Supplemental Material to: "Coupled Cluster Theory for Molecular Polaritons: Changing Ground and Excited States"

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I. MOLECULAR STRUCTURES

Here we provide the geometrical structure for the investigated molecules.

A. p-Nitroaniline (pNA)

Geometry of pNA calculated at the DFT/B3LYP level of theory using a 6-31G+* basis set.

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16

N   -2.15746458      0.00000000      0.00000000
C   -0.70321472      0.00000000      0.00000000
C   -0.01145721      1.21693110      0.00000000
H   -0.56773625      2.14697503      0.00000000
C    1.37482052      1.21656683      0.00000000
H    1.91425302      2.16055505      0.00000000
C    2.09546989      0.00000000      0.00000000
N    3.46611936      0.00000000      0.00000000
H    3.99010150      0.86140500      0.00000000
H    3.99010150     -0.86140500      0.00000000
C    1.37482052     -1.21656683      0.00000000
H    1.91425302     -2.16055505      0.00000000
C   -0.01145721     -1.21693110      0.00000000
H   -0.56773625     -2.14697503      0.00000000
O   -2.73965974      1.09143620      0.00000000
O   -2.73965974     -1.09143620      0.00000000
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B. Pyrrole

Geometry of Pyrrole calculated at the CCSD level of theory using a cc-pVDZ basis set.

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10

N     0.00000000      0.00000000      0.00000000
H     0.00000000      0.00000000      1.01019949
C     1.12779983      0.00000000     -0.79129811
C     0.71810282      0.00000000     -2.11542468
C    -0.71808175      0.00000000     -2.11543102
C    -1.12779084      0.00000000     -0.79130781
H    -2.12399903      0.00000000     -0.35161374
H    -1.37447592      0.00000000     -2.98538446
H     1.37450412      0.00000000     -2.98537279
H     2.12400236      0.00000000     -0.35159139
```