

Supplementary Information for:

**Interplay between Anion-Receptor and Anion-Solvent Interactions in Halide Receptor  
Complexes Characterized with Ultrafast Infrared Spectroscopies**

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Content:

**Fig. S1.** Computational results for the 1,3-alternate conformer of isolated OMCP.

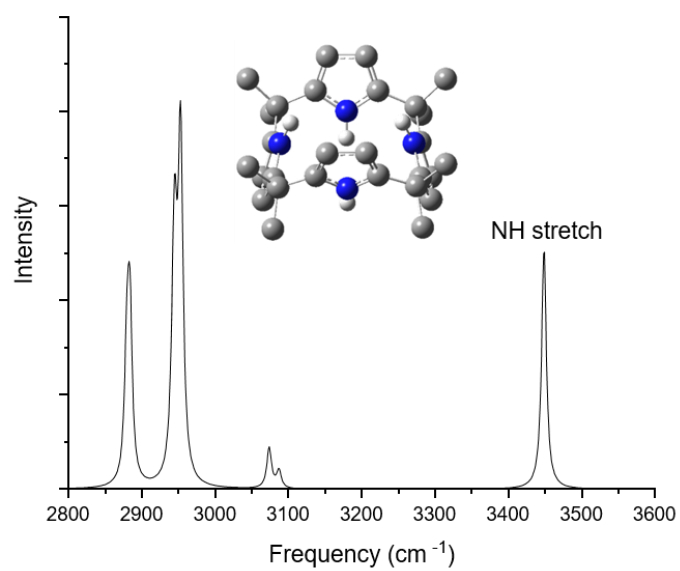
**Fig. S2.** Representative 2D IR spectra at longer pump-probe waiting times.

**Fig. S3.** Isotropic transient absorption spectra of OMCP·Cl<sup>-</sup> in DCM and OMCP·Br<sup>-</sup> in TCM.

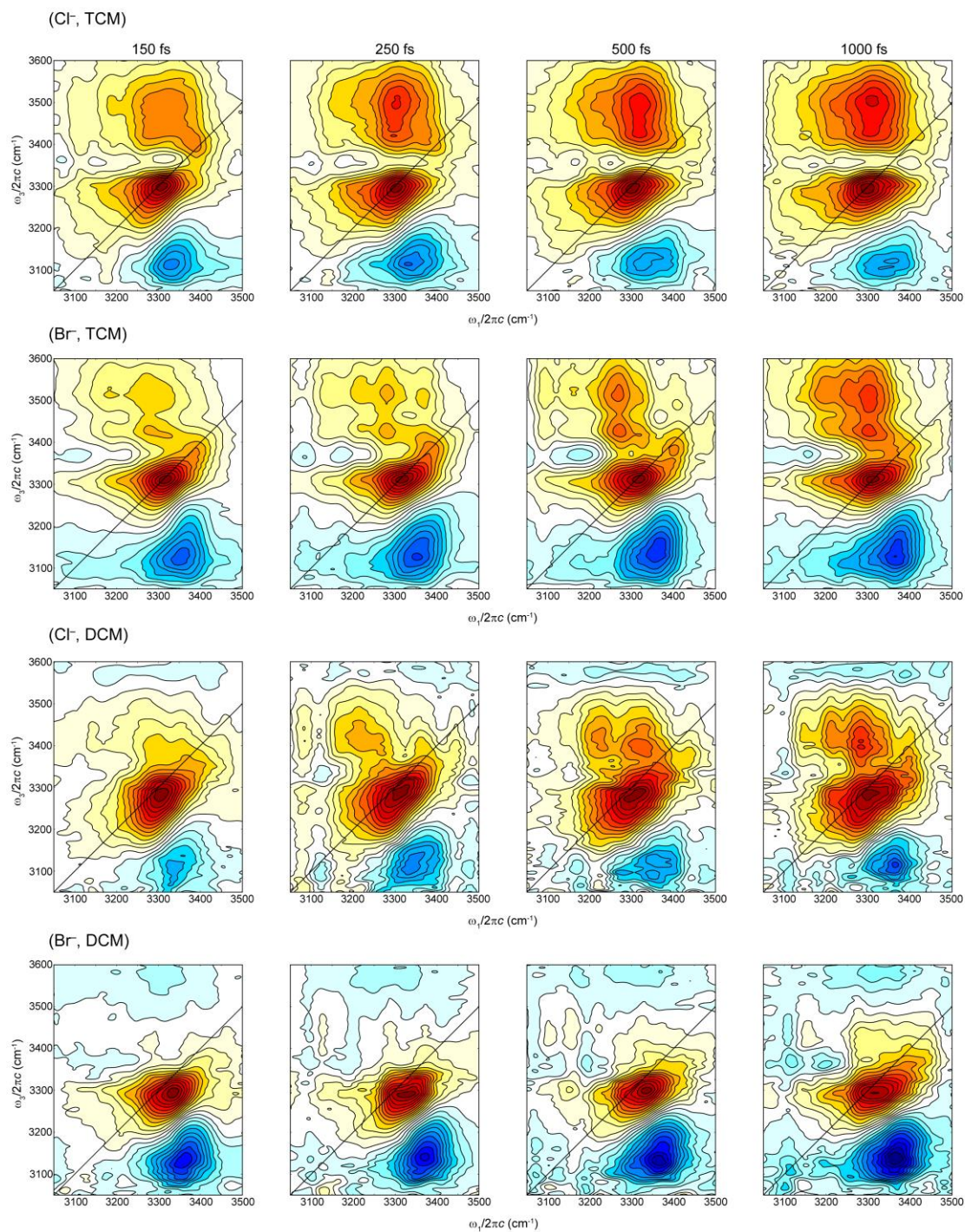
**Fig. S4.** Decay dynamics of the NH ground state bleaches, combination band bleach, and TCM solvent cross peaks.

**Fig. S5.** FTIR spectrum of OMCP·Cl<sup>-</sup> in TCM at 50 °C.

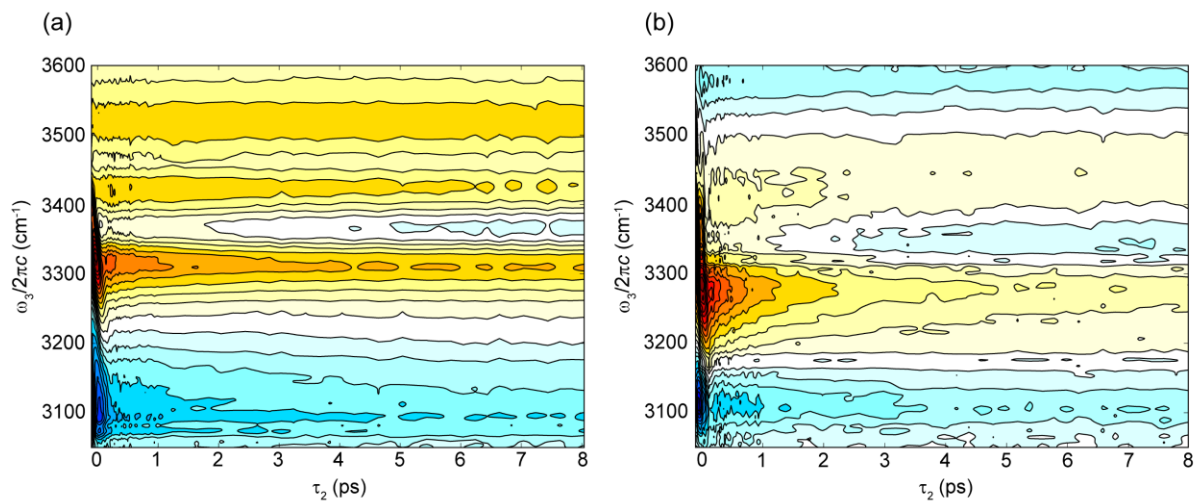
Cartesian coordinates (in Å) for all calculated optimized structures.



