -1.32952200 | -2.85903400 |
| H  | -1.52718300 | 0.18536400  | -2.38573200 |
| H  | -3.55850000 | 1.08635300  | 1.28671800  |
| C  | -3.63457800 | -1.85485400 | -0.48977700 |
| H  | -4.37218900 | -1.65845300 | 0.30546600  |
| H  | -4.15753700 | -2.29906800 | -1.35250500 |
| H  | -2.90506900 | -2.58484400 | -0.10564600 |
| C  | -3.96768800 | 0.50688500  | -1.36214700 |
| H  | -4.46600700 | 0.16988700  | -2.28533300 |
| H  | -4.75193000 | 0.66427900  | -0.60327800 |
| H  | -3.47432000 | 1.47153200  | -1.56629500 |
| C  | 1.29624500  | 0.90710100  | -0.51760100 |
| C  | 1.35301500  | 1.98115100  | 0.38428500  |
| C  | 1.24742400  | 1.09018600  | -1.90842100 |
| C  | 1.26713200  | 3.28177200  | -0.13836200 |
| H  | 1.38863000  | 1.80117800  | 1.46034300  |
| C  | 1.16763300  | 2.40311900  | -2.40180200 |
| H  | 1.25983000  | 0.23833700  | -2.59049000 |
| C  | 1.17312200  | 3.49779200  | -1.52302800 |
| H  | 1.27402700  | 4.12786500  | 0.55617900  |
| H  | 1.10923700  | 2.55989300  | -3.48396300 |
| H  | 1.11669500  | 4.51700400  | -1.91678300 |
| I  | 2.38567200  | -1.11228000 | 0.21307600  |



**T1-A2-TS4-5**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.84913300 | -0.73906300 | -2.02857300 |
| C | -2.91645900 | -0.50956900 | -0.94168600 |
| N | -2.15351700 | -0.07074600 | 0.25604000  |
| C | -2.54033300 | 0.69935000  | 1.21442300  |
| C | -1.53285000 | 1.03790800  | 2.32279300  |
| O | -1.90504000 | 1.82115900  | 3.20668400  |

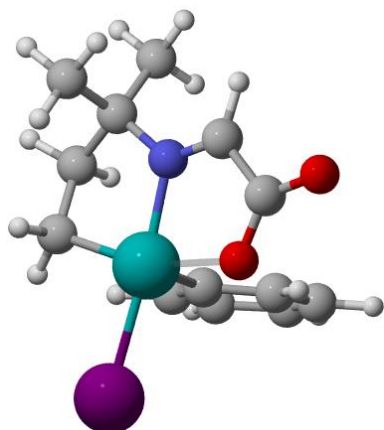
|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -0.36837400 | 0.45767500  | 2.20445400  |
| C  | -0.67546400 | -1.54691900 | -1.46169000 |
| H  | -0.97895600 | -2.55824900 | -1.13137000 |
| H  | 0.17130000  | -1.63678900 | -2.15893900 |
| Pd | -0.19744200 | -0.58929400 | 0.29151400  |
| H  | -2.30959900 | -1.25170400 | -2.89652400 |
| H  | -1.49096600 | 0.24541500  | -2.38425200 |
| H  | -3.55289600 | 1.12736400  | 1.25439400  |
| C  | -4.03910900 | 0.45027900  | -1.33900400 |
| H  | -4.53589000 | 0.08494700  | -2.25179600 |
| H  | -4.80925400 | 0.53623900  | -0.55538100 |
| H  | -3.63263200 | 1.45512200  | -1.54405600 |
| C  | 1.30546300  | 0.90267800  | -0.51405300 |
| C  | 1.36506400  | 1.97662000  | 0.38784200  |
| C  | 1.26704000  | 1.08588900  | -1.90529900 |
| C  | 1.29296200  | 3.27772700  | -0.13565900 |
| H  | 1.39267600  | 1.79660700  | 1.46415800  |
| C  | 1.20106900  | 2.39922500  | -2.39958100 |
| H  | 1.27708000  | 0.23347200  | -2.58678400 |
| C  | 1.20982900  | 3.49406900  | -1.52098700 |
| H  | 1.30217000  | 4.12399500  | 0.55863600  |
| H  | 1.15131500  | 2.55624600  | -3.48214000 |
| H  | 1.16445000  | 4.51359900  | -1.91533900 |
| I  | 2.37957300  | -1.12357800 | 0.21861200  |
| H  | -3.34152100 | -1.49597300 | -0.66513400 |



**T1-A1-TS4-5**

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.39535900 | -0.69958100 | 2.70895300  |
| C | 2.70058300 | -0.85608500 | 1.91528100  |
| N | 2.36897100 | -0.53379200 | 0.51571400  |
| C | 3.13274000 | -0.03182000 | -0.39188400 |
| C | 2.51956500 | 0.24327900  | -1.77277400 |
| O | 3.24722400 | 0.77322200  | -2.62274400 |
| O | 1.26886100 | -0.11361400 | -1.89740400 |
| C | 0.25532600 | -1.40905400 | 1.96262700  |

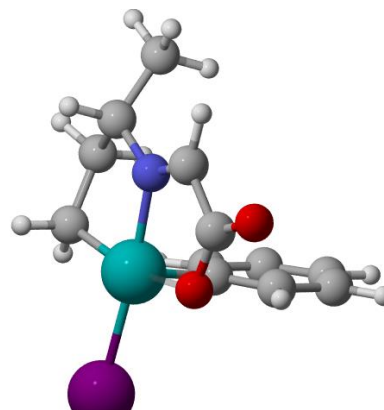
|    |             |             |             |
|----|-------------|-------------|-------------|
| H  | 0.42295100  | -2.49906500 | 1.87329700  |
| H  | -0.73522500 | -1.23402200 | 2.40912100  |
| Pd | 0.41796400  | -0.74075300 | 0.02260700  |
| H  | 1.52347100  | -1.10552500 | 3.73209300  |
| H  | 1.16196900  | 0.37573600  | 2.81005800  |
| H  | 4.18919300  | 0.21139600  | -0.19625500 |
| C  | -0.91123800 | 1.08164000  | 0.15455800  |
| C  | -0.54458600 | 1.95801500  | -0.87849700 |
| C  | -1.18758500 | 1.52261200  | 1.45809100  |
| C  | -0.36617500 | 3.31319500  | -0.55600900 |
| H  | -0.33653700 | 1.57902200  | -1.88084400 |
| C  | -1.00538500 | 2.88487200  | 1.74921000  |
| H  | -1.52531400 | 0.82796700  | 2.22910300  |
| C  | -0.59274700 | 3.77959600  | 0.74930500  |
| H  | -0.04561800 | 4.00231000  | -1.34381600 |
| H  | -1.19873300 | 3.23988700  | 2.76685100  |
| H  | -0.45977200 | 4.83993600  | 0.98376500  |
| I  | -2.14848300 | -0.87329900 | -0.54115100 |
| H  | 3.02958500  | -1.91254600 | 1.93348800  |
| H  | 3.53064100  | -0.22591600 | 2.28224700  |



**T1-A3-Int5**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.94426900 | -0.68050900 | -2.07592100 |
| C  | -3.00162800 | -0.36491900 | -0.98976300 |
| N  | -2.21126200 | 0.08834000  | 0.19900700  |
| C  | -2.64464100 | 0.68020000  | 1.25410400  |
| C  | -1.65857800 | 0.94118700  | 2.40694200  |
| O  | -2.09857800 | 1.55039700  | 3.38977600  |
| O  | -0.45435700 | 0.47485200  | 2.21933600  |
| C  | -0.71990200 | -1.41041800 | -1.51652700 |
| H  | -0.94688700 | -2.41677200 | -1.11801700 |
| H  | 0.11797300  | -1.48990500 | -2.22229800 |
| Pd | -0.22647800 | -0.41494100 | 0.21398400  |
| H  | -2.41643700 | -1.28041900 | -2.87861600 |

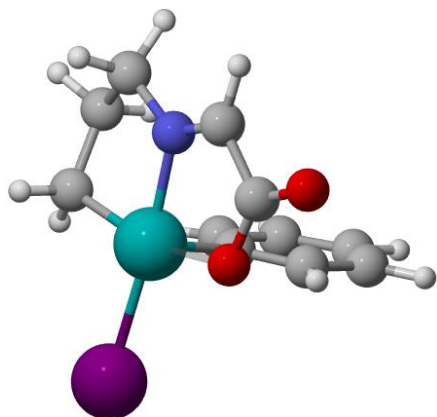
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.62249600 | 0.26992100  | -2.53567500 |
| H | -3.69676600 | 0.98057700  | 1.37208200  |
| C | -3.76503200 | -1.63502800 | -0.55786800 |
| H | -4.48077100 | -1.40442700 | 0.24801100  |
| H | -4.32428100 | -2.04207700 | -1.41581300 |
| H | -3.07518800 | -2.41179100 | -0.19085900 |
| C | -3.96527700 | 0.73869100  | -1.45230800 |
| H | -4.47511000 | 0.42193200  | -2.37648700 |
| H | -4.74210600 | 0.94629900  | -0.69810500 |
| H | -3.41394300 | 1.67016000  | -1.65938300 |
| C | 0.40534700  | 1.28581200  | -0.69970000 |
| C | 0.50376900  | 2.39672000  | 0.14164800  |
| C | 0.69832700  | 1.34512200  | -2.06416000 |
| C | 0.84324900  | 3.63528200  | -0.43713800 |
| H | 0.33912900  | 2.30286800  | 1.21617600  |
| C | 1.03642300  | 2.59460400  | -2.61826200 |
| H | 0.69537000  | 0.45633800  | -2.69543000 |
| C | 1.09950600  | 3.73917200  | -1.81146200 |
| H | 0.91074500  | 4.51516400  | 0.21086900  |
| H | 1.26818100  | 2.65260400  | -3.68684300 |
| H | 1.36703400  | 4.70563400  | -2.24942100 |
| I | 2.23393400  | -1.25434500 | 0.23968100  |



**T1-A2-Int5**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.05779700 | -0.69763400 | -2.11284100 |
| C  | -3.10601100 | -0.38964900 | -1.02841300 |
| N  | -2.34331900 | 0.04907200  | 0.17152700  |
| C  | -2.77883800 | 0.65623100  | 1.21690600  |
| C  | -1.79718900 | 0.91384600  | 2.37510000  |
| O  | -2.23924500 | 1.53126500  | 3.35185000  |
| O  | -0.59561300 | 0.43717100  | 2.19799000  |
| C  | -0.85437000 | -1.45026400 | -1.53732000 |
| H  | -1.12191600 | -2.44458400 | -1.13038300 |
| H  | -0.01052400 | -1.56041800 | -2.23174900 |
| Pd | -0.35696600 | -0.46100900 | 0.19710000  |

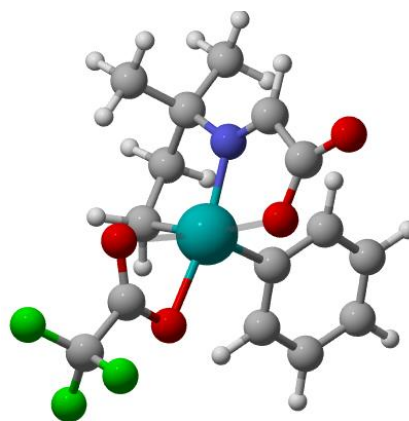
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.53016700 | -1.28851400 | -2.92178000 |
| H | -1.72470400 | 0.25447300  | -2.56244800 |
| H | -3.82770500 | 0.97114100  | 1.32413000  |
| C | -4.16513200 | 0.62824500  | -1.46048700 |
| H | -4.67739200 | 0.27016600  | -2.36764600 |
| H | -4.93239300 | 0.78346800  | -0.68520100 |
| H | -3.69097400 | 1.59747800  | -1.68727500 |
| C | 0.30306100  | 1.23270900  | -0.71028400 |
| C | 0.40333200  | 2.34440000  | 0.12960700  |
| C | 0.61272700  | 1.28549100  | -2.07142600 |
| C | 0.76075400  | 3.57829800  | -0.44848700 |
| H | 0.22676600  | 2.25460300  | 1.20259600  |
| C | 0.96865600  | 2.53025600  | -2.62481800 |
| H | 0.60881000  | 0.39472000  | -2.69997500 |
| C | 1.03332100  | 3.67625800  | -1.82008000 |
| H | 0.82956800  | 4.45911800  | 0.19809700  |
| H | 1.21328700  | 2.58330800  | -3.69078000 |
| H | 1.31510300  | 4.63899700  | -2.25728700 |
| I | 2.09783400  | -1.31500600 | 0.23474700  |
| H | -3.59362100 | -1.33889300 | -0.72744700 |



