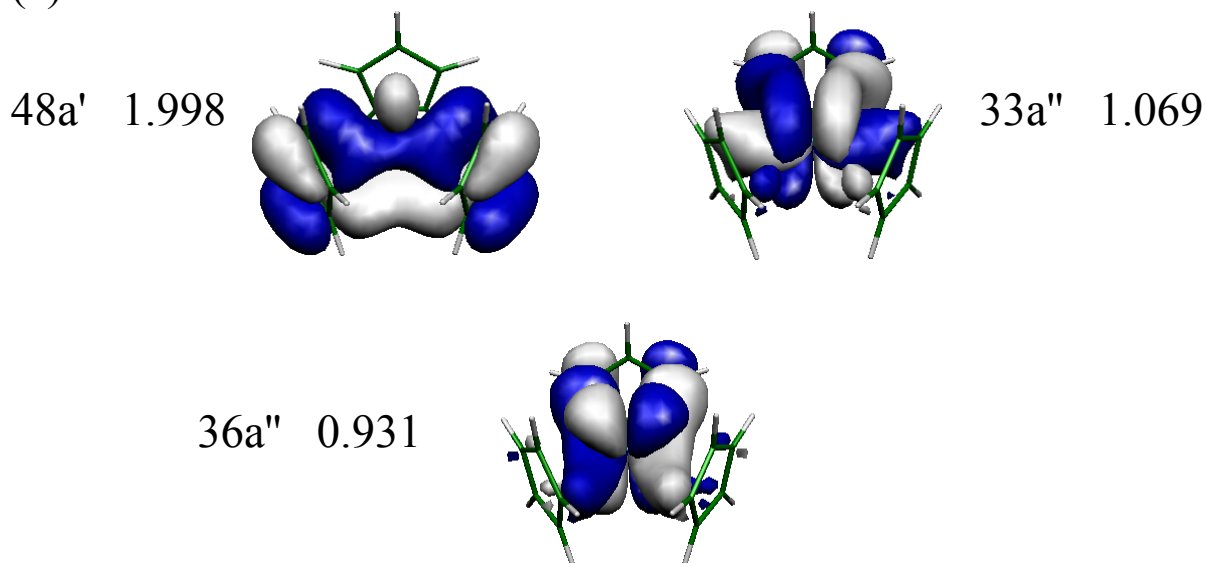


Figure S1: Natural orbitals and occupations for the $\tilde{A}^1A'$ (first excited) state of CeCp_3^+ . (a) Unaltered NOs and (b) linear combinations $33a'' + 36a''$ and $33a'' - 36a''$ (see computational details for discussion of this process). Active space II, basis A, 10 state average.

(a)



(b)