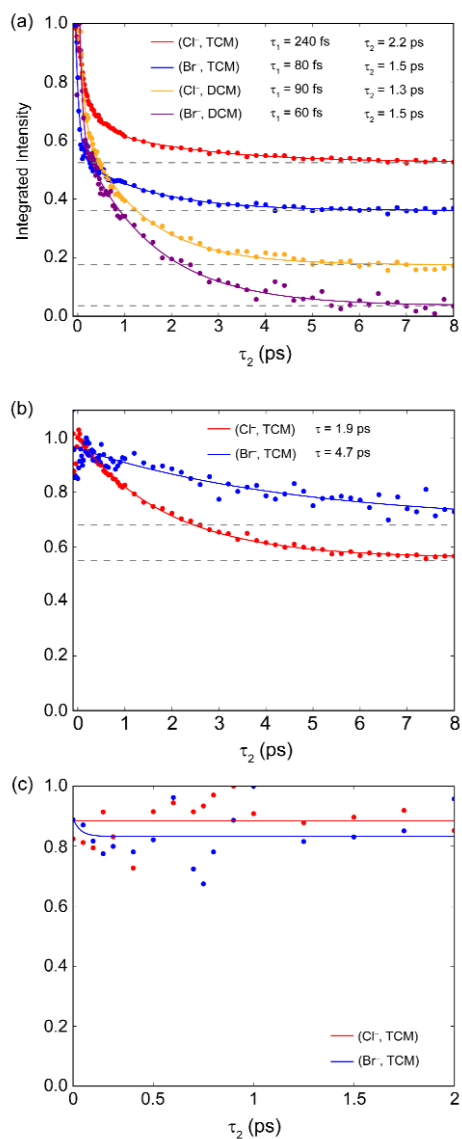
**Fig. S1.** Calculated IR spectrum (B3LYP/6-311++G(d,p), scaled by 0.951) of the isolated OMCP molecule. The 1,3-alternate arrangement of the pyrrole NH groups results in a single NH stretch transition near 3450 cm<sup>-1</sup>.



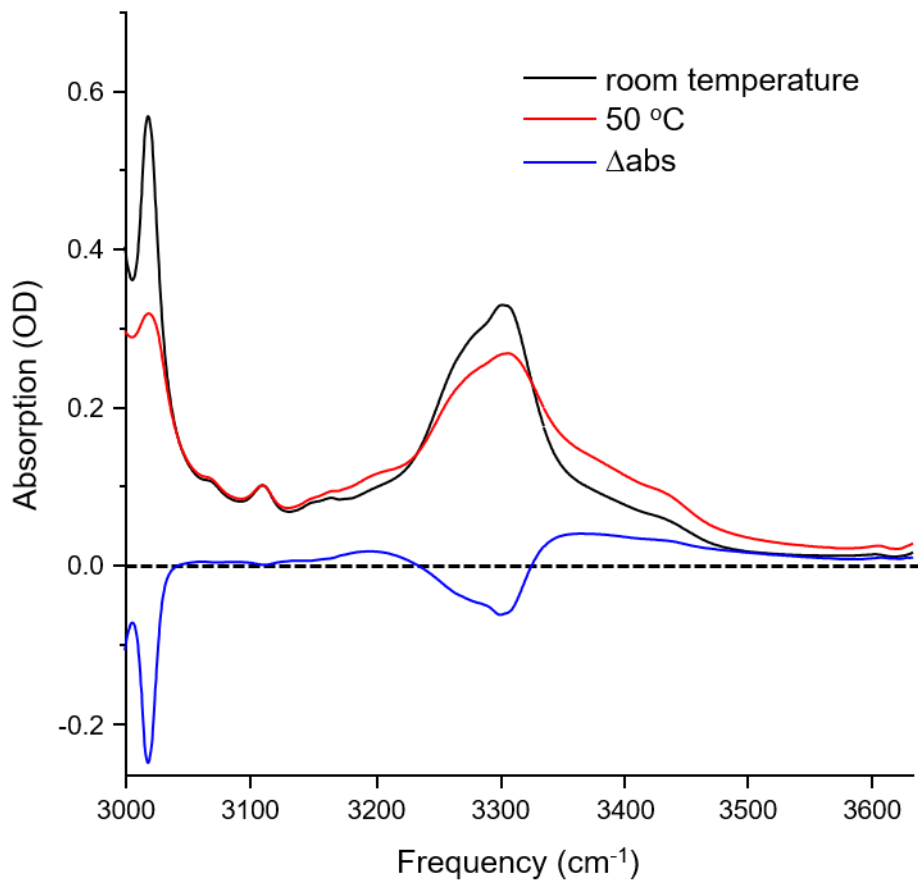
**Fig. S2.** 2D IR spectra at pump-probe waiting times of 150 fs, 250 fs, 500 fs, and 1000 fs.



**Fig. S3.** Isotropic transient absorption spectra of (a) OMCP·Br<sup>-</sup> in TCM and (b) OMCP·Cl<sup>-</sup> in DCM.



**Fig. S4.** Dynamics of the (a) NH stretch bleaches, (b) combination band transition near  $3400\text{ cm}^{-1}$ , and (c) cross peak to the TCM background feature near  $3500\text{ cm}^{-1}$ . Red: OMCP·Cl<sup>-</sup> in TCM. Blue: OMCP·Br<sup>-</sup> in TCM. Orange: OMCP·Cl<sup>-</sup> in DCM. Purple: OMCP·Br<sup>-</sup> in DCM. Time constants from fits to a biexponential decay function (solid lines) are shown inset in (a) and fits to monoexponential decays are shown in (b).



**Fig. S5.** FTIR spectra of OMCP·Cl<sup>-</sup> in TCM at room temperature (black), at 50 °C (red), and the difference (blue). Broadening of the NH stretches with increasing temperature results in the same difference profile as is observed in the transient absorption spectra at longer pump-probe waiting times.