**T1-A1-Int5**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.20819800 | -0.67572300 | -2.16791500 |
| C  | -3.23502400 | -0.41262400 | -1.05861800 |
| N  | -2.48836500 | 0.05823300  | 0.12367100  |
| C  | -2.93129600 | 0.67763200  | 1.15801600  |
| C  | -1.94889800 | 0.95193500  | 2.31161700  |
| O  | -2.38529800 | 1.59110000  | 3.27662400  |
| O  | -0.75164700 | 0.46077300  | 2.14355300  |
| C  | -0.99003900 | -1.42023700 | -1.60471000 |
| H  | -1.24489400 | -2.42217200 | -1.20822300 |
| H  | -0.14823100 | -1.51304800 | -2.30414600 |
| Pd | -0.49807300 | -0.44163900 | 0.14194600  |
| H  | -2.67673400 | -1.26222800 | -2.98207600 |
| H  | -1.89027300 | 0.28697800  | -2.60265200 |

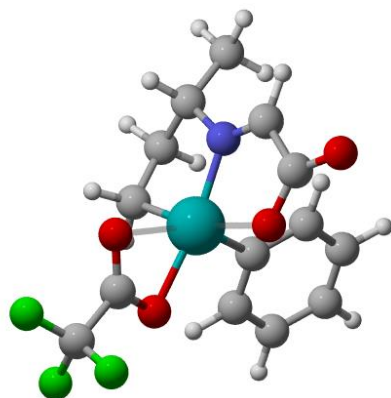
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.98436800 | 0.98609600  | 1.25218100  |
| C | 0.17335300  | 1.26096400  | -0.74517900 |
| C | 0.30962900  | 2.35320500  | 0.11464900  |
| C | 0.45515400  | 1.33504400  | -2.11113700 |
| C | 0.67388100  | 3.59262400  | -0.44718400 |
| H | 0.15224800  | 2.24503700  | 1.18907500  |
| C | 0.81852600  | 2.58520200  | -2.64765400 |
| H | 0.42496900  | 0.45746100  | -2.75709200 |
| C | 0.91855400  | 3.71362600  | -1.82217800 |
| H | 0.77010100  | 4.45920600  | 0.21492200  |
| H | 1.04054000  | 2.65564400  | -3.71753800 |
| H | 1.20593800  | 4.68046400  | -2.24646400 |
| I | 1.95793600  | -1.28947600 | 0.17080300  |
| H | -3.73532200 | -1.35502000 | -0.76540300 |
| H | -4.01378100 | 0.31579900  | -1.34424100 |



**T1-A3-Int6**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.83366800 | 0.72842000  | -2.20276800 |
| C  | -2.59519200 | -0.47343500 | -1.59570500 |
| N  | -2.00880800 | -0.63646400 | -0.22086600 |
| C  | -2.48565300 | -1.26925100 | 0.79233600  |
| C  | -1.61994200 | -1.37559900 | 2.06557400  |
| O  | -2.15415400 | -1.88312500 | 3.05825400  |
| O  | -0.40754500 | -0.91751900 | 1.93865600  |
| C  | -0.32215900 | 0.62485100  | -1.97982100 |
| H  | 0.17121300  | -0.16947900 | -2.56233900 |
| H  | 0.20432500  | 1.58144500  | -2.10416300 |
| Pd | -0.12194800 | -0.02923500 | -0.03528800 |
| H  | -2.06857400 | 0.79400700  | -3.28259700 |
| H  | -2.20779800 | 1.65239600  | -1.72899500 |
| H  | -3.48382700 | -1.72935400 | 0.77032300  |
| C  | -2.28452000 | -1.78459600 | -2.34923600 |
| H  | -2.82610700 | -2.62944400 | -1.89349900 |
| H  | -2.60173200 | -1.69025200 | -3.40049000 |

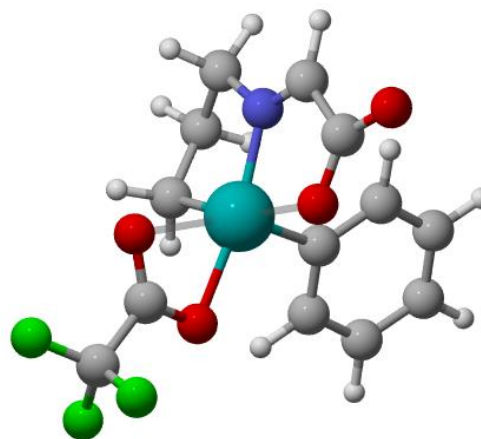
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.20787300 | -2.01461600 | -2.32227800 |
| C | -4.10457100 | -0.20876900 | -1.51243000 |
| H | -4.50096100 | -0.03139700 | -2.52488200 |
| H | -4.65063500 | -1.06817400 | -1.09014200 |
| H | -4.31079300 | 0.68289600  | -0.89815800 |
| C | -0.66670900 | 1.79807600  | 0.59343700  |
| C | -1.90874700 | 2.08624900  | 1.16769000  |
| C | 0.33306000  | 2.76812500  | 0.46676700  |
| C | -2.15218100 | 3.39599100  | 1.62233100  |
| H | -2.67971700 | 1.32481100  | 1.29036800  |
| C | 0.07139200  | 4.07208900  | 0.92631100  |
| H | 1.30686800  | 2.51649900  | 0.03833200  |
| C | -1.16931800 | 4.38819300  | 1.49898400  |
| H | -3.11792900 | 3.62715400  | 2.08374000  |
| H | 0.85091600  | 4.83529800  | 0.83314700  |
| H | -1.36681400 | 5.40381700  | 1.85521500  |
| O | 1.95751100  | 0.27345200  | -0.02891500 |
| C | 2.22799400  | -0.92287200 | -0.43843900 |
| O | 1.33495000  | -1.76060800 | -0.73464100 |
| C | 3.72385600  | -1.30343600 | -0.51365100 |
| F | 4.16899300  | -1.65198300 | 0.71833300  |
| F | 4.46255100  | -0.25673600 | -0.95669600 |
| F | 3.90960000  | -2.34694200 | -1.35098300 |



**T1-A2-Int6**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.87797100 | 0.70165000  | -2.30065200 |
| C | -2.66418300 | -0.47698700 | -1.70027500 |
| N | -2.07545200 | -0.71724900 | -0.34872100 |
| C | -2.56547200 | -1.36498100 | 0.64891800  |
| C | -1.71454300 | -1.49138500 | 1.93129600  |
| O | -2.26044800 | -2.02504600 | 2.90398200  |
| O | -0.50759800 | -1.01345000 | 1.83570900  |
| C | -0.37287400 | 0.52730400  | -2.07864100 |
| H | 0.06429700  | -0.31517400 | -2.64062800 |
| H | 0.20843800  | 1.44710900  | -2.23224100 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Pd | -0.19065600 | -0.10755100 | -0.12635800 |
| H  | -2.10886100 | 0.77925700  | -3.38043700 |
| H  | -2.22062700 | 1.63556500  | -1.82193500 |
| H  | -3.56729200 | -1.81597300 | 0.61287400  |
| C  | -4.17797300 | -0.26130500 | -1.64401500 |
| H  | -4.55990700 | -0.06656500 | -2.65853700 |
| H  | -4.71109500 | -1.14265500 | -1.25325800 |
| H  | -4.41610000 | 0.60892800  | -1.01018100 |
| C  | -0.75550200 | 1.71578300  | 0.49566100  |
| C  | -1.97963000 | 1.97332300  | 1.12068600  |
| C  | 0.20839900  | 2.71323100  | 0.31567000  |
| C  | -2.24372300 | 3.28118500  | 1.56898700  |
| H  | -2.71993300 | 1.19020400  | 1.28809500  |
| C  | -0.07381000 | 4.01501500  | 0.76924700  |
| H  | 1.17234700  | 2.48430000  | -0.14629000 |
| C  | -1.29852100 | 4.30125800  | 1.38996500  |
| H  | -3.19482500 | 3.48889500  | 2.07022500  |
| H  | 0.67746700  | 4.79999400  | 0.63433800  |
| H  | -1.51214100 | 5.31528200  | 1.74140000  |
| O  | 1.87745000  | 0.23081700  | -0.07127400 |
| C  | 2.18366600  | -0.96296500 | -0.46598800 |
| O  | 1.31684800  | -1.81894000 | -0.78293300 |
| C  | 3.68925100  | -1.31017400 | -0.49529600 |
| F  | 4.11331600  | -1.61157700 | 0.75638500  |
| F  | 4.41298600  | -0.25827300 | -0.95176400 |
| F  | 3.91976000  | -2.37201800 | -1.29692300 |
| H  | -2.42733700 | -1.39321000 | -2.27697200 |

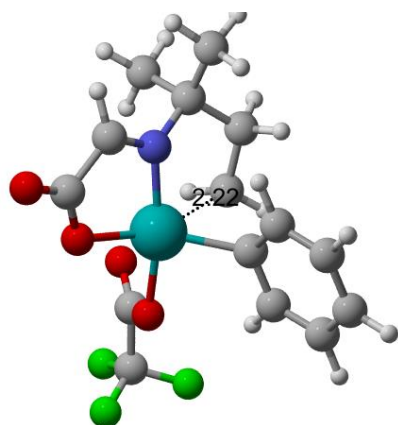


**T1-A1-Int6**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.00357700 | 0.64918900  | -2.39297300 |
| C | -2.74479900 | -0.55498000 | -1.79878200 |
| N | -2.21272200 | -0.76025500 | -0.43277800 |
| C | -2.72768200 | -1.40120900 | 0.55581700  |
| C | -1.90634900 | -1.50648300 | 1.85946100  |

