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Supplementary Material

Substituted naphthalenes: stability, conformational flexibility and description of bonding based on ETS-NOCV method

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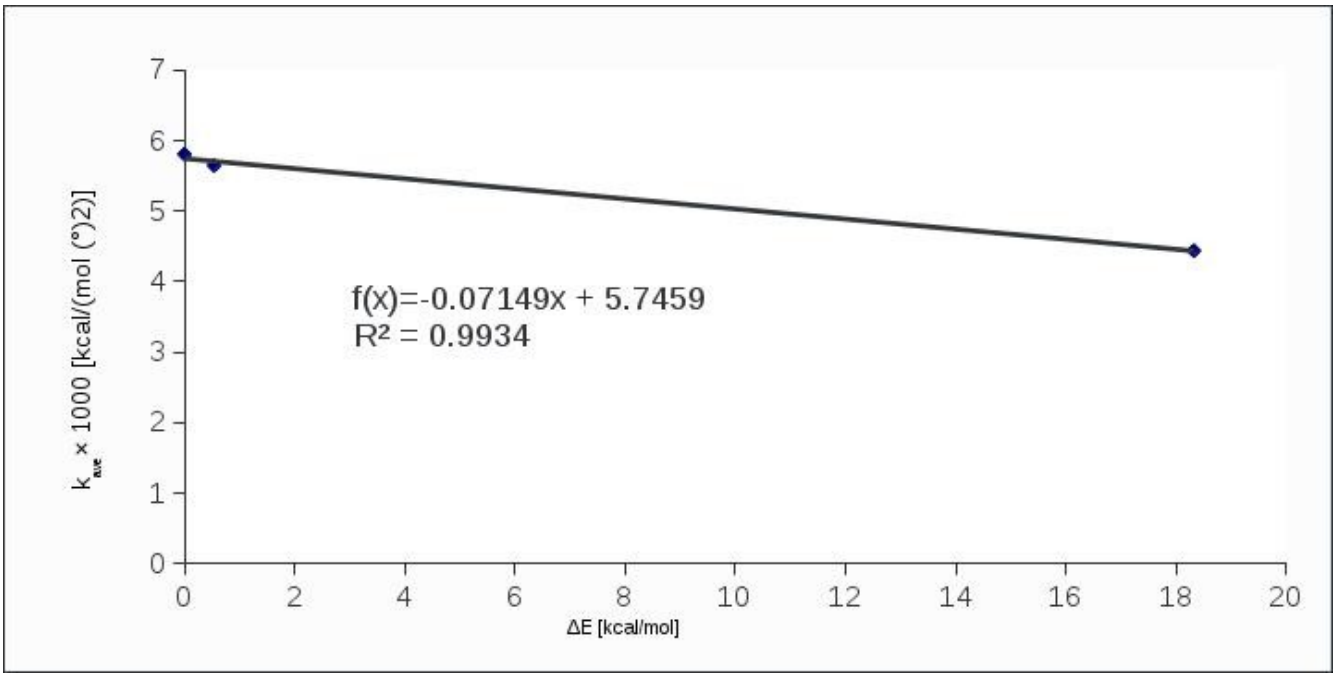
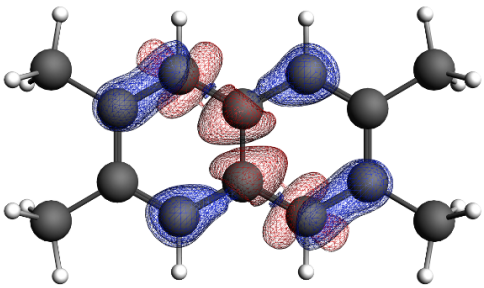
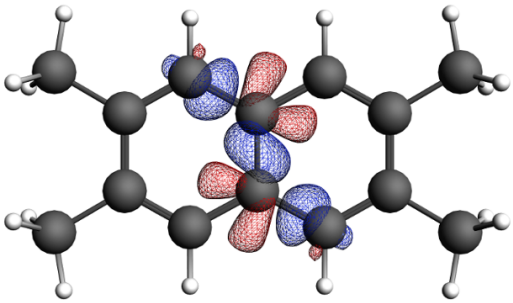


