Supplementary Information

The Structure of Au_6Y^+ in the Gas Phase

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Figure S1. Vibrational spectrum of Au_6Y^+·Ne calculated with BP86 functional and cc-pVDZ-PP (for Au and Y) and cc-pVTZ (for Ne) basis sets.

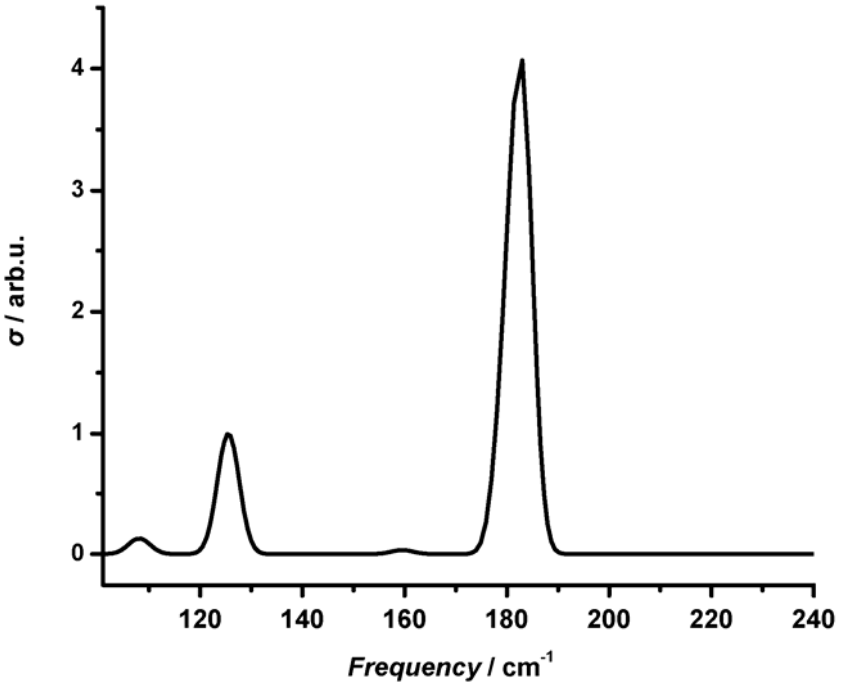
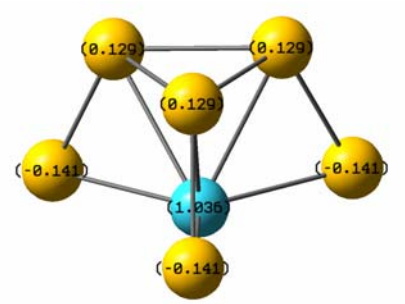


Figure S2. NBO charges distributed on each atom of Au_6Y^+ at the level of BP86/cc-pVDZ-PP.



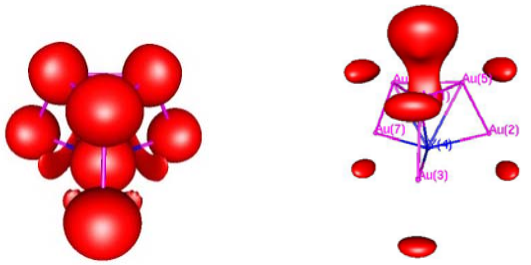
Movie S1. Movie of the calculated band at 123 cm^{-1} for Au_6Y^+ which is assigned to Y-atom displacement (cf. Movie S1 in ESI).

Movie S2. The calculated Au–Y stretching mode (a_1) centered at 179 cm^{-1} (cf. Movie S2 in ESI).

Movie S3. The calculated Au–Y stretching mode (e) centered at 183 cm^{-1} (cf. Movie S3 in ESI).

Electron Localizability Indicator (ELI-D)

The electron localizability indicator (ELI-D) (Figure a) of Au_6Y^+ exhibits localization domains around the nuclei representing the cores, and also other domains around the Y atom that may be responsible for the bonding in this cluster. Note that in the partial ELI-D maps (Figure b), the central basin around the Y atom is connected with one of the three-membered gold cycle.



(a) **(b)**