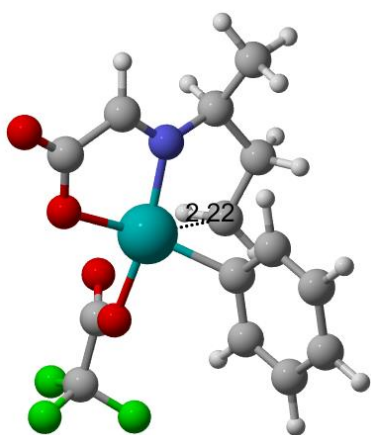


|    |             |             |             |    |             |             |             |
|----|-------------|-------------|-------------|----|-------------|-------------|-------------|
| O  | -2.47005400 | -2.02974900 | 2.82736500  | C  | -2.74665900 | -1.47045400 | 0.85280900  |
| O  | -0.69846800 | -1.02707200 | 1.78146600  | C  | -1.82776000 | -1.98622800 | 1.95541700  |
| C  | -0.49671700 | 0.51191900  | -2.13757800 | O  | -2.28659100 | -2.63641100 | 2.89276000  |
| H  | -0.02839700 | -0.31988800 | -2.69048400 | O  | -0.54722900 | -1.73136800 | 1.73804700  |
| H  | 0.06484500  | 1.44582400  | -2.27920100 | C  | -0.47597500 | 0.63097300  | -1.71894300 |
| Pd | -0.34034400 | -0.12451100 | -0.17881100 | H  | 0.00089300  | -0.32485600 | -2.01438700 |
| H  | -2.21478200 | 0.71807900  | -3.47725400 | H  | 0.10664700  | 1.43470900  | -2.18047300 |
| H  | -2.37819300 | 1.57314400  | -1.92177500 | Pd | -0.26795500 | -0.31569900 | 0.27360700  |
| H  | -3.72495000 | -1.86137400 | 0.48705300  | H  | -2.10598100 | 0.68294000  | -3.11315900 |
| C  | -0.92529100 | 1.69732200  | 0.43060900  | H  | -2.33979600 | 1.72365300  | -1.70358100 |
| C  | -2.17347500 | 1.95639900  | 1.00439500  | H  | -3.77478000 | -1.85057400 | 0.76855800  |
| C  | 0.05112900  | 2.68999500  | 0.29879900  | C  | -2.68944600 | -1.69235600 | -2.18069100 |
| C  | -2.44796000 | 3.26159600  | 1.45446300  | H  | -3.27557800 | -2.50042100 | -1.71382500 |
| H  | -2.92657500 | 1.17745800  | 1.12970300  | H  | -3.06434700 | -1.53340400 | -3.20465800 |
| C  | -0.24206800 | 3.98903000  | 0.75323400  | H  | -1.63813600 | -2.01791900 | -2.23609500 |
| H  | 1.03137200  | 2.45989100  | -0.12666200 | C  | -4.28926500 | 0.05146400  | -1.23820600 |
| C  | -1.48948900 | 4.27679100  | 1.32612800  | H  | -4.68256000 | 0.31894700  | -2.23209000 |
| H  | -3.41844800 | 3.47076000  | 1.91628000  | H  | -4.92346200 | -0.75626300 | -0.83840900 |
| H  | 0.51862900  | 4.77054100  | 0.65652900  | H  | -4.38297100 | 0.93212100  | -0.58186700 |
| H  | -1.71129400 | 5.28858200  | 1.67889000  | C  | -0.19609300 | 1.75591600  | 0.00690100  |
| O  | 1.72399300  | 0.22580200  | -0.08997900 | C  | -1.34512100 | 2.40376300  | 0.49528100  |
| C  | 2.04418500  | -0.96666300 | -0.47799400 | C  | 1.05040100  | 2.40941400  | 0.01091800  |
| O  | 1.18744600  | -1.82800800 | -0.80738300 | C  | -1.23920200 | 3.70479400  | 1.01692700  |
| C  | 3.55215400  | -1.30453900 | -0.48257200 | H  | -2.31248600 | 1.89450200  | 0.50930900  |
| F  | 3.95645000  | -1.60624600 | 0.77548200  | C  | 1.13791700  | 3.71018800  | 0.52669300  |
| F  | 4.27680100  | -0.24719800 | -0.92434600 | H  | 1.94599400  | 1.90085500  | -0.35038700 |
| F  | 3.80218400  | -2.36314300 | -1.28252500 | C  | -0.00116100 | 4.36253900  | 1.02818800  |
| H  | -2.51019400 | -1.47376500 | -2.36788900 | H  | -2.13157700 | 4.19379500  | 1.42044900  |
| H  | -3.84126800 | -0.43426600 | -1.76502000 | H  | 2.10977900  | 4.21375000  | 0.53441400  |
|    |             |             |             | H  | 0.07768000  | 5.37812800  | 1.42746600  |
|    |             |             |             | O  | 1.75736900  | -0.28996200 | 0.55334600  |
|    |             |             |             | C  | 2.35046700  | -0.95135600 | -0.40485000 |
|    |             |             |             | O  | 1.84795700  | -1.56248800 | -1.35416000 |
|    |             |             |             | C  | 3.89528900  | -0.79533200 | -0.29954200 |
|    |             |             |             | F  | 4.35059900  | -0.94229900 | 0.96549000  |
|    |             |             |             | F  | 4.22721100  | 0.46732100  | -0.72226100 |
|    |             |             |             | F  | 4.53587200  | -1.67879500 | -1.09173300 |



### T1-A3-TS6-7

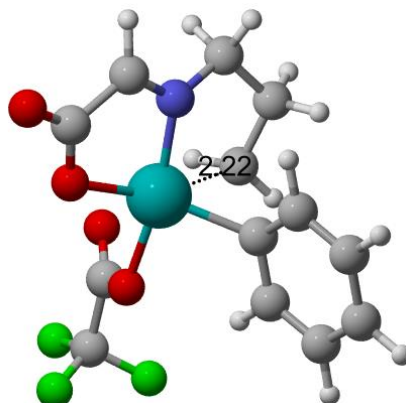
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.96615400 | 0.73487300  | -2.01691500 |
| C | -2.82119500 | -0.38122200 | -1.37111200 |
| N | -2.22364300 | -0.68029500 | -0.02393900 |



**T1-A2-TS6-7**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.97023000 | 0.74173800  | -2.02215300 |
| C  | -2.85566800 | -0.31193800 | -1.32834700 |
| N  | -2.22751600 | -0.70307600 | -0.02901600 |
| C  | -2.72837700 | -1.56790800 | 0.78842300  |
| C  | -1.81078600 | -2.09949400 | 1.88280200  |
| O  | -2.26233500 | -2.80775000 | 2.78092600  |
| O  | -0.53915700 | -1.77740100 | 1.71017100  |
| C  | -0.48333800 | 0.60205300  | -1.71882400 |
| H  | -0.04019000 | -0.37663400 | -1.99365700 |
| H  | 0.12441400  | 1.37581800  | -2.19865300 |
| Pd | -0.27431400 | -0.32035600 | 0.28711800  |
| H  | -2.11064800 | 0.64364700  | -3.11520600 |
| H  | -2.31267600 | 1.75508100  | -1.75335900 |
| H  | -3.74057700 | -1.97989400 | 0.66629300  |
| C  | -4.30761900 | 0.14900900  | -1.15651700 |
| H  | -4.72554100 | 0.42072300  | -2.13899900 |
| H  | -4.94793200 | -0.63797700 | -0.72790100 |
| H  | -4.35722000 | 1.03613400  | -0.50369200 |
| C  | -0.19662100 | 1.74745900  | -0.01229600 |
| C  | -1.34196600 | 2.40128300  | 0.47806800  |
| C  | 1.04879400  | 2.40345000  | -0.02559900 |
| C  | -1.23388500 | 3.70840400  | 0.98339200  |
| H  | -2.30886900 | 1.89178500  | 0.50550500  |
| C  | 1.13910400  | 3.71059400  | 0.47297200  |
| H  | 1.94313900  | 1.89310900  | -0.38733000 |
| C  | 0.00342200  | 4.36760700  | 0.97611400  |
| H  | -2.12349200 | 4.20140700  | 1.38808500  |
| H  | 2.11031300  | 4.21535500  | 0.46678600  |
| H  | 0.08429400  | 5.38819300  | 1.36204300  |
| O  | 1.74452300  | -0.28322400 | 0.58975800  |
| C  | 2.35956900  | -0.93067600 | -0.36511000 |
| O  | 1.88010100  | -1.53692700 | -1.32826000 |

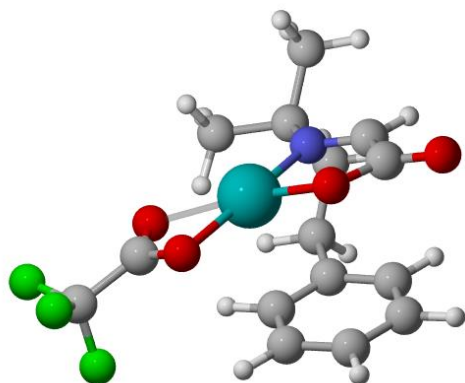
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.90087700  | -0.75882300 | -0.23360100 |
| F | 4.33623300  | -0.88540900 | 1.04041000  |
| F | 4.22750500  | 0.50220600  | -0.66648000 |
| F | 4.56349100  | -1.64514200 | -1.00396600 |
| H | -2.82926100 | -1.24072300 | -1.92960300 |



**T1-A1-TS6-7**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -1.98016300 | 0.76377900  | -2.01147500 |
| C  | -2.82994200 | -0.31016900 | -1.31554200 |
| N  | -2.22563700 | -0.68650300 | -0.01532200 |
| C  | -2.74616900 | -1.51941700 | 0.82194900  |
| C  | -1.82708300 | -2.05617800 | 1.91413100  |
| O  | -2.28170300 | -2.74821200 | 2.82307200  |
| O  | -0.55129400 | -1.76019300 | 1.72437000  |
| C  | -0.48889400 | 0.61691100  | -1.71907300 |
| H  | -0.05223200 | -0.36133000 | -2.00533400 |
| H  | 0.11873300  | 1.39423000  | -2.19315300 |
| Pd | -0.27054900 | -0.31671800 | 0.28506400  |
| H  | -2.12905800 | 0.67779400  | -3.10418500 |
| H  | -2.31869900 | 1.77191200  | -1.72525200 |
| H  | -3.77211300 | -1.90155900 | 0.70992300  |
| C  | -0.19127500 | 1.75294800  | 0.00251200  |
| C  | -1.33431800 | 2.40737900  | 0.49678500  |
| C  | 1.05604500  | 2.40455400  | -0.01297300 |
| C  | -1.22060800 | 3.71268400  | 1.00599600  |
| H  | -2.30387200 | 1.90230500  | 0.52416900  |
| C  | 1.15125300  | 3.70979000  | 0.49002900  |
| H  | 1.94775700  | 1.89261500  | -0.37880600 |
| C  | 0.01870500  | 4.36811200  | 0.99819100  |
| H  | -2.10783700 | 4.20701100  | 1.41420700  |
| H  | 2.12388900  | 4.21176600  | 0.48292700  |
| H  | 0.10340300  | 5.38706800  | 1.38754500  |
| O  | 1.74907600  | -0.28787300 | 0.57704100  |
| C  | 2.35508100  | -0.93505600 | -0.38398500 |
| O  | 1.86539500  | -1.53722200 | -1.34456300 |

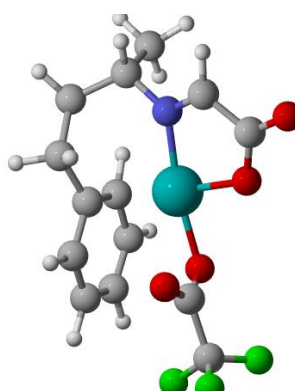
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.89781400  | -0.76909700 | -0.26310600 |
| F | 4.34178600  | -0.90608900 | 1.00679100  |
| F | 4.22518700  | 0.49383900  | -0.68953000 |
| F | 4.55143000  | -1.65219600 | -1.04458400 |
| H | -2.84064200 | -1.23517200 | -1.91924000 |
| H | -3.87625700 | 0.00881600  | -1.16579900 |



### T1-A3-Int7

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.85610900 | 0.88034700  | -1.99383700 |
| C  | -2.38213200 | -0.54622400 | -1.59589200 |
| N  | -1.86863400 | -0.53857400 | -0.17791000 |
| C  | -2.64423300 | -0.21148300 | 0.80548400  |
| C  | -2.06665000 | -0.25463400 | 2.19533800  |
| O  | -2.73578700 | 0.01764400  | 3.19111100  |
| O  | -0.79738800 | -0.63873700 | 2.22241800  |
| C  | -1.77465100 | 1.97578000  | -2.13829200 |
| H  | -1.07602500 | 1.70474500  | -2.94820200 |
| H  | -2.28859700 | 2.89673300  | -2.47161000 |
| Pd | 0.03410000  | -0.82438100 | 0.41871900  |
| H  | -3.38059700 | 0.77551900  | -2.96108000 |
| H  | -3.62216700 | 1.21114100  | -1.26866100 |
| H  | -3.69491400 | 0.07175900  | 0.66210800  |
| C  | -1.27541300 | -1.05123600 | -2.52799200 |
| H  | -0.96623100 | -2.07169400 | -2.25157300 |
| H  | -1.65703500 | -1.07082200 | -3.56207200 |
| H  | -0.38131700 | -0.41531600 | -2.49656900 |
| C  | -3.57817300 | -1.52324700 | -1.64524400 |
| H  | -3.91535200 | -1.63893100 | -2.68777200 |
| H  | -3.28025200 | -2.51299900 | -1.26326500 |
| H  | -4.43302100 | -1.16111800 | -1.05082700 |
| C  | -0.99482000 | 2.24919900  | -0.86734900 |
| C  | -1.64616500 | 2.72274800  | 0.28997600  |
| C  | 0.38057900  | 1.96494500  | -0.79226300 |
| C  | -0.94941200 | 2.87283900  | 1.49736600  |
| H  | -2.71542700 | 2.96252200  | 0.24957900  |

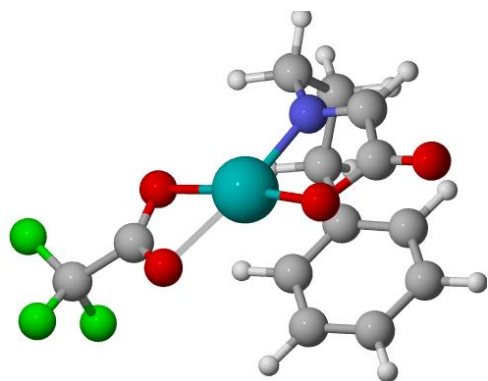
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.08913400  | 2.12717800  | 0.41462100  |
| H | 0.90606800  | 1.59662000  | -1.67979900 |
| C | 0.42166000  | 2.57042000  | 1.56446300  |
| H | -1.47872300 | 3.21372300  | 2.39214700  |
| H | 2.15587200  | 1.88723400  | 0.45043600  |
| H | 0.96057800  | 2.66737000  | 2.51090400  |
| O | 2.07974000  | -1.08357900 | 0.91604800  |
| C | 2.38265500  | -1.09698500 | -0.32613400 |
| O | 1.47446300  | -1.07354600 | -1.22335700 |
| C | 3.86291400  | -1.01500300 | -0.73876700 |
| F | 4.65826300  | -1.63015800 | 0.15978500  |
| F | 4.21932300  | 0.30087700  | -0.80077600 |
| F | 4.06059100  | -1.56573000 | -1.95584100 |



