

Abstract Submitted
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$[\text{Te}_2\text{As}_2]^{2-}$: A Planar Motif with Potential for Ferromagnetism¹

SHIV KHANNA, ARTHUR REBER, MEICHUN QIAN, Virginia Commonwealth University, ANGEL UGRINOV, AYUSMAN SEN, Pennsylvania State University — Here we report the synthesis and crystal structure of $[\text{K}(18\text{-crown-6})]_2[\text{Te}_2\text{As}_2]$, the first four-membered ring Zintl anion of elements from groups XV and XVI, isolated from an ethylenediamine solution of As, K, and As_2Te_3 at room temperature. X-ray analysis indicates that the $[\text{Te}_2\text{As}_2]^{2-}$ anion has an unexpected planar rhombic structure with alternating bonds. First-principles electronic structure investigations within the density functional framework, indicate that the $\text{Te}_2\text{As}_2\text{K}_2$ motif possesses a triplet ground state where the spin configuration leads to a distortion of the square geometry into rhombus structure marked by two Te-As shorter bond length pairs joined by longer bond lengths. A NICS analysis reveals that the triplet motif has a net aromatic character. Supercell calculations on the periodic solid show that the spin moments on the individual motifs order ferromagnetically thus offering the potential of an aromatic ferromagnet made of traditionally non-magnetic elements.

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