Insights: Publications

Crystal structures of 4-chloropyridine-2-carbo¬nitrile and 6-chloropyridine-2-carbonitrile exhibit different intermolecular n-stacking, C—H···Nnitrile and C—H···Npyridine interactions

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The two title compounds are isomers of $C_6H_3ClN_2$ containing a pyridine ring, a nitrile group, and a chloro substituent. The molecules of each compound pack together in the solid state with offset face-to-face π-stacking, and intermolecular C—H···$N_{nitrile}$ and C—H···$N_{pyridine}$ interactions. 4-Chloropyridine-2-carbonitrile, (I), exhibits pairwise centrosymmetric head-to-head C—H···$N_{nitrile}$ and C—H···$N_{pyridine}$ interactions, forming one-dimensional chains, which are π-stacked in an offset face-to-face fashion. The intermolecular packing of the isomeric 6-chloropyridine-2-carbonitrile, (II), which differs only in the position of the chloro substituent on the pyridine ring, exhibits head-to-tail C—H···$N_{nitrile}$ and C—H···$N_{pyridine}$ interactions, forming two-dimensional sheets which are π-stacked in an offset face-to-face fashion. In contrast to (I), the offset face-to-face π-stacking in (II) is formed between molecules with alternating orientations of the chloro and nitrile substituents.

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