### T1-A2-Int7

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.95475600 | 1.00809500  | -2.19207700 |
| C  | -3.46079600 | -0.20140400 | -1.35596700 |
| N  | -2.37894800 | -0.93487400 | -0.66190000 |
| C  | -2.48066000 | -2.21790900 | -0.51966900 |
| C  | -1.45469200 | -2.93655400 | 0.32763000  |
| O  | -1.56517300 | -4.14365600 | 0.54670300  |
| O  | -0.50736300 | -2.15242100 | 0.80756300  |
| C  | -1.44779100 | 1.09062800  | -2.47366500 |
| H  | -1.06112100 | 0.12745200  | -2.85457500 |
| H  | -1.30465200 | 1.81676800  | -3.29565700 |
| Pd | -0.63697300 | -0.23338400 | 0.14437300  |
| H  | -3.48442900 | 0.97652100  | -3.15866800 |
| H  | -3.27887200 | 1.94706000  | -1.70909100 |
| H  | -3.31805200 | -2.78203600 | -0.95866400 |
| C  | -4.50191800 | 0.22106200  | -0.30506900 |
| H  | -5.31379000 | 0.78698300  | -0.79034100 |
| H  | -4.93517300 | -0.65757500 | 0.19873900  |
| H  | -4.04032100 | 0.86213300  | 0.46444500  |
| C  | -0.57491400 | 1.56240800  | -1.31415800 |
| C  | -1.11444400 | 2.03161700  | -0.06795500 |

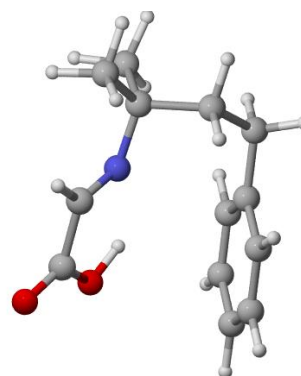
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.80291800  | 1.83846300  | -1.58579000 |
| C | -0.30658800 | 2.77795400  | 0.83456600  |
| H | -2.19261800 | 1.99583400  | 0.10945800  |
| C | 1.57463200  | 2.56463600  | -0.69080000 |
| H | 1.23586500  | 1.47470100  | -2.52191300 |
| C | 1.02200400  | 3.03552100  | 0.52764000  |
| H | -0.74500400 | 3.13397600  | 1.77076900  |
| H | 2.62709600  | 2.75553600  | -0.91483700 |
| H | 1.65055900  | 3.59514500  | 1.22540900  |
| O | 1.12699000  | 0.13138300  | 1.06204800  |
| C | 2.13238800  | -0.32789400 | 0.36309300  |
| O | 2.13069800  | -0.82552300 | -0.76363800 |
| C | 3.47542200  | -0.08324400 | 1.11456300  |
| F | 3.39687100  | -0.39198700 | 2.43085000  |
| F | 3.81403700  | 1.24263600  | 1.01920300  |
| F | 4.47731400  | -0.80201400 | 0.56689000  |
| H | -3.93305700 | -0.93023100 | -2.04219200 |



**T1-A1-Int7**

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.61592000 | 0.57547100  | -2.38417400 |
| C  | -2.15444200 | -0.80339100 | -1.87041800 |
| N  | -1.86930500 | -0.81931600 | -0.42402100 |
| C  | -2.78142000 | -0.70985000 | 0.48610000  |
| C  | -2.29150300 | -0.67140400 | 1.91514200  |
| O  | -3.06316700 | -0.56007700 | 2.86624100  |
| O  | -0.97228700 | -0.77652400 | 2.01695600  |
| C  | -1.55484100 | 1.69620500  | -2.32872500 |
| H  | -0.66779600 | 1.38268800  | -2.90765100 |
| H  | -1.97380200 | 2.57758900  | -2.85044800 |
| Pd | -0.01506700 | -0.81614100 | 0.25385600  |
| H  | -2.93016100 | 0.42977200  | -3.43336200 |
| H  | -3.52278100 | 0.87871600  | -1.82979200 |
| H  | -3.85074600 | -0.64165800 | 0.24199500  |
| C  | -1.12265000 | 2.08080400  | -0.92523600 |
| C  | -2.06902700 | 2.43173700  | 0.05829500  |

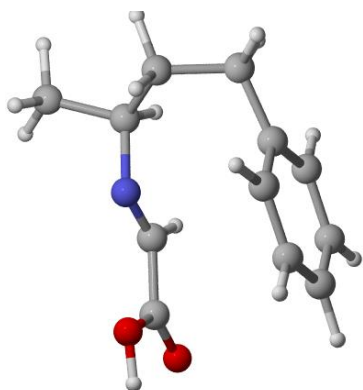
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.23706400  | 2.03767600  | -0.56097400 |
| C | -1.67313800 | 2.68510600  | 1.37933900  |
| H | -3.13185400 | 2.48838600  | -0.20441400 |
| C | 0.64114200  | 2.30785300  | 0.76032200  |
| H | 0.98615000  | 1.77586500  | -1.31559200 |
| C | -0.31584500 | 2.61584100  | 1.73641800  |
| H | -2.42607700 | 2.92492900  | 2.13617900  |
| H | 1.70096600  | 2.24664500  | 1.02398700  |
| H | -0.01067500 | 2.79089200  | 2.77179800  |
| O | 2.11680300  | -0.82055700 | 0.61830200  |
| C | 2.28379300  | -0.80867800 | -0.64494700 |
| O | 1.28251200  | -0.88883800 | -1.44459700 |
| C | 3.68256700  | -0.56792100 | -1.23857700 |
| F | 4.65298300  | -0.94272600 | -0.38225300 |
| F | 3.81644500  | 0.76638700  | -1.48880700 |
| F | 3.83656500  | -1.23536400 | -2.40340500 |
| H | -1.23159700 | -1.11986800 | -2.38211200 |
| H | -2.93466800 | -1.56066600 | -2.06821500 |



**T1-A3-Product**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.77901000 | 0.95288100  | -2.00581100 |
| C | -2.48794000 | -0.51355600 | -1.56322000 |
| N | -1.91167600 | -0.45006200 | -0.21037300 |
| C | -2.52511700 | -0.88348500 | 0.82665700  |
| C | -1.82289700 | -0.74303000 | 2.15893500  |
| O | -2.31062500 | -1.15545300 | 3.20158500  |
| O | -0.62179300 | -0.13330500 | 2.07922400  |
| C | -1.58038800 | 1.91865400  | -2.11606700 |
| H | -0.83012000 | 1.50717100  | -2.81345200 |
| H | -1.95582200 | 2.84495700  | -2.59148900 |
| H | -3.27188700 | 0.89435900  | -2.99395300 |
| H | -3.52726000 | 1.37084800  | -1.30714900 |
| H | -3.52134300 | -1.35639300 | 0.85767400  |
| C | -1.40279000 | -1.15855900 | -2.45188200 |
| H | -1.27407200 | -2.22085300 | -2.18663400 |
| H | -1.68839000 | -1.09782400 | -3.51555400 |

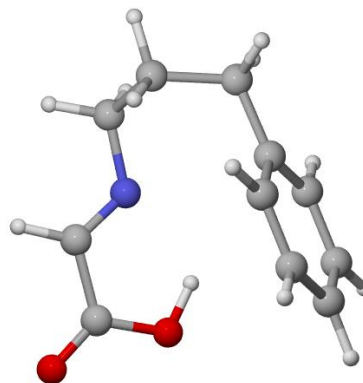
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.43356100 | -0.65639300 | -2.31113900 |
| C | -3.79651600 | -1.32099000 | -1.66401000 |
| H | -4.12335100 | -1.37575000 | -2.71513300 |
| H | -3.65742800 | -2.35330000 | -1.30016200 |
| H | -4.61236700 | -0.85468900 | -1.08516700 |
| C | -0.90916300 | 2.27868800  | -0.80496700 |
| C | -1.63007000 | 2.92432500  | 0.21930200  |
| C | 0.45094700  | 1.98830000  | -0.58467900 |
| C | -1.01423900 | 3.25589600  | 1.43412100  |
| H | -2.68836400 | 3.16510400  | 0.06547500  |
| C | 1.07426800  | 2.32347600  | 0.62820800  |
| H | 1.02507800  | 1.48872100  | -1.37354800 |
| C | 0.34135300  | 2.95671100  | 1.64371400  |
| H | -1.59445500 | 3.74665700  | 2.22200700  |
| H | 2.13097500  | 2.08238900  | 0.78210000  |
| H | 0.81953500  | 3.20502100  | 2.59570500  |
| H | -0.51354700 | 0.11880300  | 1.12169100  |



### T1-A2-Product

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.42653500 | 1.42041400  | -1.72276400 |
| C | -3.23544200 | -0.09006200 | -1.45032000 |
| N | -2.53740100 | -0.26962900 | -0.17323100 |
| C | -1.51458400 | -1.04002700 | -0.15358400 |
| C | -0.74889500 | -1.30716500 | 1.10382600  |
| O | 0.21113000  | -2.07060300 | 1.14409300  |
| O | -1.22108200 | -0.63694200 | 2.18980600  |
| C | -2.18566100 | 2.13231800  | -2.31369100 |
| H | -2.02097300 | 1.77476900  | -3.34657000 |
| H | -2.40470800 | 3.21411800  | -2.38637600 |
| H | -4.27485300 | 1.55189200  | -2.41914200 |
| H | -3.71728200 | 1.89193100  | -0.76683100 |
| H | -1.09347200 | -1.55453100 | -1.03861200 |
| C | -4.59833700 | -0.79637300 | -1.32012500 |
| H | -5.17389900 | -0.69053900 | -2.25484900 |
| H | -4.46458200 | -1.86977300 | -1.10917100 |

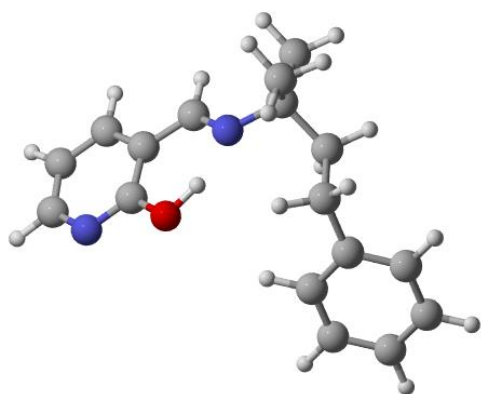
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.17882100 | -0.35444200 | -0.49333400 |
| C | -0.93207900 | 1.89519200  | -1.49900000 |
| C | -0.82837500 | 2.38844800  | -0.18343500 |
| C | 0.09910000  | 1.07657200  | -1.99402300 |
| C | 0.26095600  | 2.04432400  | 0.62760400  |
| H | -1.62680900 | 3.02120200  | 0.21916800  |
| C | 1.18779700  | 0.72050200  | -1.18360300 |
| H | 0.02800600  | 0.68599100  | -3.01582200 |
| C | 1.26753600  | 1.19866100  | 0.13423600  |
| H | 0.31557200  | 2.42198700  | 1.65344000  |
| H | 1.96900300  | 0.06127100  | -1.57506100 |
| H | 2.10783000  | 0.90914100  | 0.77257600  |
| H | -2.66803500 | -0.54987700 | -2.29270100 |
| H | -0.62106400 | -0.90911000 | 2.91804400  |



