

AB INITIO STUDY
OF MIXED CLUSTERS OF WATER
AND N,N'-DIMETHYLETHYLENEUREA

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S u m m a r y

Intermolecular interactions between a single water and two N,N'-dimethylethyleneurea (DMEU) molecules have been investigated using local and density-fitting approximations of the standard Møller–Plesset perturbation theory (DF-LMP2) with the aug-cc-pVTZ basis set. Six stable configurations have been found. In the first three, the water molecule intercalates between two DMEU molecules. In the next three configurations, the water molecule is attached to a stacked DMEU dimer, and these structures are more stable than the first three. These results support the view that DMEU molecules can form contact pairs in dilute aqueous solutions.