Density Functional Study of Ga_8 and Ga_{13} Clusters

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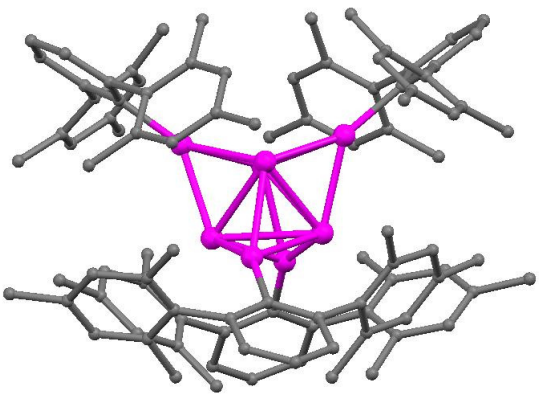
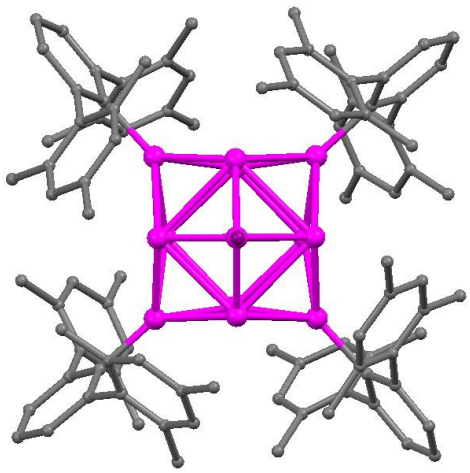
The outstanding success of terphenyl-based ligands in low coordination main group and transition metal chemistry[1] and spectacular findings in this field inspired the calculation and synthesis of compounds showing unusual binding and oxidation state behaviour stabilized by this type of ligand system. Here we report the density functional study and experimental characterization of Ga_8 and Ga_{13} clusters. Both of them show interesting structural motives and are representatives of the rare class of uncharged clusters of main group 3. Structural studies and bonding characteristics will be discussed and compared to data obtained by X-ray-diffraction[2]. Calculations were performed on the CC2/(def2-)TZVP level as implemented in *Turbomole* and on the PW91/TZ2P level as implemented in *ADF*.





[1] E. Rivard, P.P. Power, *Inorg. Chem.*, **2007**, *46*, 10047.
[2] P. Wilfling, M. Flock, R.C. Fischer, *unpublished results*.