Cartesian coordinates (in Å) for the optimized OMCP structure.

| Atom | Atomic Number | x        | y        | z        |
|------|---------------|----------|----------|----------|
| 1    | 6             | 2.872561 | -0.37396 | -0.61908 |
| 2    | 6             | 2.988033 | -0.94272 | -1.87057 |
| 3    | 6             | 2.26608  | -2.17495 | -1.85912 |
| 4    | 6             | 1.723103 | -2.33486 | -0.60106 |
| 5    | 7             | 2.10562  | -1.23487 | 0.138569 |
| 6    | 1             | 1.763163 | -1.0254  | 1.064517 |
| 7    | 1             | 3.538747 | -0.53599 | -2.70396 |
| 8    | 1             | 2.174219 | -2.86563 | -2.68238 |
| 9    | 6             | 0.897016 | -3.44771 | 0.019314 |
| 10   | 6             | -3.44803 | -0.89705 | -0.0193  |
| 11   | 6             | -2.98798 | 0.942689 | -1.87061 |
| 12   | 6             | -2.26563 | 2.174688 | -1.85932 |
| 13   | 1             | -3.53868 | 0.535972 | -2.70401 |
| 14   | 6             | -1.72313 | 2.33483  | -0.60109 |
| 15   | 1             | -2.17347 | 2.865208 | -2.68268 |
| 16   | 6             | -0.89708 | 3.447727 | 0.019301 |
| 17   | 6             | 0.942638 | 2.987697 | 1.870608 |
| 18   | 6             | 2.334993 | 1.723056 | 0.601074 |
| 19   | 6             | 2.174701 | 2.265454 | 1.859326 |
| 20   | 1             | 0.535984 | 3.538539 | 2.70396  |
| 21   | 1             | 2.865289 | 2.173529 | 2.682661 |
| 22   | 6             | 3.447941 | 0.897061 | -0.01929 |
| 23   | 7             | -1.235   | -2.10551 | -0.13863 |
| 24   | 1             | -1.02527 | -1.76254 | -1.06434 |
| 25   | 7             | -2.10541 | 1.234604 | 0.138435 |
| 26   | 1             | -1.76307 | 1.025103 | 1.064415 |
| 27   | 6             | -2.87266 | 0.373945 | -0.6191  |
| 28   | 7             | 1.234927 | 2.105534 | -0.13863 |
| 29   | 1             | 1.025216 | 1.762581 | -1.06435 |
| 30   | 6             | 0.373901 | 2.872296 | 0.619109 |
| 31   | 6             | 1.72177  | -4.15625 | 1.119489 |
| 32   | 1             | 1.152645 | -4.97921 | 1.559797 |
| 33   | 1             | 2.638177 | -4.56336 | 0.687126 |
| 34   | 1             | 2.00235  | -3.4699  | 1.921381 |
| 35   | 6             | 0.5335   | -4.4939  | -1.06037 |
| 36   | 1             | 1.436214 | -4.93976 | -1.48613 |
| 37   | 1             | -0.06662 | -5.28919 | -0.61342 |
| 38   | 1             | -0.04442 | -4.05124 | -1.87455 |
| 39   | 6             | -4.49428 | -0.53355 | 1.060364 |
| 40   | 1             | -5.28989 | 0.066107 | 0.613344 |

|    |   |          |          |          |
|----|---|----------|----------|----------|
| 41 | 1 | -4.93973 | -1.4363  | 1.48645  |
| 42 | 1 | -4.05177 | 0.044744 | 1.874368 |
| 43 | 6 | -4.15651 | -1.72175 | -1.11952 |
| 44 | 1 | -4.56334 | -2.6383  | -0.6872  |
| 45 | 1 | -4.97966 | -1.15276 | -1.55967 |
| 46 | 1 | -3.47015 | -2.00213 | -1.92147 |
| 47 | 6 | -1.72181 | 4.156351 | 1.119458 |
| 48 | 1 | -1.15274 | 4.979465 | 1.559558 |
| 49 | 1 | -2.63832 | 4.563263 | 0.687141 |
| 50 | 1 | -2.00219 | 3.470125 | 1.921526 |
| 51 | 6 | -0.53351 | 4.493879 | -1.0604  |
| 52 | 1 | -1.4362  | 4.939826 | -1.48611 |
| 53 | 1 | 0.066725 | 5.28912  | -0.6135  |
| 54 | 1 | 0.04432  | 4.051151 | -1.8746  |
| 55 | 6 | 4.494238 | 0.533631 | 1.060358 |
| 56 | 1 | 5.28981  | -0.0661  | 0.613355 |
| 57 | 1 | 4.939755 | 1.436409 | 1.486328 |
| 58 | 1 | 4.051767 | -0.04456 | 1.874448 |
| 59 | 6 | 4.156367 | 1.7218   | -1.11951 |
| 60 | 1 | 4.563153 | 2.638383 | -0.68723 |
| 61 | 1 | 4.979536 | 1.152843 | -1.55967 |
| 62 | 1 | 3.469973 | 2.002115 | -1.92146 |
| 63 | 6 | -2.33507 | -1.72304 | 0.601065 |
| 64 | 6 | -0.37397 | -2.87226 | 0.61912  |
| 65 | 6 | -2.17474 | -2.26534 | 1.85935  |
| 66 | 1 | -2.86531 | -2.17337 | 2.682698 |
| 67 | 6 | -0.94266 | -2.98756 | 1.870649 |
| 68 | 1 | -0.53598 | -3.53835 | 2.704025 |



Cartesian coordinates (in Å) for the optimized OMCP·Cl<sup>-</sup> structure.

