

P.08.08.3*Acta Cryst.* (2005). A61, C329**Cl...Cl Interactions in Dichloromethane**

Marcin Podsiadło, Andrzej Katrusiak, *Department of Chemistry, Adam Mickiewicz University in Poznań, Poland.* E-mail: marcinpodsiadlo@interia.pl

Dichloromethane, CH₂Cl₂, 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 ₂ Cl 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

P.08.08.4*Acta Cryst.* (2005). A61, C329**Molecular Packing Preferences of "Bridge-Flipped" Isomeric Molecules**

William H. Ojala, Charles R. Ojala, Ann M. Brigino, Jessica E. Engebretson, Tera L. Deal, Heather M. Sexe, Jonathan M. Smieja, Vinita M. Solomon, *Department of Chemistry, University of St. Thomas, St. Paul, MN 55105 USA.* E-mail: whojala@stthomas.edu

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 benzyldeneanilines (Ar-CH=N-Ar' vs. Ar-N=CH-Ar') and among aryhydrazones (Ar-CH=N-NH-Ar' vs. Ar-NH=N=CH-Ar'). The common occurrence of disordered benzyldeneaniline 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 benzyldeneanilines 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

P.08.08.5*Acta Cryst.* (2005). A61, C329**A Conserved Core in the SufE Sulfur-acceptor Protein Mediates Interdomain Interactions in Variety of Redox Protein Complexes**

Alexandre P. Kuzin¹, Sharon Goldsmith-Fishman², William C. Edstrom¹, Jordi Benach¹, Ritu Shastri³, Rong Xiao³, Thomas B.

Acton³, Barry Honig², Gaetano T. Monterlione³, John F. Hunt¹, ¹*Department of Biological Sciences and Northeast Structural Genomics Consortium, 705B MUDD, MC2452, 1212 Amsterdam Avenue, New York, NY 10027, USA.* ²*Department of Biochemistry and Molecular Biophysics, Howard Hughes Medical Institute, and Structural Genomics Consortium, Columbia University College of Physicians and Surgeons, New York, NY 10032, USA.* ³*Center for Advanced Biotechnology and Medicine, Department of Molecular Biology and Biochemistry, and Northeast Structural Genomics Consortium, Robert Wood Johnson Medical School and Rutgers University, Piscataway, NJ 08854, USA.* E-mail: ak2197@columbia.edu

High sequence homology cystein desulfurase IscS and SufS presumably play the same 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 cluster (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 hydrophobic 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 interactions in diverse redox protein systems in the course of evolution.

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

P.08.08.6*Acta Cryst.* (2005). A61, C329**Halogen-substituted Drugs and their Intermolecular Interactions**

Penelope W. Coddington, *Department of Chemistry, University of Victoria, Victoria, BC, V8W 3V6, Canada.* E-mail: pcoddington@uvic.ca

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 known 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.

[1] Schmidt G.M.J., *J.Chem. Soc.*, 1964, 2014. [2] Allen F.H., et al., *J. Chem Inf. Comput. Sci.*, 1991, **31**, 187. [3] Brammer L., et al., *Crystal Growth & Design*, 2001, **1**, 277. [4] Dunitz J.D., *ChemBiochem*, 2004, **5**, 614. [5] Lommerse J.P.M., et al., *J. Am. Chem. Soc.*, 1996, **118**, 3108. [6] van den Berg J.-A., Seddon K.R., *Crystal Growth & Design*, 2003, **3**, 643. [7] Price S.L., et al., *J. Am. Chem. Soc.*, 1994, **116**, 4910.

Keywords: structural systematics, drug design, halogens