Advanced Physical Chemistry

Interesting Structures in the Cambridge Structural Database

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Molecules of General Interest

Aspirin	ACSALA
Buckminsterfullerene	NOBLEV
DDT	OPTCET
Norethisterone (oral contraceptive)	NETIND01
Penicillin G	BZPENK01
Prozac	FUDCOW

Symmetry examples for the classroom

STHDMO, *sym*-dihydrosulfido-bis(μ-1,5,9,13-tetrathiacyclohexadecane)-dimolybdenum(II) trifluoromethanesulfonate dihydrate in a $P\bar{1}$ cell. No atoms at the corners of the cell!

- Mo-Mo bond distance (2.823 Å) and atomic radius of Mo (1.45 Å) established that there is a metal-metal bond. Oxidation state of Mo(II) was deduced from the X-ray structure.
- 1/2 molecule in the *asymmetric unit*. Two asymmetric units in the cell.
- *Inversion center* at the center of the cell, as well as at the corners.
- *Symmetry* operator in space group $P\bar{1}$:

x, y, z	identity	.48650(5),.58076(4), .40292(5)
$\bar{x},\bar{y},\bar{z}$	inversion center	.5135, ?, ?[1]

SAHCYB10, *S*-8-azaadenosyl-L-homocysteine (8-aza-SAH) in a $P2_12_12_1$ cell.

- Atom type and coordinates: N(6)A .1329(28), .3342(6), .4847(3)
- Distances and angles: hybridization, bond order, resonance
- Intermolecular interactions (show molecule), hydrogen bonds from -NH_2 to N of adenine
- Intermolecular interactions (show packing), hydrogen bonds between H_2O and OH on ribose
- 4 symmetry operators, 2 molecules in each asymmetric unit, 4 asymmetric units in the cell

[1] Items in yellow are to be answered by the class

Additional symmetry examples

Refcode	**Name**	**Space Group**	**Z'**	**Z**
TMZDAN10	4,4,17a,17a-Tetramethyl-4,17a-diaza-D-homo-5a-androstane dimethiodide	$P1$	1	1
TMZBCO10	*syn*-3,4,6,7-Tetramethyl-1,5-diazabicyclo(3.3.0)octa-3,6-diene-2,8-dione	Pc	1	2
YUXXIY	(18-Crown-6)-potassium bis(pyridine)-tetrakis(isothiocyanato)-indium(iii) pyridine solvate	$P\bar{1}$	.5	1
FUWPUI	2-benzoyl-3-phenylindole	$P\bar{1}$	1	2
JETLID	sodium bis(5-oxoproline)-platinum(II) dihydrate	$P2_1$	1	2
TMTBZS	aqua-benzenesulfonato-trimethyl-tin	$P2_1/c$	1	4
TMTPSW01	1,1,7,7-Tetramethyl-3,5,9,11-tetraphenyl-tricyclohexasiloxane	$C2/c$	.5	4