| Atom | Atomic Number | x        | y        | z        |
|------|---------------|----------|----------|----------|
| 1    | 6             | 2.923869 | -1.12638 | -0.35831 |
| 2    | 6             | 3.777233 | -0.70007 | -1.35778 |
| 3    | 6             | 3.773163 | 0.723597 | -1.35697 |
| 4    | 6             | 2.917138 | 1.144124 | -0.35729 |
| 5    | 7             | 2.413583 | 0.007036 | 0.239431 |
| 6    | 1             | 1.743059 | 0.00476  | 1.007406 |
| 7    | 1             | 4.345445 | -1.33379 | -2.02032 |
| 8    | 1             | 4.337378 | 1.360833 | -2.01963 |
| 9    | 6             | 2.53549  | 2.550464 | 0.090662 |
| 10   | 6             | 0.700277 | 3.770699 | -1.36301 |
| 11   | 6             | -0.72335 | 3.766936 | -1.36257 |
| 12   | 1             | 1.334224 | 4.335891 | -2.02788 |
| 13   | 6             | -1.14433 | 2.914665 | -0.35987 |
| 14   | 1             | -1.36021 | 4.32836  | -2.02796 |
| 15   | 6             | -2.55069 | 2.535541 | 0.090206 |
| 16   | 6             | -3.77707 | 0.700145 | -1.35814 |
| 17   | 6             | -3.77301 | -0.72352 | -1.35739 |
| 18   | 1             | -4.3452  | 1.333894 | -2.02071 |
| 19   | 6             | -2.9171  | -1.1441  | -0.35763 |
| 20   | 1             | -4.33715 | -1.36073 | -2.02015 |
| 21   | 6             | -2.5355  | -2.55047 | 0.090285 |
| 22   | 6             | -0.70015 | -3.77063 | -1.36328 |
| 23   | 6             | 1.144365 | -2.91464 | -0.35992 |
| 24   | 6             | 0.723481 | -3.76687 | -1.36269 |
| 25   | 1             | -1.33403 | -4.33578 | -2.02824 |
| 26   | 1             | 1.360404 | -4.32826 | -2.02805 |
| 27   | 6             | 2.550677 | -2.53555 | 0.090319 |
| 28   | 7             | -0.00746 | 2.413536 | 0.239235 |
| 29   | 1             | -0.0061  | 1.74486  | 1.008688 |
| 30   | 6             | 1.126261 | 2.921172 | -0.36009 |
| 31   | 7             | -2.41362 | -0.00705 | 0.239204 |
| 32   | 1             | -1.74319 | -0.00481 | 1.007262 |
| 33   | 6             | -2.92384 | 1.126398 | -0.35854 |
| 34   | 7             | 0.007432 | -2.41355 | 0.239112 |
| 35   | 1             | 0.006004 | -1.74492 | 1.008602 |
| 36   | 6             | -1.12623 | -2.92115 | -0.36035 |
| 37   | 6             | 3.530367 | 3.552089 | -0.5297  |
| 38   | 1             | 3.286159 | 4.567927 | -0.20992 |
| 39   | 1             | 4.547196 | 3.317434 | -0.20605 |
| 40   | 1             | 3.506531 | 3.52463  | -1.62079 |

|    |    |          |          |          |
|----|----|----------|----------|----------|
| 41 | 6  | 2.651089 | 2.66984  | 1.633097 |
| 42 | 1  | 3.673477 | 2.439423 | 1.947807 |
| 43 | 1  | 2.409372 | 3.690323 | 1.945399 |
| 44 | 1  | 1.978039 | 1.990519 | 2.159252 |
| 45 | 6  | -3.55191 | 3.531314 | -0.52933 |
| 46 | 1  | -4.56735 | 3.290067 | -0.20612 |
| 47 | 1  | -3.31407 | 4.548335 | -0.20862 |
| 48 | 1  | -3.52754 | 3.505008 | -1.62045 |
| 49 | 6  | -2.66751 | 2.652077 | 1.632787 |
| 50 | 1  | -2.43392 | 3.673921 | 1.947007 |
| 51 | 1  | -3.68813 | 2.413083 | 1.946677 |
| 52 | 1  | -1.98931 | 1.97723  | 2.158054 |
| 53 | 6  | -3.53032 | -3.55206 | -0.53022 |
| 54 | 1  | -3.28615 | -4.56791 | -0.21045 |
| 55 | 1  | -4.54718 | -3.31741 | -0.20667 |
| 56 | 1  | -3.50636 | -3.52457 | -1.6213  |
| 57 | 6  | -2.65125 | -2.66992 | 1.632702 |
| 58 | 1  | -3.67367 | -2.4395  | 1.947326 |
| 59 | 1  | -2.40958 | -3.69042 | 1.944979 |
| 60 | 1  | -1.97824 | -1.99063 | 2.158953 |
| 61 | 6  | 3.551951 | -3.53129 | -0.52918 |
| 62 | 1  | 4.567371 | -3.29005 | -0.20587 |
| 63 | 1  | 3.314087 | -4.54832 | -0.20853 |
| 64 | 1  | 3.527675 | -3.50493 | -1.62029 |
| 65 | 6  | 2.667348 | -2.65217 | 1.632904 |
| 66 | 1  | 2.433722 | -3.67402 | 1.947048 |
| 67 | 1  | 3.687939 | -2.4132  | 1.946905 |
| 68 | 1  | 1.989104 | -1.97734 | 2.158143 |
| 69 | 17 | -0.00012 | -7.5E-05 | 2.545599 |

Cartesian coordinates (in Å) for the optimized OMCP·Br<sup>-</sup> structure.

| Atom | Atomic Number | x        | y        | z        |
|------|---------------|----------|----------|----------|
| 1    | 6             | 2.982326 | -0.95563 | -0.56122 |
| 2    | 6             | 3.785432 | -0.4813  | -1.5801  |
| 3    | 6             | 3.698256 | 0.939348 | -1.58016 |
| 4    | 6             | 2.843616 | 1.312173 | -0.56096 |
| 5    | 7             | 2.420917 | 0.148027 | 0.048191 |
| 6    | 1             | 1.782036 | 0.109081 | 0.839948 |
| 7    | 1             | 4.372396 | -1.08175 | -2.2571  |
| 8    | 1             | 4.206865 | 1.606683 | -2.25794 |
| 9    | 6             | 2.386114 | 2.696866 | -0.11471 |
| 10   | 6             | 0.481643 | 3.783591 | -1.58145 |
| 11   | 6             | -0.939   | 3.696411 | -1.58182 |
| 12   | 1             | 1.082282 | 4.36975  | -2.25896 |
| 13   | 6             | -1.31213 | 2.843068 | -0.56165 |
| 14   | 1             | -1.60614 | 4.204201 | -2.26041 |
| 15   | 6             | -2.69696 | 2.38616  | -0.11521 |
| 16   | 6             | -3.78528 | 0.481396 | -1.58044 |
| 17   | 6             | -3.6981  | -0.93926 | -1.58057 |
| 18   | 1             | -4.37217 | 1.081877 | -2.25746 |
| 19   | 6             | -2.84356 | -1.31214 | -0.56131 |
| 20   | 1             | -4.20664 | -1.60655 | -2.25845 |
| 21   | 6             | -2.3861  | -2.69686 | -0.11509 |
| 22   | 6             | -0.4815  | -3.78351 | -1.5817  |
| 23   | 6             | 1.312179 | -2.84304 | -0.56169 |
| 24   | 6             | 0.939148 | -3.69633 | -1.58194 |
| 25   | 1             | -1.08207 | -4.36964 | -2.25931 |
| 26   | 1             | 1.606354 | -4.20408 | -2.26049 |
| 27   | 6             | 2.69697  | -2.38615 | -0.1151  |
| 28   | 7             | -0.14816 | 2.421059 | 0.048321 |
| 29   | 1             | -0.10951 | 1.783006 | 0.840757 |
| 30   | 6             | 0.955684 | 2.981707 | -0.56147 |
| 31   | 7             | -2.42093 | -0.14803 | 0.047956 |
| 32   | 1             | -1.78213 | -0.10913 | 0.83978  |
| 33   | 6             | -2.98227 | 0.955662 | -0.56145 |
| 34   | 7             | 0.14815  | -2.42106 | 0.048191 |
| 35   | 1             | 0.109433 | -1.78304 | 0.840655 |
| 36   | 6             | -0.95563 | -2.98168 | -0.56173 |
| 37   | 6             | 3.317614 | 3.750286 | -0.74833 |
| 38   | 1             | 3.018763 | 4.751816 | -0.43007 |
| 39   | 1             | 4.348627 | 3.574559 | -0.43241 |
| 40   | 1             | 3.286412 | 3.717077 | -1.83895 |

