Supporting Information

The Information Content of the Conditional Pair Density as a Theoretical Tool for the Analysis of the Sigma Hole in Halogen Bonded Systems

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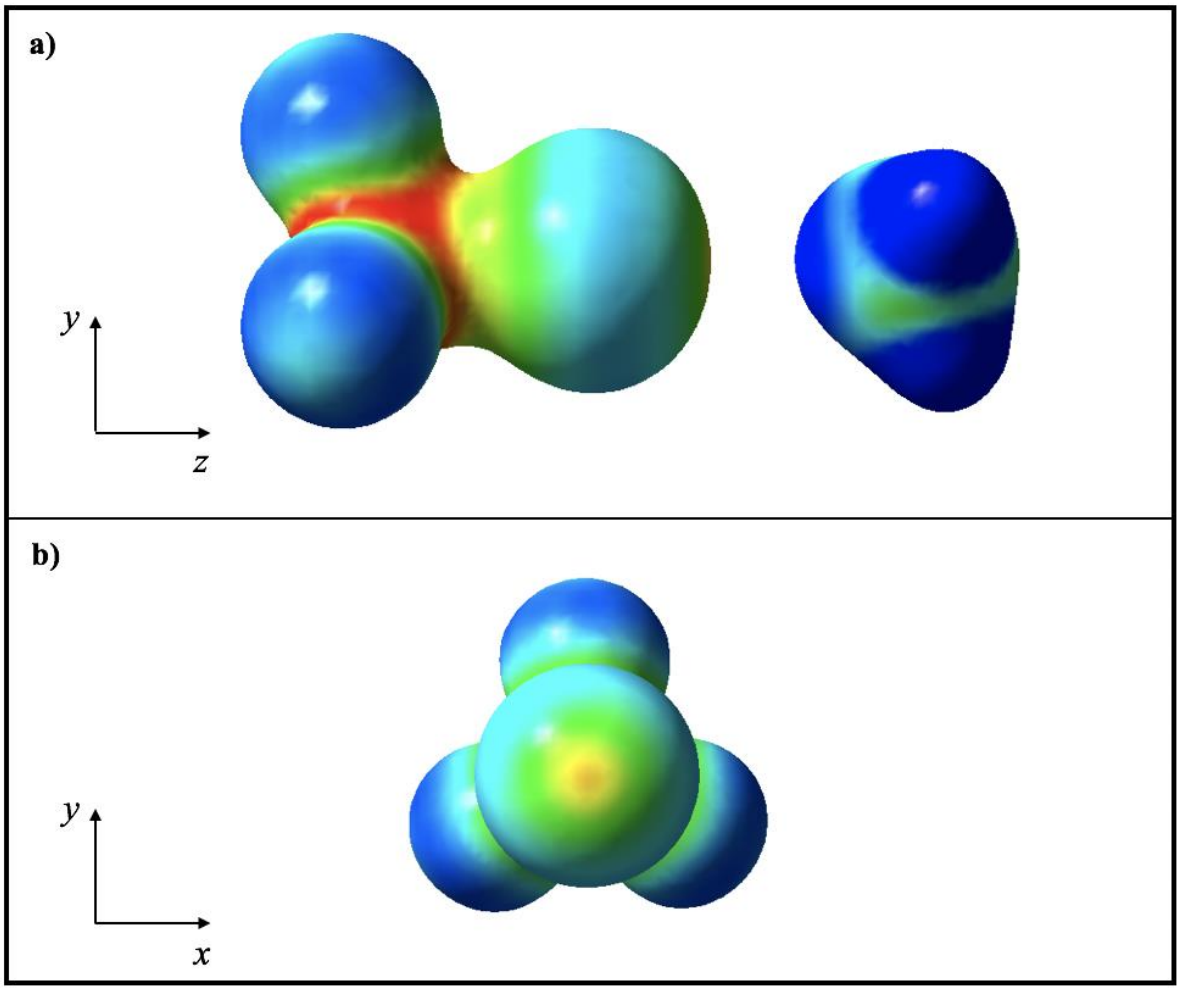
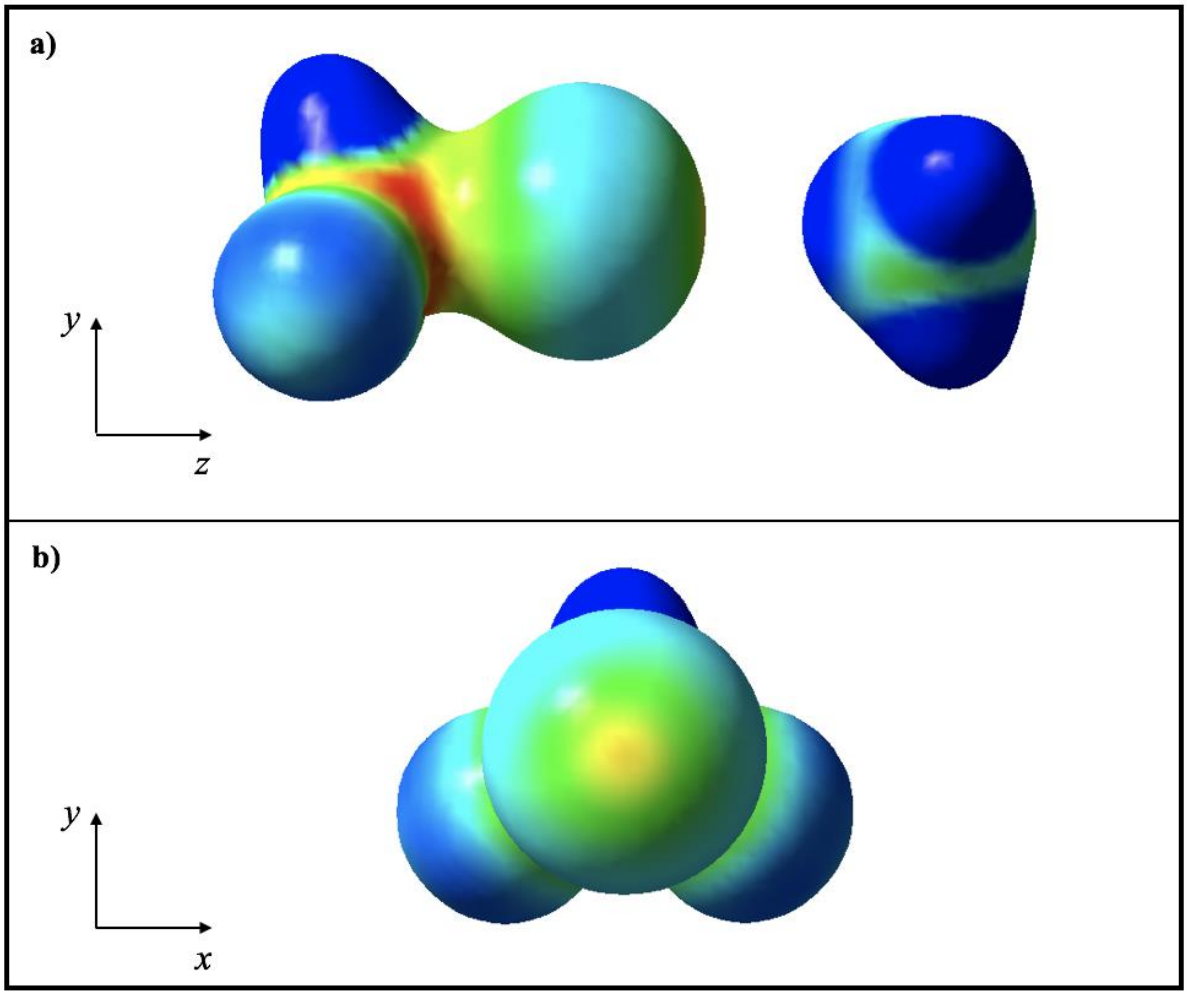
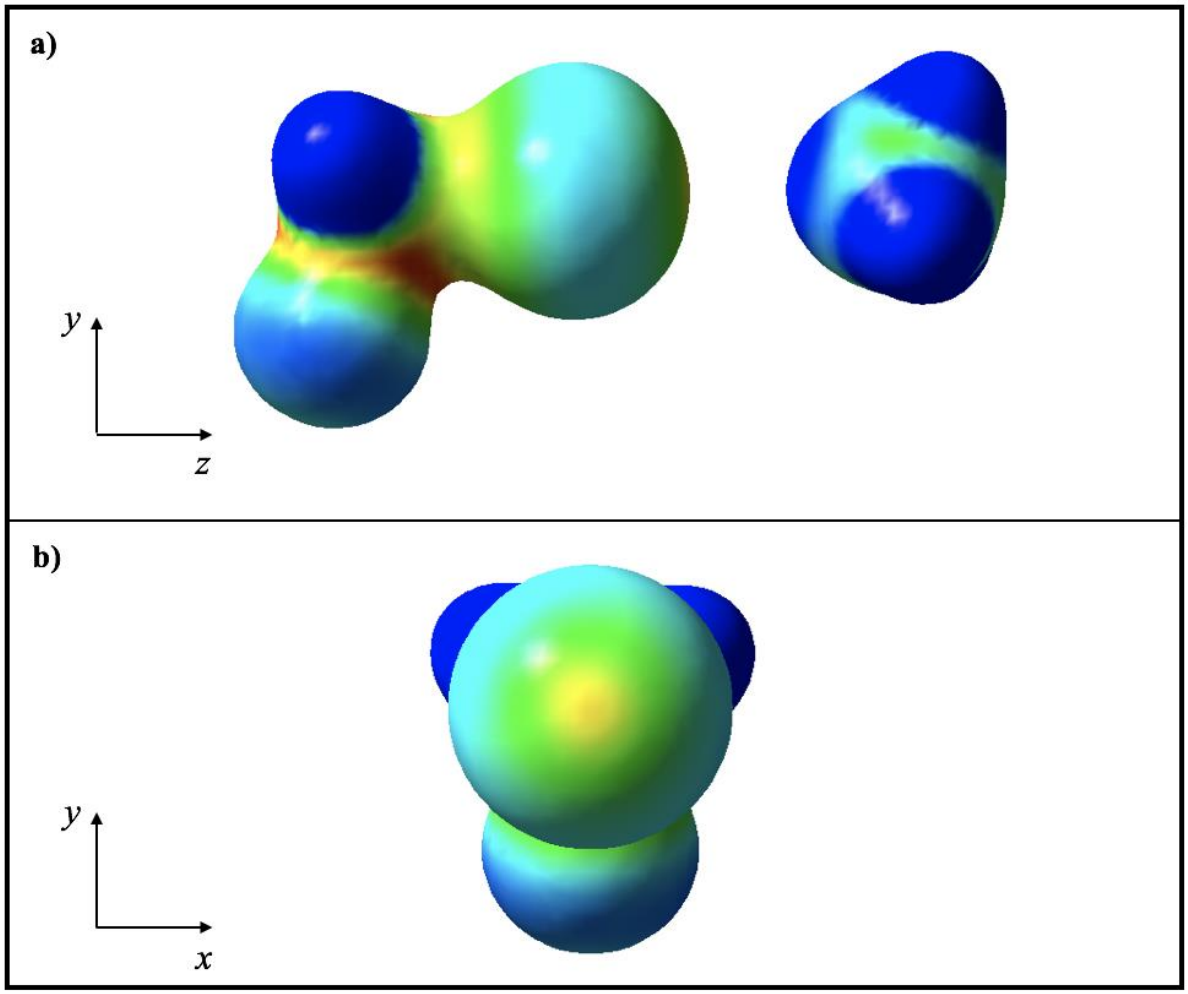
Figure S1: χ_{XC}^{σ} mapped onto the 0.04 a.u. isovalue of the electronic density for the the R—Br ··NH$_3$ complexes (R = CF_3, CHF_2, CH_2F, CH_3, CH_3CH_2, CH_2CH, and CHC). The range 0.2 – 0.5 goes from red to blue. For a sake of clarity, the NH3 molecule and map are hidden in the view of the lower part of the figures.