Figure S1

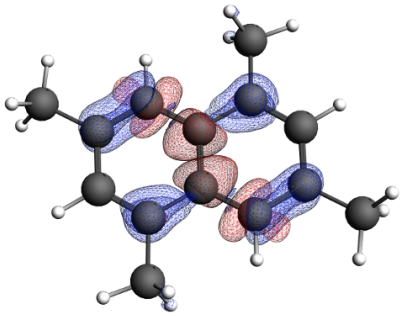
The relationship between averaged rigidity constants for 2,3,6,7-TeMN, 1,3,5,7-TeMN, and 1,4,5,8-TeMN ($k_{ave}=(k_1 + k_2)/2$), calculated at the MP2/cc-pVDZ level of theory and corresponding relative energies calculated at the B3LYP/cc-pVTZ level of theory (ΔE).



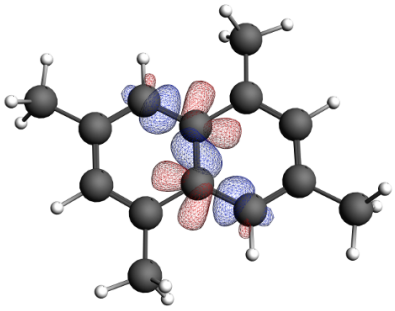
ΔEorb1= -774.7 kcal/mol



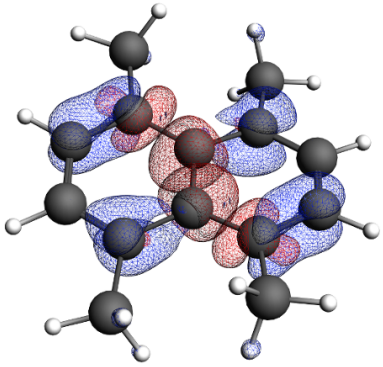
ΔEorb2= -216.2 kcal/mol



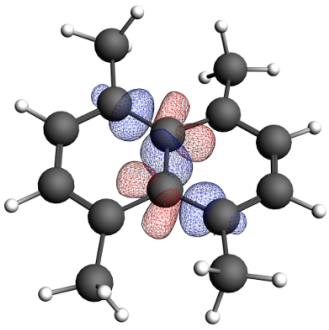
ΔEorb1= -753.9 kcal/mol



ΔEorb2= -220.9 kcal/mol



ΔEorb1= -679.6 kcal/mol



ΔEorb2= -202.9 kcal/mol

Figure S2

The deformation density plots $\Delta\rho_1$ and $\Delta\rho_2$ corresponding to most important NOCV pair of orbitals and orbital stabilization energies (ΔEorb1 and ΔEorb2) for 2,3,6,7-TeMN, 1,3,5,7-TeMN, and 1,4,5,8-TeMN obtained at the BLYP/TZ2P level of theory (the contour values: ±0.006 a.u). The direction of the charge flow in the deformation density plot Δρ is from the red to the blue region.

