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Cl···Cl Interactions in Dichloromethane

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Dichloromethane, CH_2Cl_2, has been crystallized in a diamond-anvil cell and its structure determined by X-rays at 1.33GPa/293K, and at 1.63GPa/293K. The structures are orthorhombic, space-group *Pbcn*, and isostructural with the low temperature structure [1]. The Cl···Cl intermolecular interactions have been considered as the primary reason for the layer structure of the dichloromethane crystal. The intermolecular distances and molecular geometry of low temperature and high-pressure structures are compared in the Table below.

CH_2Cl_2 at			
T:	153 K	293 K	293 K
P:	0.1 MPa	1.33 GPa	1.63 GPa
	Ref. [1]	This work	This work
C–H	0.99(13) Å	1.01 (9) Å	1.13 (12) Å
C–Cl	1.768(13) Å	1.765 (4) Å	1.769 (5) Å
Cl···Cl	2.932(4) Å	3.360 (3) Å	3.324 (5) Å
∠Cl–C–Cl	112(1) ˚	111.6(3) ˚	111.4 (4) ˚
∠ H–C–H	112(7) ˚	99 (9) ˚	102 (10) ˚

[1] Kawaguchi T., Tanaka K., Takeuchi T., Watanabe T., *Bull. Chem. Soc. Jpn*, 1973, **46**, 62-66.

Keywords: high-pressure X-ray diffraction, halogens, crystallization crystallography

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Molecular Packing Preferences of "Bridge-Flipped" Isomeric Molecules

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Molecules we have designated "bridge-flipped isomers" differ only in the orientation of a bridge of atoms connecting two major parts of the molecule, as among benzylideneanilines (Ar-CH=N-Ar' vs. Ar-N=CH-Ar') and among arylhydrazones (Ar-CH=N-NH-Ar' vs. Ar-NH-N=CH-Ar'). The common occurrence of disordered benzylideneaniline crystal structures having multiple orientations of the bridge raises the question of whether this disorder could be created artificially by means of co-crystallization of bridge-flipped isomers. Because co-crystallization would be facilitated by isostructuralism of the two components, we are examining solid-state structural features that would cause bridge-flipped isomers to assume similar molecular packing arrangements. These include (1) hydrogen bonding that might enforce similar packing arrangements; (2) Lewis acid-Lewis base interactions that might encourage similar packing arrangements; and (3) molecular planarity in benzylideneanilines that would minimize the effect of conformational differences on packing arrangements. Obstacles to isostructuralism have been found to include differences in molecular position of key H-bonding groups, differences in conformation enforced by intramolecular H-bonding, and competing intermolecular interactions (e.g. halogen-nitrile vs. halogen-halogen vs. nitrile-hydrogen). Although our studies have not resulted in the preparation of isostructural isomers to date, they have provided insight into the packing preferences of these compounds.

Keywords: intermolecular interactions and packing in small-molecule crystals, disordered molecular crystals, cocrystals

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A Conserved Core in the SufE Sulfur-acceptor Protein Mediates Interdomain Interactions in Variety of Redox Protein Complexes

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High sequence homology cystein desulfurase IscS and SufS presumably play the sane role in the oxygen-sensitive assembly process. The *isc* and *suf* operons in *E. coli* represent alternative genetic systems optimized to mediate the essential metabolic process of iron-sulfur claster (Fe-S) assembly and basal or oxidative-stress conditions. IscU has 3 invariant cystein residues that function as a template for Fe-S assembly while accepting a S atom from IscS, SufE does not have those function, but

Has been suggested to function as a shuttle protein that uses a persulfide linkage to a single invariant cystein residue to transfer a S atom from SufS to an alternative Fe-S assembly template. The structure of SufE shows the persulfide-forming cysteine occurs at the tip of a loop with elevated B-factors. The side chain of cystein is buried in hydrophopcic cavity located beneath a highly conserved surface. A conserved core structure is implicated in mediating the interactions of both SufE and IscU with mutually homologous cystein desulfurase enzyme present in their respective operons.

The core fold SufE/IscU has been adapted to mediate interdomain interations in diverse redox protein systems in the course of evolution.

Keywords: northeast structural genomics consortium, SufE er30, IscU IscS X-ray

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Halogen-substituted Drugs and their Intermolecular Interactions

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Halogen substitution is an important tool in drug design. Halogenation alters physicochemical properties and enhances the potency of membrane-soluble anesthetics. The presence and identity of halogen (X) substituents pendant on an aromatic nucleus in anticonvulsant and anxiolytic drugs have significant consequences for activity. Explanations of the Structure-activity effects of halogens have been limited to considerations of membrane solubility and the steric effects of X substituents on aromatic rings even though much is know about the effect of halogens on crystal packing. Crystal engineering originated with a study of the packing of Cl substituents [1]. Subsequent investigations using the CSD [2] and theoretical calculations have established the intermolecular interactions important in crystals of halogen compounds: (a) X atoms are potential H-bond acceptors able to interact with strong and weak H-bond donors [3], although the evidence is equivocal for C-F as a H-bond acceptor [4]; (b) C-H•••X interactions are weakly attractive yet highly dependant on the molecular environment of the halogen [5, 6] and (c) X•••aromatic ring and X•••H are stronger interactions than X•••X [7]. Structure activity relationships in CNS drugs will be interpreted in light of these intermolecular interactions to explain identify key factors for binding.

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Keywords: structural systematics, drug design, halogens

P8