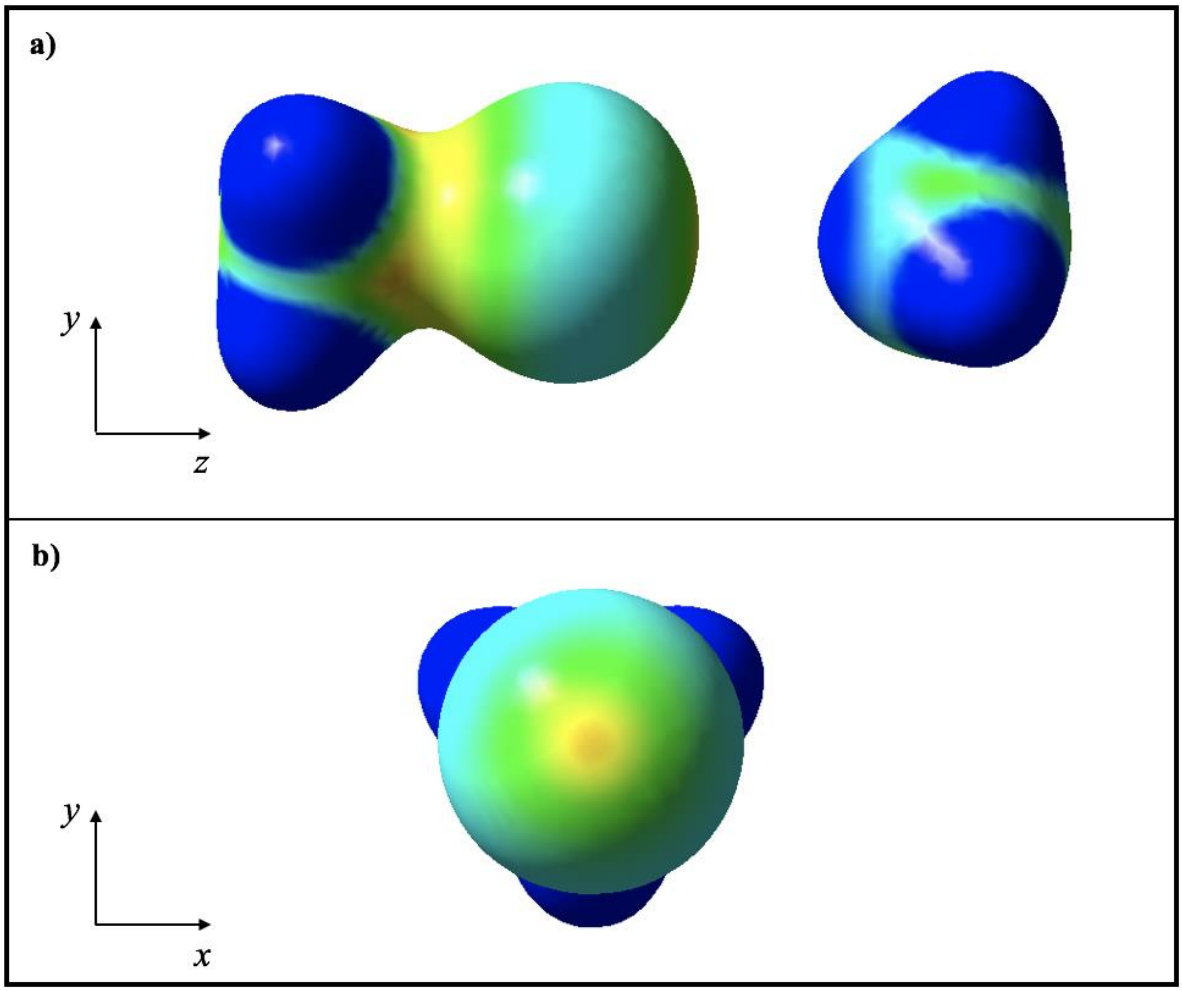
CF_3—Br ··NH$_3$



