

# Planar tetracoordinate fluorine atoms

Castillo-Toraya G.

Orozco-Ic M.

Dzib E.

Zarate X.

Ortiz-Chi F.

Cui Z.-H.

Barroso J.

Merino G.

Among the list of planar tetracoordinate atoms, fluorine is missing. So far, there are no theoretical or experimental reports suggesting their existence. Herein, we introduce the first six combinations ( $\text{Fln4}^+$ ,  $\text{FTl4}^+$ ,  $\text{FGaln3}^+$ ,  $\text{Fln2Tl2}^+$ ,  $\text{Fln3Tl}^+$ , and  $\text{FlnTl3}^+$ ) whose global minima contain a planar tetracoordinate fluorine. The bonding analyses indicate that the interactions between the fluorine and the peripheral atoms are significantly electrostatic, which is also reflected in the electronic delocalization. As opposed to other planar tetracoordinate systems with carbon, nitrogen, or oxygen atoms, the fluorine in the ptFs does not act as a  $\sigma$ -acceptor, restraining any back-donation. On the other hand,  $\sigma$ -electrons show a diatropic response, which would characterize these clusters as  $\sigma$ -aromatic. © The Royal Society of Chemistry.