Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Anharmonic vibrations from the Chloride•••Amide Ionic Hydrogen Bonds in Cl^-(*N*-methylacetamide)$_1$(H_2O)$_{0-2}$$Ar_2$ Cluster Ions. Combined IRPD experiments and BOMD simulations.

Supplementary Information

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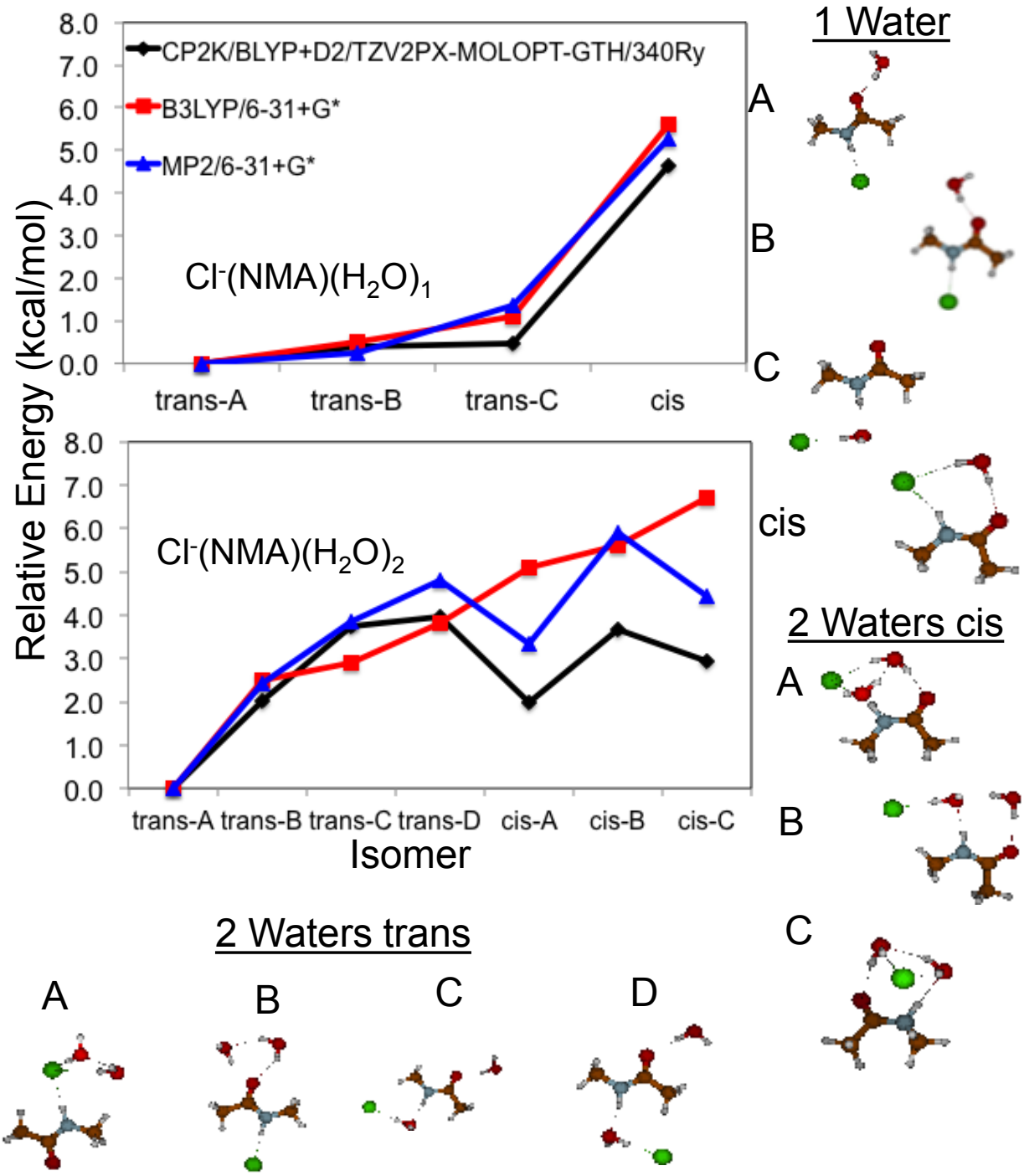
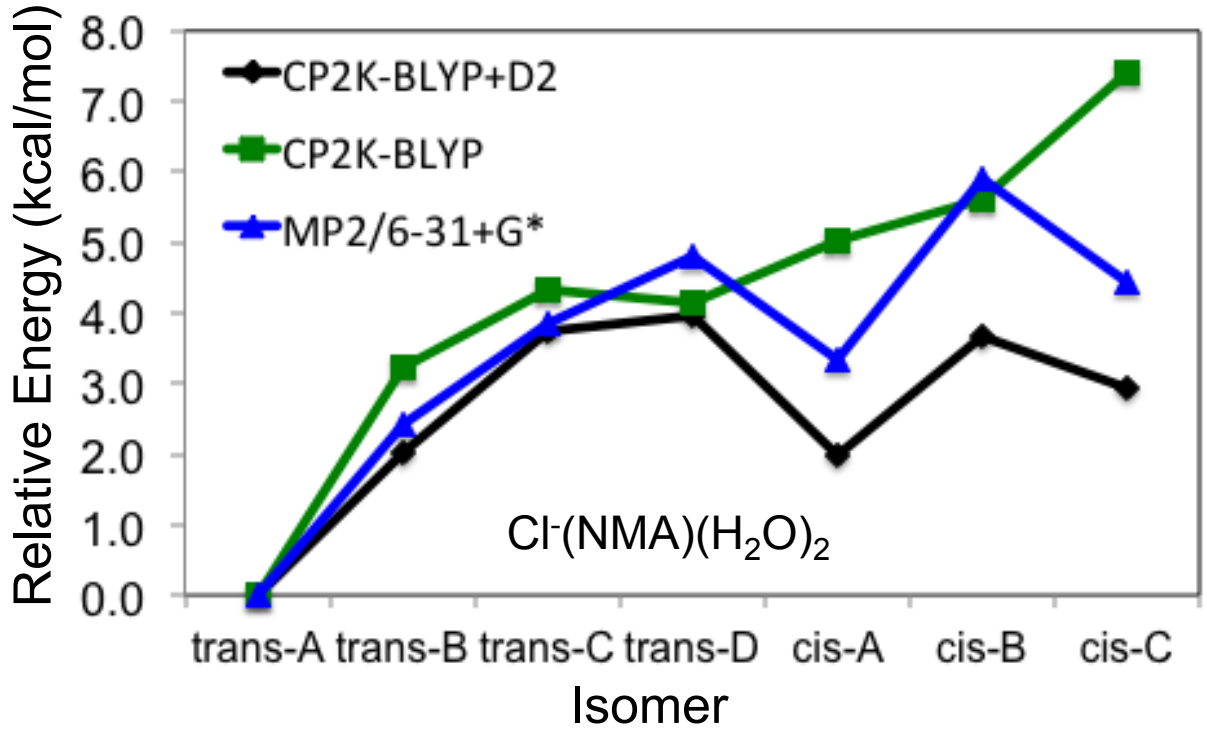


SI Figure 1: Relative energies of several isomers of $Cl^-(NMA)(H_2O)_n$ for n=1 (top panel) and n=2 (bottom) calculated with various approaches for comparison. The structures of all the isomers are also shown.



SI Figure 2: Comparison of the relative energies for $Cl^-(NMA)(H_2O)_2$ to show the impact of dispersion on the CP2K calculations. The calculations which include dispersion match the relative energies from the MP2 calculations more closely than the calculations not including dispersion.