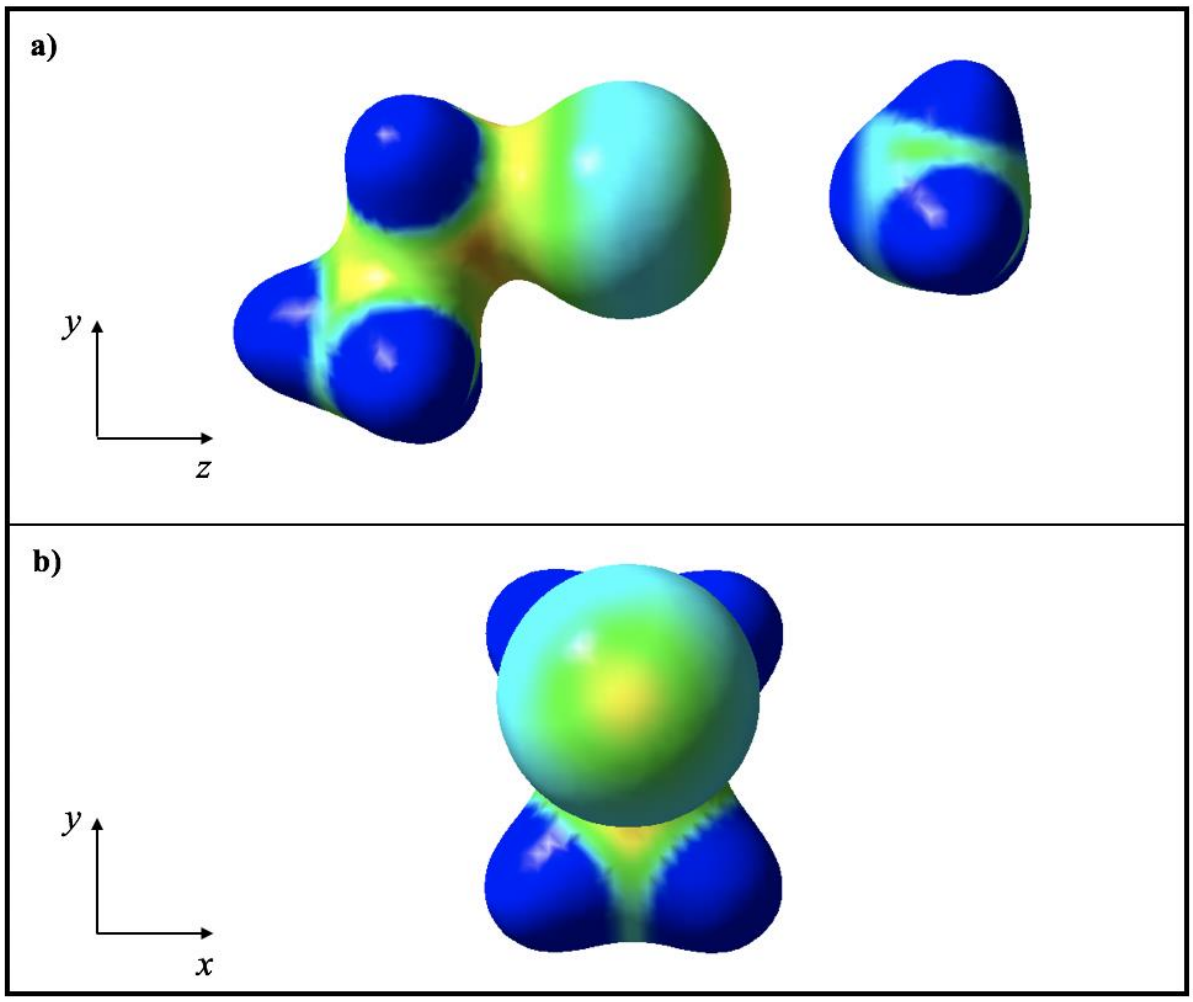
CHF_2—Br ··· NH_3



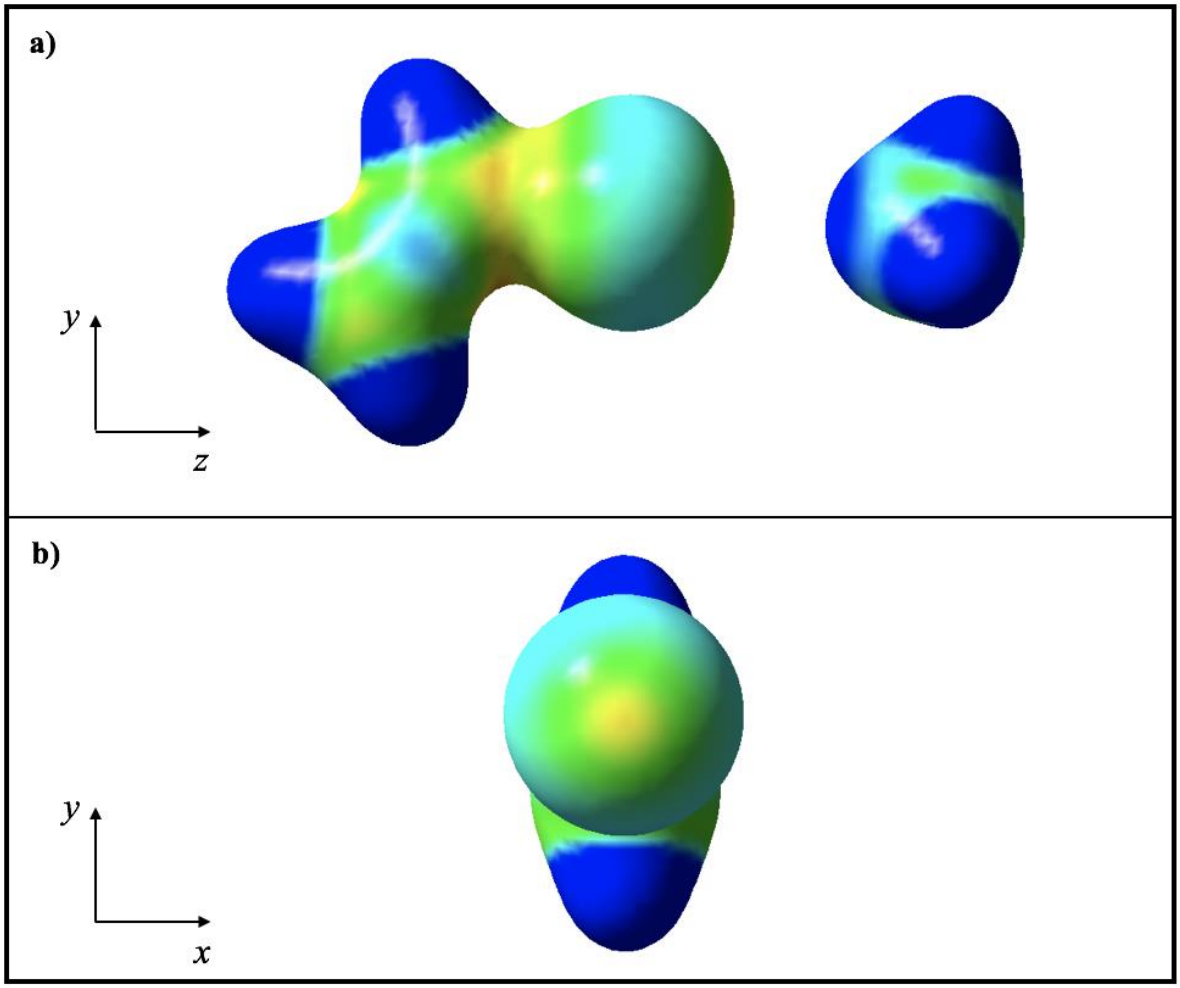