|    |    |          |          |          |
|----|----|----------|----------|----------|
| 41 | 6  | 2.5067   | 2.834474 | 1.424968 |
| 42 | 1  | 3.543192 | 2.666321 | 1.732685 |
| 43 | 1  | 2.208969 | 3.841629 | 1.731865 |
| 44 | 1  | 1.879545 | 2.122718 | 1.964636 |
| 45 | 6  | -3.75008 | 3.317793 | -0.74913 |
| 46 | 1  | -4.75172 | 3.019343 | -0.43085 |
| 47 | 1  | -3.57404 | 4.348837 | -0.4335  |
| 48 | 1  | -3.71682 | 3.286266 | -1.83975 |
| 49 | 6  | -2.83453 | 2.507279 | 1.424427 |
| 50 | 1  | -2.66584 | 3.543762 | 1.731886 |
| 51 | 1  | -3.84185 | 2.210158 | 1.731362 |
| 52 | 1  | -2.12316 | 1.87985  | 1.964292 |
| 53 | 6  | -3.31755 | -3.75024 | -0.74885 |
| 54 | 1  | -3.01873 | -4.75179 | -0.43063 |
| 55 | 1  | -4.34859 | -3.57453 | -0.43303 |
| 56 | 1  | -3.28624 | -3.71697 | -1.83947 |
| 57 | 6  | -2.50684 | -2.83455 | 1.424567 |
| 58 | 1  | -3.54336 | -2.66641 | 1.732197 |
| 59 | 1  | -2.20914 | -3.84172 | 1.731438 |
| 60 | 1  | -1.87973 | -2.12283 | 1.964335 |
| 61 | 6  | 3.750143 | -3.31775 | -0.74898 |
| 62 | 1  | 4.751756 | -3.01932 | -0.43058 |
| 63 | 1  | 3.574081 | -4.34881 | -0.43342 |
| 64 | 1  | 3.716989 | -3.28616 | -1.83959 |
| 65 | 6  | 2.834391 | -2.50736 | 1.424548 |
| 66 | 1  | 2.665667 | -3.54386 | 1.731931 |
| 67 | 1  | 3.841686 | -2.21027 | 1.731597 |
| 68 | 1  | 2.122976 | -1.87996 | 1.964383 |
| 69 | 35 | -0.00012 | -7.5E-05 | 2.623975 |

Cartesian coordinates (in Å) for the optimized OMCP·Cl<sup>-</sup>·2TCM structure.

| Atom | Atomic Number | x        | y        | z        |
|------|---------------|----------|----------|----------|
| 1    | 6             | 2.168898 | -2.61743 | -1.60045 |
| 2    | 6             | 3.305581 | -3.36832 | -1.29597 |
| 3    | 6             | 3.307028 | -3.60661 | 0.088418 |
| 4    | 6             | 2.17147  | -3.00095 | 0.628971 |
| 5    | 7             | 1.506199 | -2.40001 | -0.41465 |
| 6    | 1             | 0.664642 | -1.83603 | -0.31726 |
| 7    | 1             | 4.038397 | -3.7184  | -2.00457 |
| 8    | 1             | 4.040905 | -4.17359 | 0.6376   |
| 9    | 6             | 1.692986 | -2.9294  | 2.069083 |
| 10   | 6             | 3.31491  | -1.28003 | 3.349216 |
| 11   | 6             | 3.304888 | 0.103874 | 3.591232 |
| 12   | 1             | 4.059337 | -1.98199 | 3.688094 |
| 13   | 6             | 2.15575  | 0.633638 | 3.001996 |
| 14   | 1             | 4.04045  | 0.659535 | 4.149758 |
| 15   | 6             | 1.660875 | 2.068091 | 2.936365 |
| 16   | 6             | 3.282292 | 3.379599 | 1.312231 |
| 17   | 6             | 3.292448 | 3.617973 | -0.07209 |
| 18   | 1             | 4.008622 | 3.732787 | 2.025949 |
| 19   | 6             | 2.163297 | 3.007496 | -0.62061 |
| 20   | 1             | 4.02775  | 4.188043 | -0.61613 |
| 21   | 6             | 1.695085 | 2.933984 | -2.06401 |
| 22   | 6             | 3.332482 | 1.291432 | -3.33302 |
| 23   | 6             | 2.179152 | -0.62714 | -2.99358 |
| 24   | 6             | 3.329951 | -0.09248 | -3.57511 |
| 25   | 1             | 4.076184 | 1.996512 | -3.66701 |
| 26   | 1             | 4.071548 | -0.64494 | -4.12881 |
| 27   | 6             | 1.690061 | -2.06376 | -2.93148 |
| 28   | 7             | 1.493458 | -0.41528 | 2.407582 |
| 29   | 1             | 0.646409 | -0.32289 | 1.850984 |
| 30   | 6             | 2.171623 | -1.59462 | 2.612992 |
| 31   | 7             | 1.493366 | 2.403566 | 0.41828  |
| 32   | 1             | 0.654908 | 1.836084 | 0.314899 |
| 33   | 6             | 2.146745 | 2.623784 | 1.608717 |
| 34   | 7             | 1.508436 | 0.418939 | -2.4036  |
| 35   | 1             | 0.658106 | 0.322995 | -1.85256 |
| 36   | 6             | 2.182965 | 1.601165 | -2.60448 |
| 37   | 6             | 2.327662 | -4.07489 | 2.880722 |
| 38   | 1             | 2.011242 | -4.01002 | 3.923828 |
| 39   | 1             | 2.005526 | -5.03746 | 2.4782   |
| 40   | 1             | 3.417791 | -4.04622 | 2.85608  |