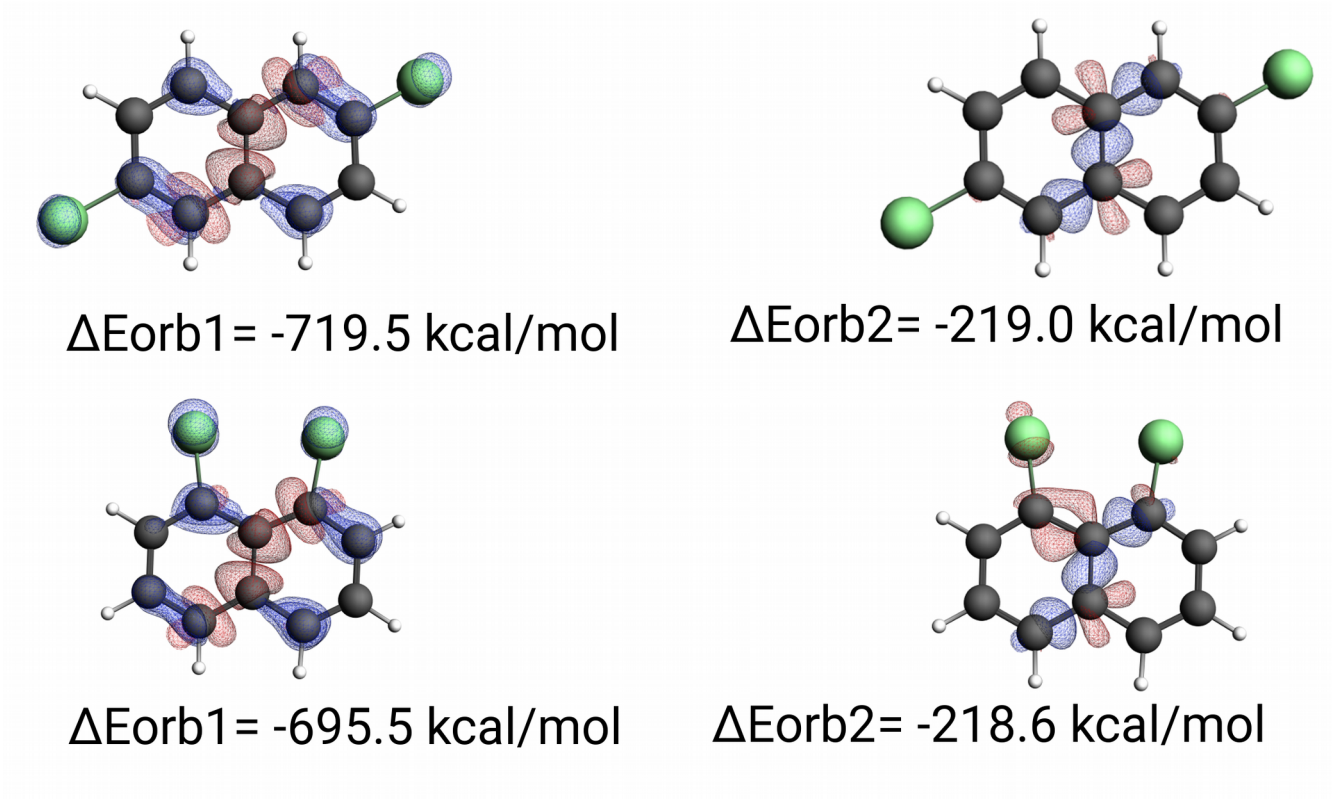
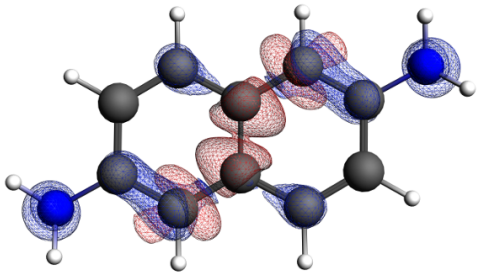
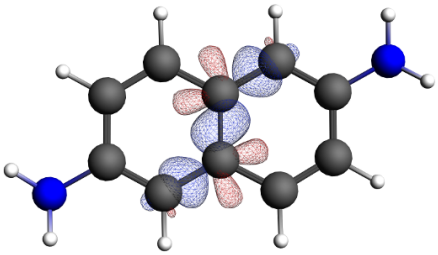


Figure S3

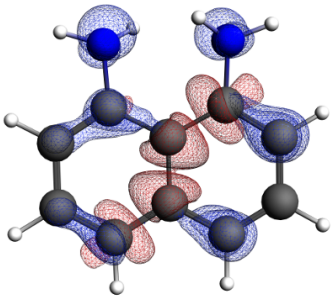
The deformation density plots $\Delta\rho_1$ and $\Delta\rho_2$ corresponding to most important NOCV pair of orbitals and orbital stabilization energies (ΔEorb1 and ΔEorb2) for 2,6-DCN and 1,8-DCN obtained at the BLYP/TZ2P level of theory (the contour values: ±0.006 a.u). The direction of the charge flow in the deformation density plot Δρ is from the red to the blue region.