$CH_2F—Br\cdots NH_3$



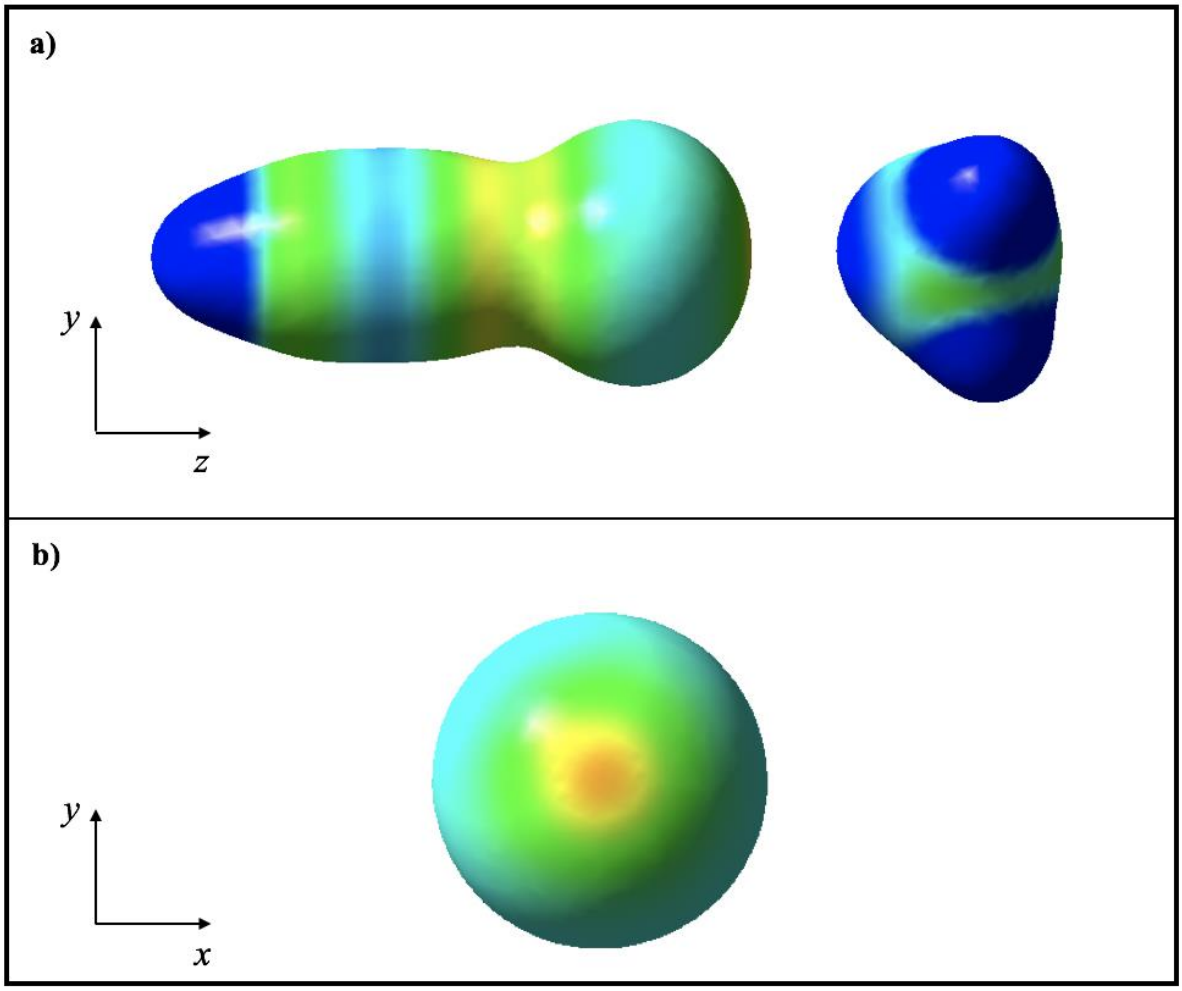
CH_3—Br ··NH_3



CH_3CH_2—Br ··· NH_3



$CH_2CH—Br \cdots NH_3$



CHC—Br ··NH$_3$