|    |    |          |          |          |
|----|----|----------|----------|----------|
| 41 | 6  | 0.15765  | -3.06376 | 2.166429 |
| 42 | 1  | -0.15882 | -4.0275  | 1.761516 |
| 43 | 1  | -0.15368 | -3.00915 | 3.2124   |
| 44 | 1  | -0.37633 | -2.28463 | 1.620815 |
| 45 | 6  | 2.277315 | 2.88001  | 4.091642 |
| 46 | 1  | 1.948726 | 3.919669 | 4.031409 |
| 47 | 1  | 1.953373 | 2.467129 | 5.049192 |
| 48 | 1  | 3.367817 | 2.868598 | 4.070991 |
| 49 | 6  | 0.123105 | 2.145547 | 3.060602 |
| 50 | 1  | -0.19044 | 1.736846 | 4.024377 |
| 51 | 1  | -0.20178 | 3.186985 | 3.005479 |
| 52 | 1  | -0.40219 | 1.593754 | 2.279612 |
| 53 | 6  | 2.330746 | 4.082056 | -2.87123 |
| 54 | 1  | 2.022384 | 4.01557  | -3.91664 |
| 55 | 1  | 2.001432 | 5.043294 | -2.47135 |
| 56 | 1  | 3.420773 | 4.058168 | -2.83852 |
| 57 | 6  | 0.159936 | 3.062178 | -2.17207 |
| 58 | 1  | -0.16325 | 4.024407 | -1.76887 |
| 59 | 1  | -0.14384 | 3.006944 | -3.22025 |
| 60 | 1  | -0.37482 | 2.280591 | -1.63075 |
| 61 | 6  | 2.318304 | -2.87283 | -4.08239 |
| 62 | 1  | 1.993957 | -3.91395 | -4.02455 |
| 63 | 1  | 1.999291 | -2.46129 | -5.04217 |
| 64 | 1  | 3.408562 | -2.85652 | -4.05399 |
| 65 | 6  | 0.153594 | -2.14805 | -3.06677 |
| 66 | 1  | -0.15495 | -1.73989 | -4.03239 |
| 67 | 1  | -0.16689 | -3.19104 | -3.01499 |
| 68 | 1  | -0.37979 | -1.59955 | -2.289   |
| 69 | 17 | -0.84011 | -0.00274 | -0.00644 |
| 70 | 6  | -3.57244 | 2.367985 | -0.01648 |
| 71 | 1  | -2.79797 | 1.606338 | -0.03495 |
| 72 | 17 | -4.19399 | 2.563039 | -1.68181 |
| 73 | 17 | -4.85892 | 1.82382  | 1.095072 |
| 74 | 17 | -2.82139 | 3.889959 | 0.567344 |
| 75 | 6  | -3.56641 | -2.37783 | 0.004509 |
| 76 | 17 | -4.85743 | -1.8332  | -1.10151 |
| 77 | 17 | -4.18345 | -2.5822  | 1.670547 |
| 78 | 17 | -2.81159 | -3.89459 | -0.5876  |
| 79 | 1  | -2.79447 | -1.61365 | 0.024587 |

Cartesian coordinates (in Å) for the optimized OMCP·Cl<sup>-</sup>·2DCM structure.

| Atom | Atomic Number | x        | y        | z        |
|------|---------------|----------|----------|----------|
| 1    | 6             | -1.80734 | 3.061799 | -0.81405 |
| 2    | 6             | -2.74054 | 3.932594 | -0.28714 |
| 3    | 6             | -2.72594 | 3.784919 | 1.129238 |
| 4    | 6             | -1.78384 | 2.826405 | 1.446094 |
| 5    | 7             | -1.23319 | 2.401575 | 0.253854 |
| 6    | 1             | -0.50828 | 1.693856 | 0.17381  |
| 7    | 1             | -3.37018 | 4.603964 | -0.8492  |
| 8    | 1             | -3.34296 | 4.324296 | 1.83034  |
| 9    | 6             | -1.35471 | 2.269313 | 2.798754 |
| 10   | 6             | -2.90992 | 0.346558 | 3.719256 |
| 11   | 6             | -2.92727 | -1.06863 | 3.568441 |
| 12   | 1             | -3.60454 | 0.932169 | 4.300478 |
| 13   | 6             | -1.8718  | -1.42163 | 2.750836 |
| 14   | 1             | -3.63764 | -1.74624 | 4.015114 |
| 15   | 6             | -1.41345 | -2.79229 | 2.265137 |
| 16   | 6             | -2.773   | -3.91062 | 0.299063 |
| 17   | 6             | -2.76482 | -3.7632  | -1.11739 |
| 18   | 1             | -3.405   | -4.57683 | 0.864605 |
| 19   | 6             | -1.81668 | -2.8124  | -1.43943 |
| 20   | 1             | -3.39    | -4.29759 | -1.81508 |
| 21   | 6             | -1.39    | -2.25907 | -2.79438 |
| 22   | 6             | -2.93334 | -0.32263 | -3.70616 |
| 23   | 6             | -1.87434 | 1.436374 | -2.74369 |
| 24   | 6             | -2.93742 | 1.092649 | -3.55535 |
| 25   | 1             | -3.63648 | -0.90208 | -4.28331 |
| 26   | 1             | -3.64438 | 1.776428 | -3.99799 |
| 27   | 6             | -1.40125 | 2.803001 | -2.26064 |
| 28   | 7             | -1.22454 | -0.25028 | 2.411631 |
| 29   | 1             | -0.4131  | -0.19385 | 1.802974 |
| 30   | 6             | -1.84435 | 0.83815  | 2.991451 |
| 31   | 7             | -1.2562  | -2.39195 | -0.25022 |
| 32   | 1             | -0.52515 | -1.69009 | -0.17436 |
| 33   | 6             | -1.82991 | -3.04742 | 0.820821 |
| 34   | 7             | -1.23551 | 0.259376 | -2.40801 |
| 35   | 1             | -0.4213  | 0.195959 | -1.8038  |
| 36   | 6             | -1.86804 | -0.82359 | -2.98438 |
| 37   | 6             | -1.95936 | 3.150743 | 3.910206 |
| 38   | 1             | -1.65406 | 2.776199 | 4.88979  |
| 39   | 1             | -1.60852 | 4.180004 | 3.804125 |
| 40   | 1             | -3.05034 | 3.158363 | 3.873834 |

|    |    |          |          |          |
|----|----|----------|----------|----------|
| 41 | 6  | 0.188432 | 2.332973 | 2.938956 |
| 42 | 1  | 0.52771  | 3.367926 | 2.840003 |
| 43 | 1  | 0.490824 | 1.95855  | 3.921251 |
| 44 | 1  | 0.706119 | 1.739392 | 2.183522 |
| 45 | 6  | -2.05319 | -3.87142 | 3.161597 |
| 46 | 1  | -1.72065 | -4.86415 | 2.849186 |
| 47 | 1  | -1.75889 | -3.71416 | 4.201657 |
| 48 | 1  | -3.14313 | -3.84671 | 3.10892  |
| 49 | 6  | 0.125921 | -2.92177 | 2.404299 |
| 50 | 1  | 0.424139 | -2.77548 | 3.446425 |
| 51 | 1  | 0.441618 | -3.92024 | 2.08692  |
| 52 | 1  | 0.662345 | -2.18945 | 1.798516 |
| 53 | 6  | -2.00843 | -3.13497 | -3.90263 |
| 54 | 1  | -1.70487 | -2.76311 | -4.88379 |
| 55 | 1  | -1.66633 | -4.16737 | -3.79845 |
| 56 | 1  | -3.09923 | -3.13277 | -3.86055 |
| 57 | 6  | 0.151699 | -2.33641 | -2.94299 |
| 58 | 1  | 0.482296 | -3.37437 | -2.84608 |
| 59 | 1  | 0.452079 | -1.96449 | -3.92685 |
| 60 | 1  | 0.678798 | -1.74779 | -2.19022 |
| 61 | 6  | -2.03656 | 3.887643 | -3.15359 |
| 62 | 1  | -1.69388 | 4.877464 | -2.84292 |
| 63 | 1  | -1.74929 | 3.727927 | -4.19524 |
| 64 | 1  | -3.12637 | 3.872274 | -3.09499 |
| 65 | 6  | 0.138381 | 2.918872 | -2.40863 |
| 66 | 1  | 0.429338 | 2.769484 | -3.45237 |
| 67 | 1  | 0.464747 | 3.914683 | -2.09368 |
| 68 | 1  | 0.671895 | 2.182168 | -1.80558 |
| 69 | 6  | 3.592849 | -2.68468 | 0.21256  |
| 70 | 1  | 3.123158 | -1.71904 | 0.04851  |
| 71 | 17 | 4.401362 | -3.20018 | -1.30785 |
| 72 | 17 | 4.745549 | -2.53685 | 1.5834   |
| 73 | 6  | 3.612019 | 2.656191 | -0.22532 |
| 74 | 17 | 4.76002  | 2.503686 | -1.5996  |
| 75 | 17 | 4.427698 | 3.164945 | 1.293486 |
| 76 | 1  | 3.137273 | 1.693039 | -0.06132 |
| 77 | 1  | 2.868554 | -3.44713 | 0.47406  |
| 78 | 1  | 2.891337 | 3.42309  | -0.48377 |
| 79 | 17 | 1.157458 | -0.00631 | -0.0042  |