### T1-A1-Product

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.65790200 | 0.67985700  | -2.34215200 |
| C | -2.29776700 | -0.72975200 | -1.82653700 |
| N | -1.89132400 | -0.68453900 | -0.42953100 |
| C | -2.63884200 | -1.21186500 | 0.46645800  |
| C | -2.20861500 | -1.08964400 | 1.90992400  |
| O | -2.83024900 | -1.61083100 | 2.82424800  |
| O | -1.08746800 | -0.35739300 | 2.08482600  |
| C | -1.50388000 | 1.70565500  | -2.30181100 |
| H | -0.63337000 | 1.29533700  | -2.84592900 |
| H | -1.82809100 | 2.59988300  | -2.86719400 |
| H | -3.00677700 | 0.56873000  | -3.38489600 |
| H | -3.51741100 | 1.05861300  | -1.75941200 |
| H | -3.58459800 | -1.75513600 | 0.27690700  |
| C | -1.07670400 | 2.12583600  | -0.90773000 |
| C | -1.98342300 | 2.76980400  | -0.04290500 |
| C | 0.22808400  | 1.87316700  | -0.44221200 |
| C | -1.60486900 | 3.13104400  | 1.25806900  |
| H | -3.00138400 | 2.98374000  | -0.38903900 |
| C | 0.61457900  | 2.23878500  | 0.85696100  |

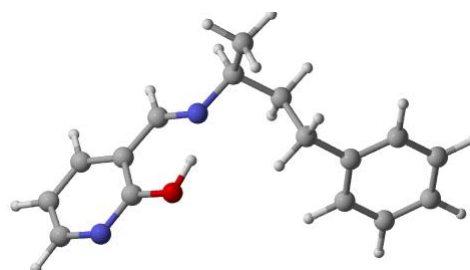
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.94269900  | 1.37008200  | -1.10339400 |
| C | -0.30437300 | 2.86480100  | 1.71435000  |
| H | -2.32787800 | 3.61924100  | 1.91930500  |
| H | 1.63121000  | 2.02606700  | 1.20290100  |
| H | -0.01128600 | 3.13581200  | 2.73285600  |
| H | -1.43988500 | -1.11543400 | -2.40955900 |
| H | -3.15848100 | -1.41353800 | -1.98923600 |
| H | -0.82392600 | -0.03588600 | 1.18126000  |



### T2-A3-Product

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.37496600 | -0.15455400 | -3.92149200 |
| C | -3.37138200 | 0.81498700  | -3.86267000 |
| C | -2.53452000 | 0.88161300  | -2.73316000 |
| C | -2.75773500 | -0.07296100 | -1.67656300 |
| C | -4.49370700 | -1.03830100 | -2.83115200 |
| H | -5.04541000 | -0.23595400 | -4.78074200 |
| H | -3.22085600 | 1.52660800  | -4.68345200 |
| H | -5.26722000 | -1.81812100 | -2.84419200 |
| O | -1.99714500 | -0.05441700 | -0.57940800 |
| C | -1.45224300 | 1.84863700  | -2.64248000 |
| H | -1.29141500 | 2.50433100  | -3.51747100 |
| N | -0.70904200 | 1.90495700  | -1.57996400 |
| C | 0.46345200  | 2.78900400  | -1.45083100 |
| C | 0.76589300  | 3.62302000  | -2.70816900 |
| H | -0.07159600 | 4.29484000  | -2.96453600 |
| H | 1.65173900  | 4.25305400  | -2.52844300 |
| H | 0.98169300  | 2.98142600  | -3.58006000 |
| C | 0.19501900  | 3.72454200  | -0.25240400 |
| H | -0.08372400 | 3.14927500  | 0.64394200  |
| H | 1.09488800  | 4.31965200  | -0.02239700 |
| H | -0.63184800 | 4.41654000  | -0.48326100 |
| C | 1.66314900  | 1.83693200  | -1.17007000 |
| H | 1.71480600  | 1.11951600  | -2.00868900 |
| H | 2.59880700  | 2.42473300  | -1.20063300 |
| C | 1.58217000  | 1.05218300  | 0.16246700  |

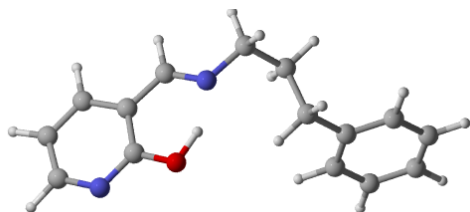
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.96553400  | 1.67555100  | 0.98933500  |
| H | 0.52681400  | 0.83068700  | 0.39393600  |
| N | -3.71756400 | -1.01646600 | -1.73446600 |
| C | 2.34313900  | -0.25401000 | 0.08864200  |
| C | 3.71203700  | -0.32748300 | 0.40800000  |
| C | 1.68756800  | -1.41744800 | -0.36318800 |
| C | 4.41403500  | -1.53586200 | 0.27851000  |
| H | 4.22943200  | 0.57058800  | 0.76587500  |
| C | 2.38624300  | -2.62637900 | -0.49250900 |
| H | 0.61843600  | -1.36719500 | -0.60197600 |
| C | 3.75277000  | -2.68871700 | -0.17360600 |
| H | 4.29830800  | -3.63291400 | -0.27112500 |
| H | 1.86103400  | -3.52352200 | -0.83652600 |
| H | 5.47780900  | -1.57843800 | 0.53534100  |
| H | -1.34262400 | 0.74246800  | -0.72232800 |



### T2-A2-Product

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.70519300 | 0.38914000  | -4.08536000 |
| C | -3.53035500 | 1.13998600  | -4.01230600 |
| C | -2.79256400 | 1.16059800  | -2.81353300 |
| C | -3.29550700 | 0.39296200  | -1.70118300 |
| C | -5.09611200 | -0.32513800 | -2.93553300 |
| H | -5.30527400 | 0.34848100  | -4.99782500 |
| H | -3.16895500 | 1.71445300  | -4.87364000 |
| H | -6.01280700 | -0.93002300 | -2.95640400 |
| O | -2.64428300 | 0.37723400  | -0.53727100 |
| C | -1.55522300 | 1.90905400  | -2.68987100 |
| H | -1.19375200 | 2.46276800  | -3.58083200 |
| N | -0.89105100 | 1.91977400  | -1.57456700 |
| C | 0.38194600  | 2.63074500  | -1.48099100 |
| C | 0.31439500  | 3.63227300  | -0.31636500 |
| H | 0.06789000  | 3.12204800  | 0.62867700  |
| H | 1.28258100  | 4.14619000  | -0.19476500 |
| H | -0.46274700 | 4.39106300  | -0.50198900 |
| C | 1.52348000  | 1.59641300  | -1.32623500 |
| H | 1.56076500  | 0.97805300  | -2.24169100 |
| H | 2.48466000  | 2.14075300  | -1.27459300 |
| C | 1.39278000  | 0.66150400  | -0.10352500 |

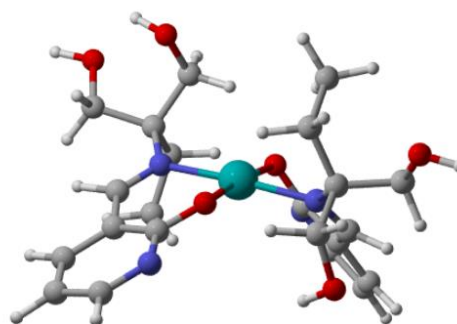
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.40797700  | 1.25635200  | 0.82697100  |
| H | 0.41506900  | 0.15071600  | -0.14363500 |
| N | -4.42649900 | -0.33662800 | -1.77108300 |
| C | 2.50923600  | -0.36028900 | -0.07495600 |
| C | 3.73702300  | -0.07149000 | 0.55232400  |
| C | 2.36134400  | -1.60174700 | -0.72432100 |
| C | 4.79039700  | -0.99773600 | 0.53324900  |
| H | 3.86315700  | 0.88948600  | 1.06520400  |
| C | 3.41160100  | -2.53140200 | -0.74624900 |
| H | 1.40821200  | -1.84028700 | -1.21066700 |
| C | 4.63067400  | -2.23147700 | -0.11761300 |
| H | 5.45004200  | -2.95734900 | -0.13028900 |
| H | 3.27607800  | -3.49416300 | -1.25004900 |
| H | 5.73575300  | -0.75830500 | 1.03142000  |
| H | 0.56676400  | 3.19190500  | -2.42424500 |
| H | -1.82322200 | 0.99454700  | -0.67154900 |



### T2-A1-Product

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -4.78917200 | 0.33772700  | -3.99052000 |
| C | -3.58048300 | 1.03567000  | -3.96109400 |
| C | -2.81409300 | 1.04786700  | -2.78008400 |
| C | -3.32427200 | 0.32732000  | -1.63969300 |
| C | -5.18429200 | -0.33372100 | -2.81638400 |
| H | -5.41221900 | 0.30528200  | -4.88777700 |
| H | -3.21437400 | 1.57491500  | -4.84295100 |
| H | -6.12757200 | -0.89647800 | -2.80300600 |
| O | -2.64647000 | 0.30621300  | -0.49160500 |
| C | -1.54181200 | 1.74066700  | -2.70166500 |
| H | -1.17587500 | 2.25624300  | -3.61348600 |
| N | -0.85302900 | 1.74755900  | -1.60051000 |
| C | 0.45584200  | 2.38276000  | -1.56397900 |
| C | 1.56629900  | 1.33039900  | -1.37594900 |
| H | 1.57987500  | 0.65948400  | -2.25461600 |
| H | 2.54291800  | 1.84787500  | -1.35738400 |
| C | 1.40351100  | 0.48587600  | -0.09365800 |
| H | 1.39165200  | 1.15876400  | 0.78431100  |
| H | 0.42419800  | -0.02263200 | -0.11917000 |
| N | -4.48839600 | -0.35140500 | -1.66766300 |
| C | 2.51281400  | -0.53431500 | 0.04648300  |

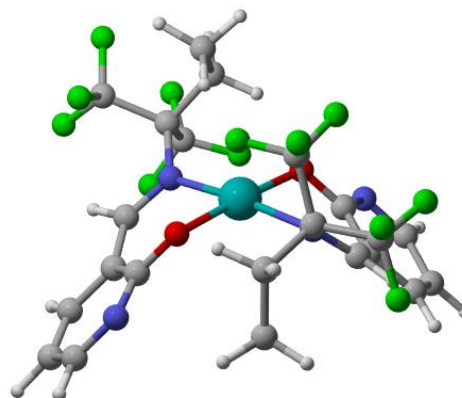
|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.72811800  | -0.19870400 | 0.67509100  |
| C | 2.37212900  | -1.82543300 | -0.49924800 |
| C | 4.77607900  | -1.12748300 | 0.75782300  |
| H | 3.84859900  | 0.80115300  | 1.10886600  |
| C | 3.41732400  | -2.75770900 | -0.41970400 |
| H | 1.42862000  | -2.10053800 | -0.98500800 |
| C | 4.62374500  | -2.41083300 | 0.20903700  |
| H | 5.43895000  | -3.13841700 | 0.27587200  |
| H | 3.28753100  | -3.75872000 | -0.84418000 |
| H | 5.71131800  | -0.85092300 | 1.25582600  |
| H | -1.80120100 | 0.88231900  | -0.65905600 |
| H | 0.64475700  | 2.97016700  | -2.48764600 |
| H | 0.47067300  | 3.08537000  | -0.70877200 |