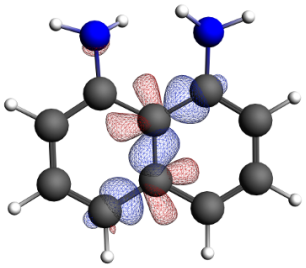
ΔEorb1= -708.3 kcal/mol



ΔEorb2= -224.2 kcal/mol



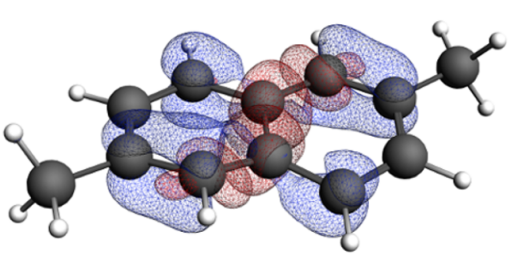
ΔEorb1= -701.3 kcal/mol

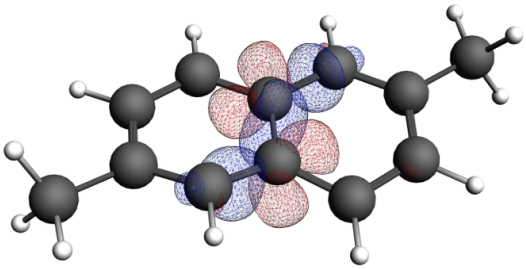


ΔEorb2= -211.9 kcal/mol

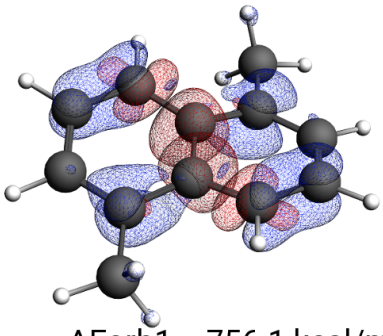
Figure S4

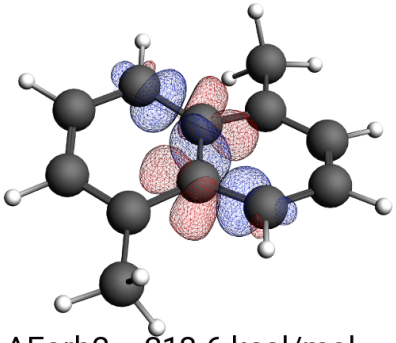
The deformation density plots $\Delta\rho_1$ and $\Delta\rho_2$ corresponding to most important NOCV pair of orbitals and orbital stabilization energies (ΔEorb1 and ΔEorb2) for 2,6-DAN and 1,8-DAN obtained at the BLYP/TZ2P level of theory (the contour values: ±0.006 a.u). The direction of the charge flow in the deformation density plot Δρ is from the red to the blue region.





ΔEorb1= -761.2 kcal/mol	0 deg	ΔEorb2= -217.2 kcal/mol
ΔEorb1= -731.3 kcal/mol	5 deg	ΔEorb2= -214.5 kcal/mol
ΔEorb1= -708.7 kcal/mol	15 deg	ΔEorb2= -211.8 kcal/mol





ΔEorb1= -756.1 kcal/mol	0 deg	ΔEorb2= -218.6 kcal/mol
ΔEorb1= -705.9 kcal/mol	5 deg	ΔEorb2= -208.7 kcal/mol
ΔEorb1= -667.4 kcal/mol	15 deg	ΔEorb2= -207.3 kcal/mol

Figure S5

The change of orbital energies ΔEorb1 and ΔEorb2 of 2,6-DMN and 1,5-DMN for two most important deformation density channels ($\Delta\rho_1$ and $\Delta\rho_2$, respectively) with the out-of-plane deformation angles 0º, 5º, and 15º obtained at the BLYP/TZ2P level of theory. The direction of the charge flow in the deformation density plot Δρ is from the red to the blue region.