Cartesian coordinates (in Å) for the optimized OMCP·Br<sup>-</sup>·2TCM structure.

| Atom | Atomic Number | x        | y        | z        |
|------|---------------|----------|----------|----------|
| 1    | 6             | 2.299462 | 2.906602 | 1.18238  |
| 2    | 6             | 3.320237 | 3.739227 | 0.76924  |
| 3    | 6             | 3.320442 | 3.760307 | -0.65397 |
| 4    | 6             | 2.29992  | 2.940171 | -1.09201 |
| 5    | 7             | 1.689613 | 2.431555 | 0.037828 |
| 6    | 1             | 0.890469 | 1.807159 | 0.029086 |
| 7    | 1             | 3.999845 | 4.276118 | 1.411897 |
| 8    | 1             | 4.000018 | 4.316205 | -1.28028 |
| 9    | 6             | 1.857953 | 2.585419 | -2.50794 |
| 10   | 6             | 3.355094 | 0.769251 | -3.69839 |
| 11   | 6             | 3.355914 | -0.65388 | -3.72058 |
| 12   | 1             | 4.048077 | 1.412609 | -4.21709 |
| 13   | 6             | 2.313757 | -1.09243 | -2.9284  |
| 14   | 1             | 4.04951  | -1.27999 | -4.25918 |
| 15   | 6             | 1.862288 | -2.50832 | -2.58605 |
| 16   | 6             | 3.326721 | -3.73568 | -0.76786 |
| 17   | 6             | 3.326111 | -3.75678 | 0.655364 |
| 18   | 1             | 4.007401 | -4.27168 | -1.41013 |
| 19   | 6             | 2.304213 | -2.93803 | 1.092794 |
| 20   | 1             | 4.006038 | -4.3118  | 1.282069 |
| 21   | 6             | 1.86074  | -2.58393 | 2.508415 |
| 22   | 6             | 3.354168 | -0.76531 | 3.699737 |
| 23   | 6             | 2.310213 | 1.094668 | 2.9292   |
| 24   | 6             | 3.352633 | 0.657817 | 3.72197  |
| 25   | 1             | 4.047905 | -1.40755 | 4.218818 |
| 26   | 1             | 4.044886 | 1.285039 | 4.260995 |
| 27   | 6             | 1.856589 | 2.509807 | 2.586618 |
| 28   | 7             | 1.689777 | 0.036833 | -2.43531 |
| 29   | 1             | 0.875723 | 0.027326 | -1.82999 |
| 30   | 6             | 2.312322 | 1.181642 | -2.89308 |
| 31   | 7             | 1.6939   | -2.43024 | -0.0374  |
| 32   | 1             | 0.894    | -1.80683 | -0.02909 |
| 33   | 6             | 2.305061 | -2.90444 | -1.18159 |
| 34   | 7             | 1.688385 | -0.0356  | 2.435707 |
| 35   | 1             | 0.874667 | -0.02734 | 1.829914 |
| 36   | 6             | 2.312551 | -1.1794  | 2.893808 |
| 37   | 6             | 2.490994 | 3.593934 | -3.48804 |
| 38   | 1             | 2.1794   | 3.365808 | -4.5099  |
| 39   | 1             | 2.168344 | 4.607706 | -3.23995 |
| 40   | 1             | 3.581431 | 3.566156 | -3.45142 |

|    |    |          |          |          |
|----|----|----------|----------|----------|
| 41 | 6  | 0.319263 | 2.710528 | -2.64198 |
| 42 | 1  | 0.003799 | 3.727814 | -2.39431 |
| 43 | 1  | 0.015644 | 2.489652 | -3.66933 |
| 44 | 1  | -0.22065 | 2.027369 | -1.9843  |
| 45 | 6  | 2.497549 | -3.48542 | -3.59607 |
| 46 | 1  | 2.177431 | -4.50697 | -3.37843 |
| 47 | 1  | 2.185115 | -3.22762 | -4.6106  |
| 48 | 1  | 3.587929 | -3.45618 | -3.55878 |
| 49 | 6  | 0.323831 | -2.63259 | -2.7241  |
| 50 | 1  | 0.020206 | -2.38258 | -3.74475 |
| 51 | 1  | 0.010406 | -3.65732 | -2.50621 |
| 52 | 1  | -0.21791 | -1.97008 | -2.0471  |
| 53 | 6  | 2.494731 | -3.59139 | 3.488974 |
| 54 | 1  | 2.182191 | -3.36366 | 4.510638 |
| 55 | 1  | 2.173758 | -4.60568 | 3.240784 |
| 56 | 1  | 3.585147 | -3.56197 | 3.452998 |
| 57 | 6  | 0.322156 | -2.71151 | 2.641368 |
| 58 | 1  | 0.008498 | -3.72927 | 2.393344 |
| 59 | 1  | 0.017444 | -2.49124 | 3.66852  |
| 60 | 1  | -0.21836 | -2.02914 | 1.983371 |
| 61 | 6  | 2.489776 | 3.487954 | 3.596932 |
| 62 | 1  | 2.168173 | 4.508988 | 3.379073 |
| 63 | 1  | 2.177215 | 3.229695 | 4.611303 |
| 64 | 1  | 3.580218 | 3.460417 | 3.560216 |
| 65 | 6  | 0.317872 | 2.631572 | 2.723976 |
| 66 | 1  | 0.014225 | 2.381101 | 3.744501 |
| 67 | 1  | 0.002859 | 3.655779 | 2.505927 |
| 68 | 1  | -0.22252 | 1.968153 | 2.046779 |
| 69 | 6  | -3.64599 | -2.58911 | 0.001549 |
| 70 | 1  | -2.86312 | -1.83189 | 0.00087  |
| 71 | 17 | -4.60221 | -2.39606 | 1.502926 |
| 72 | 17 | -4.66931 | -2.32917 | -1.44446 |
| 73 | 17 | -2.86218 | -4.19823 | -0.05266 |
| 74 | 6  | -3.64643 | 2.586085 | -0.00251 |
| 75 | 17 | -4.67042 | 2.325342 | 1.442876 |
| 76 | 17 | -4.60207 | 2.39421  | -1.50443 |
| 77 | 17 | -2.86234 | 4.194995 | 0.05309  |
| 78 | 1  | -2.86372 | 1.828695 | -0.00204 |
| 79 | 35 | -1.00456 | -0.00142 | -0.00078 |