### T2-B1-Cat

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | 1.01212100  | 2.44527100 | -1.07059600 |
| C  | 1.89873400  | 1.40138000 | -2.94255700 |
| C  | 0.76474400  | 1.65933900 | -3.73895900 |
| C  | -0.30691100 | 2.31478000 | -3.13351800 |
| C  | -0.20746300 | 2.73890200 | -1.79139900 |
| C  | -1.37464400 | 3.26942500 | -1.12555300 |
| N  | -1.38575500 | 3.90049900 | 0.01915300  |
| H  | 2.75702300  | 0.86740700 | -3.37371100 |
| H  | 0.72779900  | 1.33722400 | -4.78243000 |
| H  | -1.23447600 | 2.50709200 | -3.68592000 |
| H  | -2.33453100 | 3.06702800 | -1.61992700 |
| O  | 1.18486100  | 2.75850000 | 0.19030000  |
| Pd | 0.42163600  | 4.55226200 | 0.75741100  |
| C  | 0.19202100  | 7.46629900 | 0.92140400  |
| C  | -0.03845900 | 9.73548200 | 0.49829300  |
| C  | 1.35342000  | 9.97009400 | 0.49855100  |
| C  | 2.18251800  | 8.87986300 | 0.74554900  |
| C  | 1.62974200  | 7.59435800 | 0.95277400  |
| C  | 2.52260800  | 6.51684000 | 1.29380600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 2.25621600  | 5.23957500  | 1.38185900  |
| H | -0.73137900 | 10.56920100 | 0.31789800  |
| H | 1.75362700  | 10.97136400 | 0.32229900  |
| H | 3.27215200  | 9.00006300  | 0.78295100  |
| H | 3.54791000  | 6.84834600  | 1.51250000  |
| O | -0.43396400 | 6.34018800  | 1.12839700  |
| N | 2.03258600  | 1.76009600  | -1.65799200 |
| N | -0.61414600 | 8.54554700  | 0.70433500  |
| C | 3.31272600  | 4.30345100  | 1.87045000  |
| C | -2.67701800 | 4.20528900  | 0.68622700  |
| C | -2.46498800 | 4.24926000  | 2.21694600  |
| C | -3.73631000 | 3.13094600  | 0.31930400  |
| C | -3.20194400 | 5.58678800  | 0.17910400  |
| C | 4.01203400  | 3.58561200  | 0.68103200  |
| C | 4.37014500  | 5.06601800  | 2.71448500  |
| C | 2.65489500  | 3.24355200  | 2.80785700  |
| H | -1.74601500 | 5.05446600  | 2.43496000  |
| H | -3.42873400 | 4.54130100  | 2.66556900  |
| C | -1.98859600 | 2.92219800  | 2.82353400  |
| H | -1.06845000 | 2.56296700  | 2.33084800  |
| H | -1.76128400 | 3.05162000  | 3.89399200  |
| H | -2.75996500 | 2.13887900  | 2.73577200  |
| H | 4.94373300  | 3.16196800  | 1.09880900  |
| H | 3.38086100  | 2.74916800  | 0.34717100  |
| C | 4.31995900  | 4.48245100  | -0.52173200 |
| H | 4.91458800  | 5.37536500  | -0.25164000 |
| H | 4.89480800  | 3.91894100  | -1.27403900 |
| H | 3.39090500  | 4.82903100  | -1.00300100 |
| H | 3.32101300  | 2.36006100  | 2.82353900  |
| H | 3.85389100  | 5.77161400  | 3.39481400  |
| H | 5.05726400  | 5.63692800  | 2.05826400  |
| H | 1.69415500  | 2.93213300  | 2.37675900  |
| H | -3.28711600 | 2.11949200  | 0.41271900  |
| H | -4.05030000 | 3.28368400  | -0.73204500 |
| H | -4.24844200 | 5.66171300  | 0.52049800  |
| H | -2.59955800 | 6.39493800  | 0.62119900  |
| O | 5.10242700  | 4.08049100  | 3.46184400  |
| H | 5.86727100  | 4.53132900  | 3.86219200  |
| O | 2.39810800  | 3.73102000  | 4.12091700  |
| H | 3.28273300  | 3.76419400  | 4.53965400  |
| O | -4.84658400 | 3.30015900  | 1.20180600  |
| H | -5.62338400 | 2.90835700  | 0.76593200  |
| O | -3.21996700 | 5.65996800  | -1.24853100 |
| H | -2.31807100 | 5.92779500  | -1.50735600 |

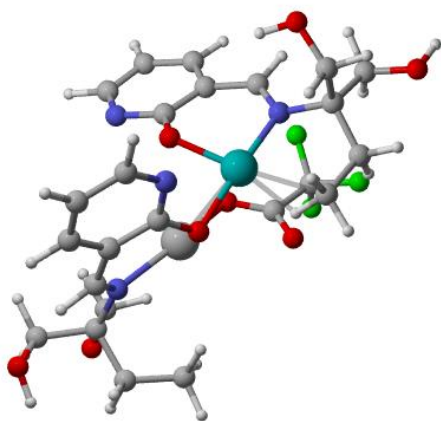


### T2-B2-Cat

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 1.08592500  | 2.64768200  | -1.33630300 |
| C  | 1.89827500  | 1.72531300  | -3.30092900 |
| C  | 0.73845700  | 2.04491600  | -4.04257100 |
| C  | -0.30526900 | 2.66042000  | -3.36103800 |
| C  | -0.15632900 | 2.99275600  | -1.99259500 |
| C  | -1.30139400 | 3.45961800  | -1.26792800 |
| N  | -1.31740300 | 3.98277500  | -0.06137800 |
| H  | 2.73519600  | 1.21507400  | -3.79778500 |
| H  | 0.66604300  | 1.79276300  | -5.10302300 |
| H  | -1.24991000 | 2.89400600  | -3.86565500 |
| H  | -2.26307000 | 3.29959900  | -1.76906100 |
| O  | 1.30230500  | 2.87481100  | -0.07151800 |
| Pd | 0.49816100  | 4.53193600  | 0.76543700  |
| C  | 0.27938800  | 7.37879600  | 1.14053400  |
| C  | -0.01717900 | 9.63850100  | 0.73316100  |
| C  | 1.34198000  | 9.85730200  | 0.41160300  |
| C  | 2.20512300  | 8.77464500  | 0.52946300  |
| C  | 1.69935600  | 7.50185600  | 0.89264600  |
| C  | 2.63666100  | 6.46357700  | 1.21077400  |
| N  | 2.37169200  | 5.19326200  | 1.41421900  |
| H  | -0.72493500 | 10.47837300 | 0.69430300  |
| H  | 1.69499400  | 10.84808300 | 0.11625000  |
| H  | 3.28128900  | 8.88896200  | 0.35394400  |
| H  | 3.66656800  | 6.81436900  | 1.33157100  |
| O  | -0.28346400 | 6.25137900  | 1.47842500  |
| N  | 2.08096400  | 1.99249500  | -2.00297400 |
| N  | -0.54356500 | 8.46466200  | 1.09751100  |
| C  | 3.39671600  | 4.29107200  | 2.00368200  |
| C  | -2.64019900 | 4.14278400  | 0.60663100  |
| C  | -2.49571800 | 4.41809500  | 2.12669700  |
| C  | -3.49902800 | 2.83868300  | 0.42364300  |
| C  | -3.40096000 | 5.35026200  | -0.03275900 |



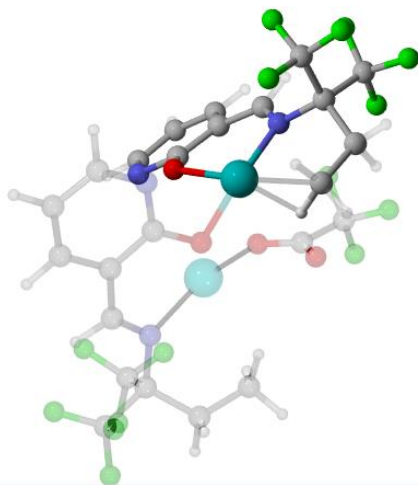
|   |             |            |             |    |             |             |             |
|---|-------------|------------|-------------|----|-------------|-------------|-------------|
| C | 3.98527400  | 3.29379800 | 0.96280900  | C  | -3.27302100 | 1.76354700  | 0.80566000  |
| C | 4.57597500  | 5.07242300 | 2.68724600  | C  | -3.11791000 | 2.37382700  | -0.50789100 |
| C | 2.66324000  | 3.48851200 | 3.13914700  | N  | -2.17750600 | 2.18548800  | -1.39125100 |
| H | -1.93664700 | 5.35798800 | 2.22048200  | H  | -3.53849600 | 0.49514800  | 4.44087500  |
| H | -3.51252700 | 4.59981200 | 2.50711000  | H  | -4.91332500 | 2.48707800  | 3.74120500  |
| C | -1.81562300 | 3.31278400 | 2.94505700  | H  | -4.67638500 | 3.31553900  | 1.36343500  |
| H | -0.80563600 | 3.08696900 | 2.56650200  | H  | -3.90703800 | 3.10823900  | -0.74646200 |
| H | -1.70315800 | 3.66279700 | 3.98363100  | O  | -1.97181900 | -0.19949300 | 0.43307400  |
| H | -2.39643200 | 2.37822000 | 2.96178000  | Pd | -0.21438100 | -0.94142800 | 1.16782300  |
| H | 4.84641600  | 2.79783100 | 1.43981600  | C  | 1.42342800  | 1.40695300  | 1.59456200  |
| H | 3.21378700  | 2.53691800 | 0.77256600  | C  | 2.68921600  | 3.32978100  | 1.34342700  |
| C | 4.37568700  | 3.91741500 | -0.38161600 | C  | 3.91737800  | 2.63690200  | 1.38811700  |
| H | 5.23956200  | 4.59404600 | -0.30501700 | C  | 3.86582700  | 1.25564400  | 1.53746900  |
| H | 4.61441000  | 3.10863800 | -1.08825000 | C  | 2.61801800  | 0.59603100  | 1.62928400  |
| H | 3.52678400  | 4.47188500 | -0.81156900 | C  | 2.62434400  | -0.83448100 | 1.76870500  |
| F | 5.41949600  | 4.23295900 | 3.32873800  | N  | 1.59839800  | -1.63544000 | 1.62864300  |
| F | 4.14161600  | 5.99222200 | 3.58536600  | H  | 2.68214300  | 4.42066300  | 1.21378600  |
| F | 5.34182000  | 5.74066600 | 1.76495000  | H  | 4.86590800  | 3.17077700  | 1.29437500  |
| F | 3.51829800  | 2.67377300 | 3.80377000  | H  | 4.78356200  | 0.65786000  | 1.56408800  |
| F | 2.08670600  | 4.32449000 | 4.03680400  | H  | 3.60216400  | -1.28194600 | 1.98410500  |
| F | 1.68766500  | 2.69074500 | 2.63407300  | O  | 0.20717300  | 0.92856300  | 1.74594200  |
| F | -3.46506600 | 5.26518600 | -1.39275100 | N  | -2.72788800 | 0.15367800  | 2.56833800  |
| F | -2.80756400 | 6.51812100 | 0.26735000  | N  | 1.48369000  | 2.75676700  | 1.44120600  |
| F | -4.68088000 | 5.38960700 | 0.43212100  | C  | 1.66322300  | -3.07880200 | 1.95803200  |
| F | -4.09747200 | 2.74965600 | -0.80455300 | C  | -2.28122100 | 2.93433200  | -2.67325600 |
| F | -4.49280800 | 2.77017800 | 1.33981600  | C  | -3.10223900 | 2.07859700  | -3.67432300 |
| F | -2.72312400 | 1.73429300 | 0.56727900  | H  | -4.13873400 | 2.03548300  | -3.28964000 |



## T2-B1-Int2

|   |             |            |            |   |            |             |             |
|---|-------------|------------|------------|---|------------|-------------|-------------|
| C | -2.63412300 | 0.56374400 | 1.27705500 | O | 0.65493700 | -1.79654800 | -1.71863400 |
| C | -3.50860600 | 0.85467800 | 3.40383300 | C | 1.65607500 | -1.05463700 | -1.61778600 |
| C | -4.26768600 | 1.97661900 | 3.02238000 | C | 3.06201500 | -1.71355100 | -1.75755700 |
| C | -4.13900100 | 2.42344800 | 1.70650800 | O | 1.71609900 | 0.21123000  | -1.42996400 |

