

Supplementary information for: Constrained Subsystem Density Functional Theory

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1 Diabatic States generated on DNA

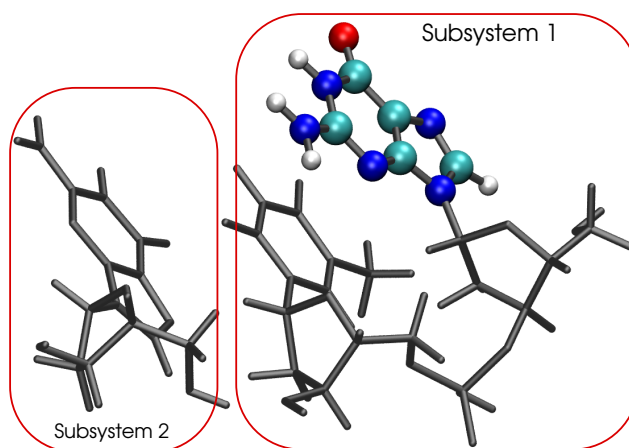


Figure S1: Diabatic state G_1 , C atoms in cyan, N atoms in blue, O atoms in red and H atoms in white. In black the non-constrained atoms.

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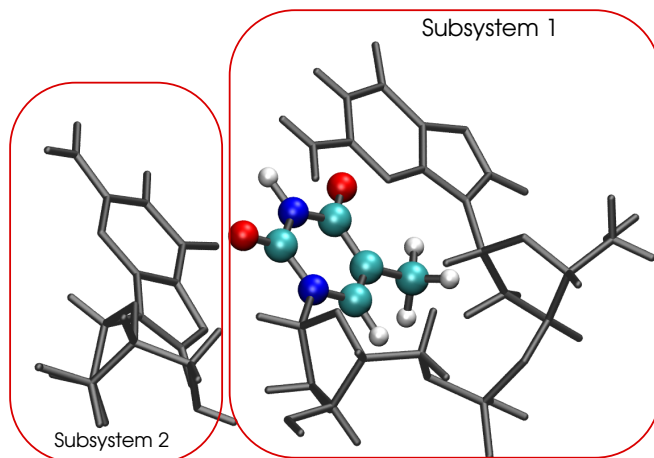


Figure S2: Diabatic state T, C atoms in cyan, N atoms in blue, O atoms in red and H atoms in white. In black the non-constrained atoms.

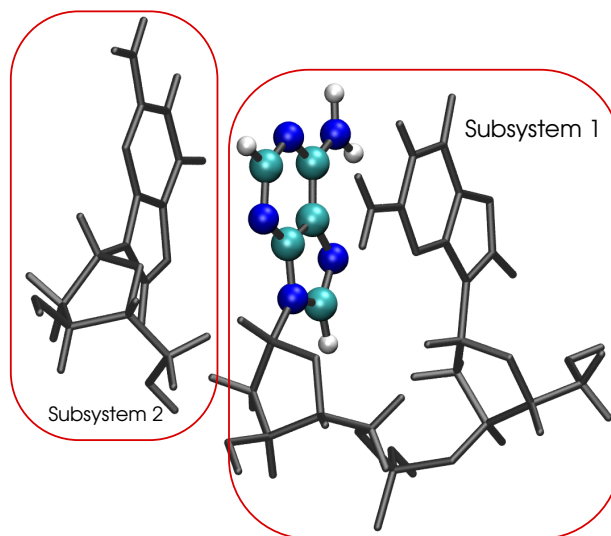


Figure S3: Diabatic state A, C atoms in cyan, N atoms in blue and H atoms in white. In black the non-constrained atoms.

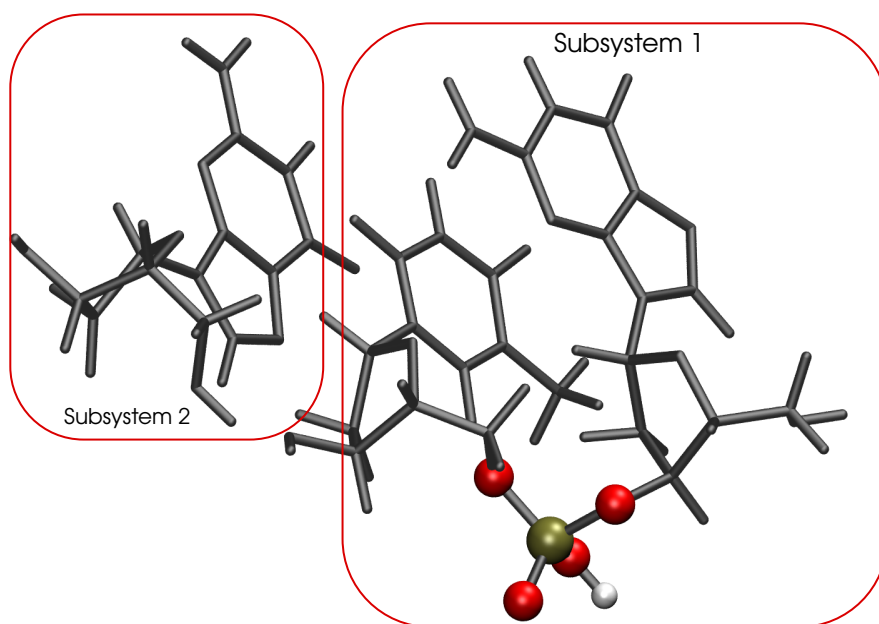


Figure S4: Diabatic state PO_4 , P atoms in yellow, O atoms in red and H atoms in white. In black the non-constrained atoms.

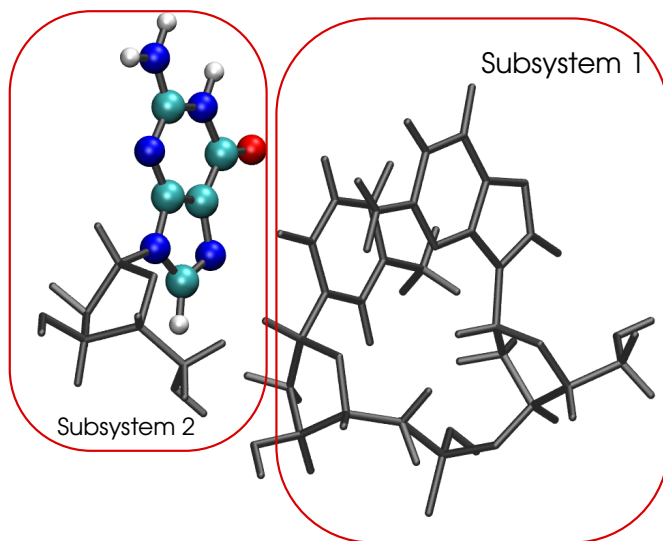


Figure S5: Diabatic state G_2 , C atoms in cyan, N atoms in blue, O atoms in red and H atoms in white. In black the non-constrained atoms.