Cartesian coordinates (in Å) for the optimized OMCP·Br<sup>-</sup>·2DCM structure.

| Atom | Atomic Number | x        | y        | z        |
|------|---------------|----------|----------|----------|
| 1    | 6             | 1.956806 | 2.985442 | 0.98199  |
| 2    | 6             | 2.962842 | 3.807333 | 0.514491 |
| 3    | 6             | 2.965187 | 3.732498 | -0.90697 |
| 4    | 6             | 1.960146 | 2.866396 | -1.28902 |
| 5    | 7             | 1.356041 | 2.424708 | -0.12821 |
| 6    | 1             | 0.573603 | 1.778383 | -0.09688 |
| 7    | 1             | 3.631162 | 4.398718 | 1.120049 |
| 8    | 1             | 3.635827 | 4.257182 | -1.56882 |
| 9    | 6             | 1.525029 | 2.410095 | -2.67737 |
| 10   | 6             | 3.02866  | 0.51531  | -3.72884 |
| 11   | 6             | 3.028472 | -0.90582 | -3.65333 |
| 12   | 1             | 3.724089 | 1.121205 | -4.28778 |
| 13   | 6             | 1.981094 | -1.28812 | -2.83892 |
| 14   | 1             | 3.724475 | -1.5676  | -4.14406 |
| 15   | 6             | 1.523938 | -2.6774  | -2.40732 |
| 16   | 6             | 2.96089  | -3.81008 | -0.50779 |
| 17   | 6             | 2.959253 | -3.73523 | 0.913684 |
| 18   | 1             | 3.630056 | -4.40247 | -1.11143 |
| 19   | 6             | 1.954456 | -2.86756 | 1.292824 |
| 20   | 1             | 3.627164 | -4.26095 | 1.577455 |
| 21   | 6             | 1.515816 | -2.41087 | 2.679937 |
| 22   | 6             | 3.01745  | -0.51701 | 3.735856 |
| 23   | 6             | 1.973642 | 1.287074 | 2.842837 |
| 24   | 6             | 3.018335 | 0.90412  | 3.66038  |
| 25   | 1             | 3.710829 | -1.12334 | 4.296857 |
| 26   | 1             | 3.713287 | 1.565451 | 4.153193 |
| 27   | 6             | 1.518784 | 2.676673 | 2.409862 |
| 28   | 7             | 1.355366 | -0.12765 | -2.42777 |
| 29   | 1             | 0.54105  | -0.09584 | -1.82202 |
| 30   | 6             | 1.981734 | 0.98237  | -2.9593  |
| 31   | 7             | 1.354367 | -2.42498 | 0.130262 |
| 32   | 1             | 0.573042 | -1.77742 | 0.096698 |
| 33   | 6             | 1.957482 | -2.98664 | -0.97819 |
| 34   | 7             | 1.348478 | 0.126982 | 2.429728 |
| 35   | 1             | 0.535853 | 0.095587 | 1.821654 |
| 36   | 6             | 1.972576 | -0.98342 | 2.963135 |
| 37   | 6             | 2.161475 | 3.346215 | -3.72493 |
| 38   | 1             | 1.85259  | 3.046323 | -4.72887 |
| 39   | 1             | 1.838243 | 4.375209 | -3.55123 |
| 40   | 1             | 3.251864 | 3.321351 | -3.68322 |

|    |    |          |          |          |
|----|----|----------|----------|----------|
| 41 | 6  | -0.01352 | 2.523712 | -2.82624 |
| 42 | 1  | -0.32887 | 3.557466 | -2.65827 |
| 43 | 1  | -0.31342 | 2.227031 | -3.83538 |
| 44 | 1  | -0.55615 | 1.891906 | -2.12103 |
| 45 | 6  | 2.158807 | -3.71916 | -3.35081 |
| 46 | 1  | 1.8329   | -4.72386 | -3.07173 |
| 47 | 1  | 1.852946 | -3.52386 | -4.38113 |
| 48 | 1  | 3.249059 | -3.69256 | -3.30948 |
| 49 | 6  | -0.01502 | -2.80505 | -2.54273 |
| 50 | 1  | -0.31678 | -2.61742 | -3.57714 |
| 51 | 1  | -0.32724 | -3.8167  | -2.26601 |
| 52 | 1  | -0.55455 | -2.10032 | -1.90735 |
| 53 | 6  | 2.148803 | -3.34734 | 3.729268 |
| 54 | 1  | 1.837496 | -3.04712 | 4.732353 |
| 55 | 1  | 1.825278 | -4.37612 | 3.554815 |
| 56 | 1  | 3.239315 | -3.32326 | 3.690422 |
| 57 | 6  | -0.02323 | -2.52357 | 2.824567 |
| 58 | 1  | -0.33874 | -3.55709 | 2.65546  |
| 59 | 1  | -0.32571 | -2.22699 | 3.832972 |
| 60 | 1  | -0.5635  | -1.89119 | 2.118076 |
| 61 | 6  | 2.151713 | 3.718011 | 3.355127 |
| 62 | 1  | 1.827303 | 4.722933 | 3.075078 |
| 63 | 1  | 1.842795 | 3.522971 | 4.384578 |
| 64 | 1  | 3.242056 | 3.690637 | 3.316892 |
| 65 | 6  | -0.02044 | 2.805563 | 2.540794 |
| 66 | 1  | -0.32526 | 2.618717 | 3.574454 |
| 67 | 1  | -0.33107 | 3.817316 | 2.26266  |
| 68 | 1  | -0.55872 | 2.100875 | 1.904307 |
| 69 | 6  | -3.69723 | -2.90551 | -0.22718 |
| 70 | 1  | -3.32718 | -1.90829 | -0.00979 |
| 71 | 17 | -4.39072 | -3.6038  | 1.276937 |
| 72 | 17 | -4.90783 | -2.79139 | -1.55    |
| 73 | 6  | -3.69659 | 2.90726  | 0.221906 |
| 74 | 17 | -4.91129 | 2.792589 | 1.540984 |
| 75 | 17 | -4.38499 | 3.607704 | -1.28347 |
| 76 | 1  | -3.32662 | 1.909989 | 0.004566 |
| 77 | 35 | -1.29432 | 0.000586 | -0.00254 |
| 78 | 1  | -2.90469 | -3.56452 | -0.5618  |
| 79 | 1  | -2.90455 | 3.565282 | 0.559644 |