

# Unique magnetic shielding and bonding in Pnictogen nortricyclane Zintl clusters

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Using first principle calculations, in-depth bonding and aromaticity pattern of bare anionic nortricyclane,  $E_7^{3-}$  ( $E = P, As, Sb, \text{ and } Bi$ ) Zintl clusters have been explored. A detailed topological analysis reveals that every cluster comprises of nine  $2c-2e$   $\sigma$ -bond with an occupation number of  $1.96\text{--}1.99 |e|$ . We find an impressive covalence in the  $E_7^{3-}$  cluster which decreases down the group from  $P_7^{3-}$  to  $Bi_7^{3-}$ . The nucleus independent chemical shift (NICS) foretell about the aromatic property of the Zintl cluster which is also decreasing along the group. In addition, the response with respect to external magnetic field of the nucleus independent shielding tensor was obtained to explore the possible formation of the shielding cone behavior. © 2020 Elsevier B.V.

Aromaticity

Chemical bonding

DFT

Magnetic shielding

Pnictogen

Zintl cluster

Aromatization

Chemical bonds

Chemical shift

Magnetism

Topology

Aromaticities

Chemical bondings

External magnetic field

First principle calculations

Nucleus independent chemical shifts

Pnicogens

Topological analysis

Zintl cluster

Magnetic shielding