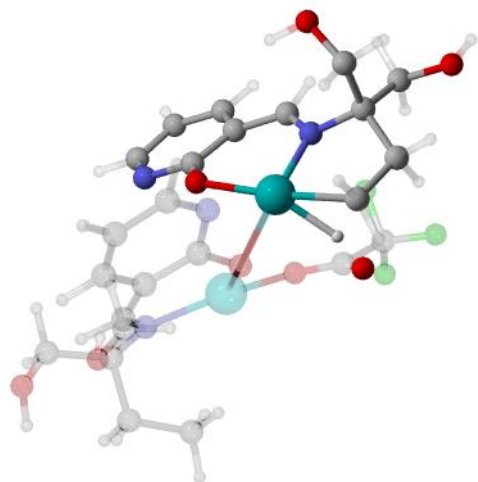
|   |             |             |             |    |             |             |             |
|---|-------------|-------------|-------------|----|-------------|-------------|-------------|
| F | 3.01597400  | -3.06881800 | -1.59755400 | H  | -4.50661600 | 2.62888100  | 3.97675600  |
| F | 3.94872300  | -1.24413500 | -0.82435200 | H  | -4.42322100 | 3.45364400  | 1.59214200  |
| F | 3.59478100  | -1.46643600 | -2.98222200 | H  | -3.78853400 | 3.27646800  | -0.50441700 |
| C | 1.12034100  | -3.22030800 | 3.41445800  | O  | -1.93503300 | -0.17052400 | 0.45361300  |
| C | 3.11184700  | -3.61420600 | 1.91468100  | Pd | -0.22051900 | -1.03545100 | 1.16724400  |
| H | -0.53571400 | -2.36801400 | 0.03893400  | C  | 1.56218400  | 1.20220000  | 1.55427800  |
| H | -1.22647100 | -3.89744000 | 0.06979300  | C  | 2.95388300  | 3.02478500  | 1.24530000  |
| H | 1.29540100  | -4.26340500 | 3.72351700  | C  | 4.13488400  | 2.25754400  | 1.35971300  |
| H | 0.03294200  | -3.01560500 | 3.42963100  | C  | 3.99303300  | 0.89306500  | 1.56942700  |
| H | 3.56196600  | -3.34912000 | 0.93678600  | C  | 2.70040800  | 0.31616500  | 1.65194600  |
| H | -2.46191900 | 4.84180100  | -1.64444400 | C  | 2.62032100  | -1.10030600 | 1.83151700  |
| H | -2.58345600 | 4.93161700  | -3.42782400 | N  | 1.54684500  | -1.84051900 | 1.66996500  |
| H | -0.29774700 | 3.80050900  | -2.46476400 | H  | 3.02054800  | 4.10442200  | 1.05582800  |
| H | -0.31080300 | 2.16680700  | -3.19751600 | H  | 5.11695100  | 2.72618400  | 1.26501900  |
| O | 1.82049600  | -2.38845000 | 4.33139000  | H  | 4.86966800  | 0.24076200  | 1.64578600  |
| H | 1.49709800  | -1.47891400 | 4.18147100  | H  | 3.55796000  | -1.59494500 | 2.10700200  |
| O | -4.31815300 | 4.41806700  | -2.35801100 | O  | 0.31605200  | 0.81537200  | 1.70246400  |
| H | -4.72152500 | 4.10097600  | -3.18716800 | N  | -2.56209000 | 0.18151600  | 2.62665900  |
| O | -0.89965000 | 3.72262300  | -4.49090900 | N  | 1.71309900  | 2.53629900  | 1.34088500  |
| H | 0.01534900  | 3.91337400  | -4.76367200 | C  | 1.51402300  | -3.28879500 | 1.96112100  |
| H | 3.69263800  | -3.14044400 | 2.73106400  | C  | -2.51310100 | 2.73529900  | -2.72671100 |
| O | 3.03202700  | -5.02855400 | 2.10295200  | C  | -2.49778100 | 1.70169700  | -3.90238800 |
| H | 3.93780800  | -5.34991500 | 2.25745300  | H  | -3.49428300 | 1.22890300  | -3.89205400 |



## T2-B2-Int2

|   |             |            |             |    |             |             |             |
|---|-------------|------------|-------------|----|-------------|-------------|-------------|
| C | -2.53993400 | 0.59698800 | 1.33441300  | Ag | -0.38133700 | 1.00541400  | -1.10551900 |
| C | -3.23927300 | 0.91305700 | 3.52101600  | O  | 0.50415500  | -1.72707700 | -1.71704000 |
| C | -3.95412900 | 2.08613500 | 3.20618100  | C  | 1.54530000  | -1.03177900 | -1.65231600 |
| C | -3.90845900 | 2.53164100 | 1.88749500  | C  | 2.90632300  | -1.74165200 | -1.90814100 |
| C | -3.16775300 | 1.82270000 | 0.91060700  | O  | 1.67265200  | 0.21909800  | -1.41303600 |
| C | -3.11465700 | 2.41229900 | -0.41220100 | F  | 2.78581400  | -3.09802700 | -1.90606500 |
| N | -2.38246900 | 2.04241100 | -1.43194000 | F  | 3.82917700  | -1.41752100 | -0.95223500 |
| H | -3.21753200 | 0.54029900 | 4.55330100  | F  | 3.42225100  | -1.37893600 | -3.11214000 |
|   |             |            |             | C  | 0.97501200  | -3.45423600 | 3.41905600  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.92035500  | -3.97546000 | 1.86479200  |
| H | -0.59798500 | -2.40886000 | -0.01543900 |
| H | -1.34316800 | -3.90798400 | -0.05793500 |
| F | 1.74443800  | -2.78009000 | 4.30575100  |
| F | 0.95165300  | -4.76275900 | 3.77728800  |
| F | -0.29147300 | -2.97416000 | 3.54075600  |
| F | 2.79585800  | -5.32293400 | 1.92240200  |
| F | 3.76686400  | -3.60831700 | 2.86986400  |
| F | 3.51647800  | -3.65977700 | 0.69365000  |
| F | -3.93215500 | 4.64783300  | -2.12720600 |
| F | -4.91357900 | 2.73305700  | -2.57548900 |
| F | -4.04214400 | 3.92797000  | -4.18574100 |
| F | -1.46604900 | 4.52230100  | -3.96043300 |
| F | -0.12967400 | 3.13118100  | -2.93206700 |
| F | -1.28941600 | 4.57748100  | -1.77019000 |

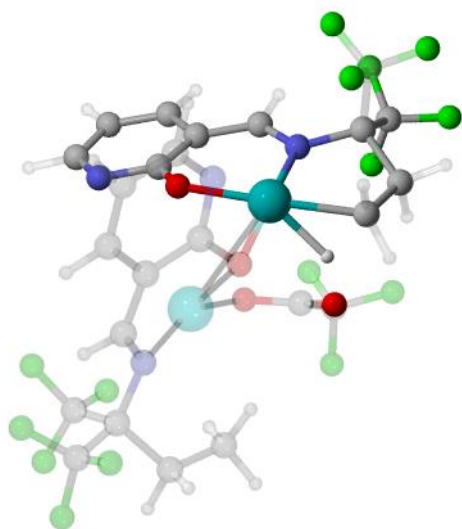


### T2-B1-TS2-3

|    |             |            |             |
|----|-------------|------------|-------------|
| C  | -1.78385400 | 5.81103100 | 0.17268700  |
| C  | -2.86595600 | 5.83882600 | 2.22567300  |
| C  | -3.69642600 | 6.91528000 | 1.86136100  |
| C  | -3.46547900 | 7.50949000 | 0.62102000  |
| C  | -2.46543900 | 7.00950200 | -0.24709100 |
| C  | -2.15386900 | 7.84992900 | -1.39376700 |
| N  | -1.16441000 | 7.77742700 | -2.24103000 |
| H  | -2.95148500 | 5.38964700 | 3.22416100  |
| H  | -4.45533300 | 7.29664500 | 2.54889400  |
| H  | -4.02496100 | 8.40271700 | 0.31823800  |
| H  | -2.84868800 | 8.70102100 | -1.49715400 |
| O  | -1.00030900 | 5.16465000 | -0.66035700 |
| Pd | 0.82812500  | 4.67078800 | 0.16583900  |
| C  | 2.34373900  | 7.19784700 | 0.15342300  |
| C  | 3.57032100  | 9.09729300 | -0.40019300 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | 4.81830800  | 8.47444500  | -0.18605500 |
| C  | 4.80152100  | 7.13872500  | 0.19810100  |
| C  | 3.57385100  | 6.45118600  | 0.35878500  |
| C  | 3.64629000  | 5.06644500  | 0.74693200  |
| N  | 2.66591900  | 4.19763900  | 0.75467800  |
| H  | 3.53643300  | 10.14723700 | -0.72451200 |
| H  | 5.75249100  | 9.02247700  | -0.32908200 |
| H  | 5.73746900  | 6.59338700  | 0.36738500  |
| H  | 4.64366800  | 4.71368200  | 1.04134600  |
| O  | 1.15182900  | 6.70244000  | 0.33827400  |
| N  | -1.93995500 | 5.29610300  | 1.42209600  |
| N  | 2.38088500  | 8.50770700  | -0.24250200 |
| C  | 2.80188400  | 2.83305200  | 1.32282700  |
| C  | -0.99971700 | 8.88756400  | -3.21652300 |
| C  | -1.66835200 | 8.49886800  | -4.56117100 |
| H  | -2.75749200 | 8.43660000  | -4.37695800 |
| C  | 0.52814200  | 9.07865100  | -3.38129400 |
| C  | -1.54401200 | 10.25878200 | -2.72575000 |
| C  | 1.86758700  | 1.90276500  | 0.52075800  |
| H  | 2.36454900  | 1.64863300  | -0.42989600 |
| H  | 1.73867700  | 0.95997300  | 1.07916300  |
| C  | 0.51745100  | 2.56520000  | 0.21634500  |
| H  | -0.14638100 | 2.68566600  | 1.08993000  |
| H  | -1.49130300 | 9.32919000  | -5.26889000 |
| C  | -1.19168200 | 7.18233900  | -5.18855500 |
| H  | -0.11428000 | 7.20810200  | -5.42249200 |
| H  | -1.37670000 | 6.32609400  | -4.51853800 |
| H  | -1.72938100 | 6.99321400  | -6.13257100 |
| Ag | 0.43667700  | 6.24590500  | -2.32822400 |
| O  | 1.44680200  | 3.08966400  | -2.26134800 |
| C  | 2.34060000  | 3.89776400  | -2.67663000 |
| C  | 3.75396800  | 3.28847400  | -2.91268800 |
| O  | 2.26970100  | 5.13838800  | -2.89006300 |
| F  | 3.77278300  | 1.94400700  | -2.74741100 |
| F  | 4.63155500  | 3.82049100  | -2.00174800 |
| F  | 4.22312100  | 3.57237800  | -4.14986900 |
| C  | 2.34348800  | 2.92976800  | 2.80956400  |
| C  | 4.25609800  | 2.32503500  | 1.26809500  |
| H  | 0.86956300  | 3.35949000  | -1.01658300 |
| H  | -0.06839000 | 2.01115800  | -0.53682200 |
| H  | 2.55845700  | 1.95463200  | 3.27581600  |
| H  | 1.25344600  | 3.11721900  | 2.84531700  |
| H  | 4.63550000  | 2.44639300  | 0.23202700  |
| H  | -1.22968200 | 10.40702900 | -1.67799400 |

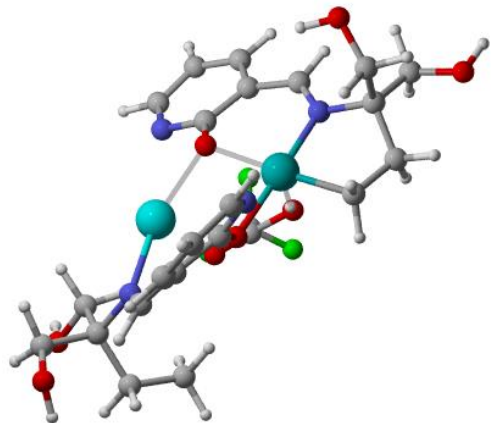
|   |             |             |             |   |             |             |             |
|---|-------------|-------------|-------------|---|-------------|-------------|-------------|
| H | -1.05764300 | 11.03692200 | -3.34351300 | C | 3.71687600  | 6.35222700  | 1.00573100  |
| H | 0.95718100  | 9.37356700  | -2.40099000 | C | 3.65542200  | 4.92874800  | 1.13033400  |
| H | 0.98321100  | 8.09655000  | -3.65077100 | N | 2.63125900  | 4.15146400  | 0.84978300  |
| O | 3.07293300  | 3.91093400  | 3.53820400  | H | 4.08982800  | 10.15904400 | 0.54061200  |
| H | 2.71717000  | 4.77847000  | 3.26522300  | H | 6.13138800  | 8.80132700  | 1.11881400  |
| O | -2.97005200 | 10.41003800 | -2.73253300 | H | 5.85511000  | 6.30642700  | 1.38798200  |
| H | -3.25268700 | 10.39480900 | -3.66549400 | H | 4.57835800  | 4.44968900  | 1.47875000  |
| O | 0.76108600  | 10.04783300 | -4.40629600 | O | 1.35425500  | 6.82992000  | 0.65595200  |
| H | 1.70396000  | 10.28598300 | -4.36365400 | N | -1.52337600 | 6.00982200  | 1.68054800  |
| H | 4.87950400  | 2.92795700  | 1.95859000  | N | 2.77363800  | 8.57396000  | 0.56691500  |
| O | 4.22641800  | 0.95554800  | 1.67450500  | C | 2.66376300  | 2.68874200  | 1.08525200  |
| H | 5.14751400  | 0.67889300  | 1.82525800  | C | -1.36034800 | 8.62624300  | -3.63035000 |



