Poster

# Insight into α-iminoamidines: Hirshfeld atom refinement and evaluation of intermolecular interaction energies

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Amidine-containing compounds represent a versatile class of biologically active compounds and an important pharmacophore in modern drug discovery, exerting numerous biological properties [1–3]. We have discovered that by variation of the iodoform reaction, aryl-methyl ketones can be converted into *α*-iminoamidines—a functionality previously unknown to chemistry (Fig. 1) [4].

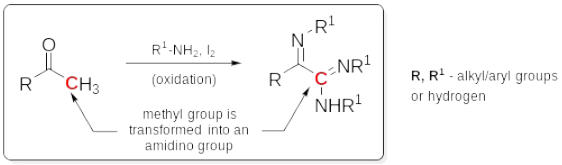


**Figure 1**. Synthetic approach to *α*-iminoamidines.

The aim of this work is detailed structural characterization of four *α*-iminoamidines through the application of quantum-crystallographic methods to gain precise structural parameters. A comparison of traditional independent atom model refinement and Hrishfeld atom refinement has been performed. Molecular structures are depicted in Fig. 2.

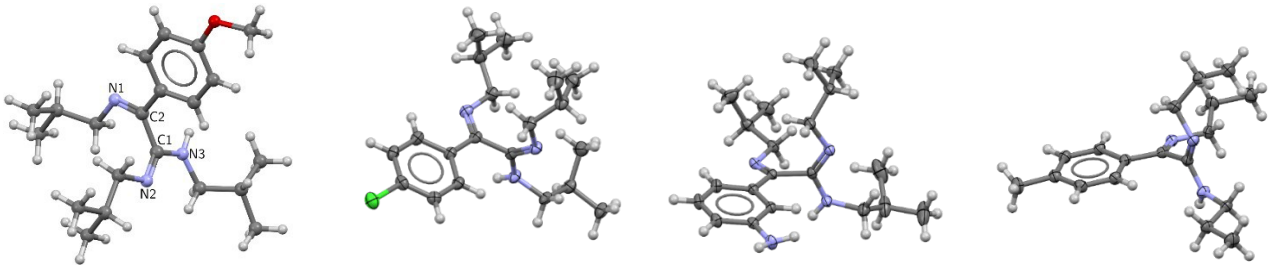


**Figure 2**. Molecular structures of the studied *α*-iminoamidines.

All molecular structural parameters conform to the range observed in structures featuring analogous fragments. Conformation of N=C−C=N fragment is quite similar in all studied molecules and the corresponding torsion angles fall within the range of 95–101 °. Intermolecular interactions were analyzed by traditional geometric approach, and an energetic perspective employing *CrystalExplorer* model energies. A common property of all analyzed compounds is the presence of hydrogen bonded dimers, related by crystallographic or non-crystallographic inversion.

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*65/2024-03/200124) and the European Research Council (ERC) under the European Union's Horizon 2020 Research and Innovation Programme (Grant agreement No. 950625).*