### T2-B2-TS2-3

|    |             |            |             |    |             |            |             |
|----|-------------|------------|-------------|----|-------------|------------|-------------|
| C  | -1.51509300 | 6.41145200 | 0.38279400  | Ag | 0.69006600  | 6.83289800 | -1.95260300 |
| C  | -2.23720500 | 6.71876200 | 2.56445200  | O  | 1.36830700  | 3.70100000 | -2.43723400 |
| C  | -2.99834100 | 7.85919600 | 2.23741200  | C  | 2.38231000  | 4.43530400 | -2.68679700 |
| C  | -2.94964200 | 8.30570100 | 0.91940800  | C  | 3.60111600  | 3.69741300 | -3.31569200 |
| C  | -2.17132400 | 7.62191200 | -0.04653300 | O  | 2.53874400  | 5.67608100 | -2.52540800 |
| C  | -2.08679900 | 8.23428500 | -1.35620400 | F  | 3.56263300  | 2.35997400 | -3.07626500 |
| N  | -1.29163300 | 7.91357900 | -2.34503000 | F  | 4.77070100  | 4.17389200 | -2.82211000 |
| H  | -2.20467500 | 6.35624800 | 3.60022200  | F  | 3.60605400  | 3.87858000 | -4.66418100 |
| H  | -3.57928600 | 8.38255500 | 3.00038700  | C  | 2.25863500  | 2.44395000 | 2.56950100  |
| H  | -3.48736700 | 9.21245600 | 0.61737100  | C  | 4.07060500  | 2.06815000 | 0.81107500  |
| H  | -2.78530300 | 9.07687700 | -1.46322900 | H  | 0.79959300  | 3.75909000 | -1.11100600 |
| O  | -0.89604800 | 5.65089800 | -0.49216800 | H  | -0.21306900 | 2.43554000 | -0.93077300 |
| Pd | 0.87181000  | 4.87860700 | 0.25986900  | F  | 3.06393600  | 3.12004300 | 3.42611400  |
| C  | 2.59243800  | 7.23167900 | 0.73744900  | F  | 2.32966300  | 1.12249200 | 2.87389600  |
| C  | 4.00292600  | 9.07554700 | 0.70037700  | F  | 0.98602600  | 2.85564400 | 2.80011500  |
| C  | 5.15632800  | 8.31961000 | 1.01696100  | F  | 3.99245000  | 0.71942700 | 0.73489800  |
| C  | 4.99671100  | 6.95060800 | 1.16536800  | F  | 4.99079700  | 2.36041700 | 1.77783100  |
|    |             |            |             | F  | 4.55685800  | 2.53059500 | -0.36577700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -2.68767800 | 10.58984900 | -3.01151400 |
| F | -3.76179100 | 8.75875300  | -3.58062700 |
| F | -2.75185700 | 9.95745900  | -5.10364100 |
| F | -0.16964500 | 10.36408100 | -4.81023400 |
| F | 1.04811600  | 8.87155800  | -3.77946800 |
| F | -0.04330400 | 10.37164900 | -2.61673200 |

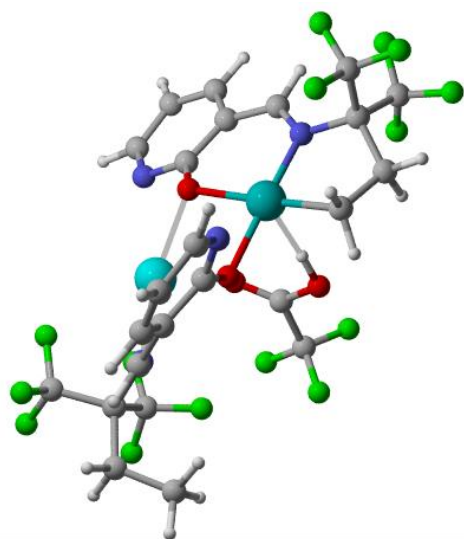


### T2-B1-Int3

|    |             |             |             |
|----|-------------|-------------|-------------|
| C  | -2.61344200 | 0.39609700  | 1.18922100  |
| C  | -3.85620700 | 0.16753800  | 3.14247500  |
| C  | -4.89535500 | 0.99648500  | 2.68206100  |
| C  | -4.72299600 | 1.60391300  | 1.43663800  |
| C  | -3.55361500 | 1.37687600  | 0.67828600  |
| C  | -3.41156100 | 2.14131500  | -0.55096200 |
| N  | -2.30578200 | 2.44620700  | -1.17646400 |
| H  | -3.91316300 | -0.28182800 | 4.14331800  |
| H  | -5.78236400 | 1.17842900  | 3.29360100  |
| H  | -5.47520100 | 2.29953000  | 1.04544400  |
| H  | -4.35572900 | 2.54654700  | -0.95618200 |
| O  | -1.62536100 | -0.01280600 | 0.43696200  |
| Pd | -0.00434100 | -0.91399500 | 1.34613200  |
| C  | 2.24913900  | 1.10399000  | 0.96875900  |
| C  | 3.97935600  | 2.39082900  | 0.09358300  |
| C  | 4.97924200  | 1.55647900  | 0.62980400  |
| C  | 4.56561700  | 0.40957800  | 1.30451800  |
| C  | 3.19016500  | 0.12191300  | 1.46595800  |
| C  | 2.84108600  | -1.15085900 | 2.06246000  |
| N  | 1.66158300  | -1.72200100 | 2.08271600  |
| H  | 4.25512800  | 3.27178200  | -0.50024100 |
| H  | 6.03703200  | 1.78415500  | 0.48006200  |
| H  | 5.30298300  | -0.30203000 | 1.69472300  |
| H  | 3.68981100  | -1.70610300 | 2.48630200  |
| O  | 0.96497800  | 1.01204600  | 1.17630800  |
| N  | -2.75694500 | -0.13446700 | 2.43578800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| N  | 2.66423400  | 2.18448700  | 0.24811600  |
| C  | 1.41969600  | -3.03863000 | 2.73176300  |
| C  | -2.40580600 | 3.18560400  | -2.45791600 |
| C  | -2.98348400 | 2.25018500  | -3.55041600 |
| H  | -4.03140500 | 2.02486900  | -3.27678900 |
| C  | -0.96403900 | 3.61145800  | -2.81388000 |
| C  | -3.24754700 | 4.48706000  | -2.33387400 |
| C  | 0.35253300  | -3.72717200 | 1.85446100  |
| H  | 0.85125500  | -4.05194700 | 0.92276800  |
| H  | 0.00215200  | -4.64289300 | 2.36402700  |
| C  | -0.79912200 | -2.76420500 | 1.52631000  |
| H  | -1.54174000 | -2.66000100 | 2.33482500  |
| H  | -2.99923400 | 2.81548800  | -4.49988800 |
| C  | -2.21306400 | 0.93529100  | -3.73363400 |
| H  | -1.19060300 | 1.11270700  | -4.10311200 |
| H  | -2.13085000 | 0.38531400  | -2.78266500 |
| H  | -2.72609300 | 0.29096000  | -4.46664800 |
| Ag | -0.33547700 | 2.04960100  | -0.30838800 |
| O  | 1.70913200  | -1.35011300 | -1.14802100 |
| C  | 1.66990300  | -0.32956000 | -1.99738900 |
| C  | 2.95731100  | -0.30602000 | -2.86373400 |
| O  | 0.79448500  | 0.51631100  | -2.12701900 |
| F  | 2.90366300  | 0.70089400  | -3.76014500 |
| F  | 3.11345500  | -1.47449200 | -3.53478600 |
| F  | 4.04687500  | -0.11981800 | -2.07341200 |
| C  | 0.86882200  | -2.73388200 | 4.15515800  |
| C  | 2.69641000  | -3.88909700 | 2.85594100  |
| H  | 0.94939300  | -1.27178900 | -0.45458800 |
| H  | -1.32255400 | -3.02856300 | 0.59288200  |
| H  | 0.77016400  | -3.69776900 | 4.68000200  |
| H  | -0.12597800 | -2.25963700 | 4.06732700  |
| H  | 3.19655300  | -3.94239200 | 1.86382500  |
| H  | -2.96291500 | 4.99625700  | -1.39682600 |
| H  | -2.97283600 | 5.14370900  | -3.18163700 |
| H  | -0.59796100 | 4.30168200  | -2.01850100 |
| H  | -0.31737800 | 2.71077300  | -2.80486700 |
| O  | 1.77003500  | -1.93421800 | 4.91775800  |
| H  | 1.69949100  | -1.02932600 | 4.55697000  |
| O  | -4.66696600 | 4.29918800  | -2.26182800 |
| H  | -4.95523200 | 4.00605700  | -3.14612100 |
| O  | -0.97685500 | 4.24064000  | -4.09701500 |
| H  | -0.04940500 | 4.38531600  | -4.35503900 |
| H  | 3.38349400  | -3.40711600 | 3.57960700  |
| O  | 2.29491700  | -5.18150400 | 3.31659300  |

H 3.08743500 -5.62083900 3.67213300



### T2-B2-Int3

C -2.55028500 0.04673200 0.85603100  
 C -4.09039200 -0.28796400 2.56400200  
 C -5.10045200 0.45798700 1.91968900  
 C -4.76702800 1.07605100 0.71848200  
 C -3.46916900 0.93607000 0.16660200  
 C -3.18529500 1.70712200 -1.01990300  
 N -2.02175500 1.94641800 -1.57497300  
 H -4.28636900 -0.74449000 3.54361800  
 H -6.09016800 0.56705100 2.36904700  
 H -5.49498100 1.70902700 0.19629600  
 H -4.09034600 2.15306300 -1.46729100  
 O -1.41043900 -0.26153900 0.30970600  
 Pd 0.09876000 -1.03426500 1.50532800  
 C 2.07778200 1.25787700 1.59054100  
 C 3.71645500 2.85980200 1.19781600  
 C 4.71227400 2.12669600 1.88183200  
 C 4.36187800 0.87809200 2.38157100  
 C 3.04146300 0.37990500 2.22452900  
 C 2.80118700 -0.97269300 2.65130600  
 N 1.73226800 -1.70707500 2.42206500  
 H 3.96303900 3.82530800 0.73740100  
 H 5.72666800 2.52014300 1.97849400  
 H 5.10767500 0.24749100 2.87962300  
 H 3.63989400 -1.44332600 3.17943000  
 O 0.81479900 0.96953200 1.49772300  
 N -2.86571200 -0.49340900 2.06753600  
 N 2.45182400 2.45482300 1.05031100  
 C 1.64831300 -3.12340500 2.86646300

C -1.99349600 2.77752900 -2.79026100  
 C -3.21416300 2.63402300 -3.74543300  
 H -4.09584300 3.04457200 -3.22826200  
 C -0.69498100 2.37840700 -3.56378500  
 C -1.90425200 4.26978100 -2.34750700  
 C 0.63841600 -3.82782400 1.92399500  
 H 1.18958200 -4.05235800 0.99569800  
 H 0.34373600 -4.79449100 2.36874800  
 C -0.56662000 -2.93613800 1.59679600  
 H -1.32742200 -2.91458300 2.39116600  
 H -3.03294600 3.30494900 -4.59921100  
 C -3.50027900 1.20901900 -4.23972400  
 H -2.69742800 0.83477600 -4.89082000  
 H -3.61205500 0.49863300 -3.40545900  
 H -4.43800000 1.20482800 -4.81806700  
 Ag -0.12856700 1.82869600 -0.36983200  
 O 1.06538400 -1.82293700 -1.30785300  
 C 1.53020000 -0.74652500 -1.93061600  
 C 1.87808900 -1.08324700 -3.40596000  
 O 1.69592300 0.37784100 -1.47173500  
 F 2.85210000 -2.02896700 -3.45458900  
 F 2.31496100 0.01599600 -4.05095300  
 F 0.78731600 -1.56245200 -4.05517900  
 C 1.15854500 -3.13075900 4.34187000  
 C 3.00889500 -3.87532500 2.75188500  
 H 0.79580300 -1.56530800 -0.34803200  
 H -1.03671800 -3.22989700 0.64456700  
 F 1.99807100 -2.43098200 5.14983300  
 F 1.08250400 -4.40208100 4.81634500  
 F -0.06915000 -2.56979000 4.45417000  
 F 2.83183400 -5.21289700 2.86809300  
 F 3.92286000 -3.51261800 3.70086700  
 F 3.56920100 -3.63166800 1.53846100  
 F -0.91986300 4.49675200 -1.43934300  
 F -3.07692500 4.64549300 -1.76414000  
 F -1.68562100 5.08995400 -3.40755000  
 F -0.68796100 2.89223100 -4.81881100  
 F -0.60695300 1.02825000 -3.66405500  
 F 0.43872100 2.81607200 -2.94705300