04.1-05 GEOMETRY OF THE $\rangle\overset{+}{N}=C\langle$ MOIETY : STRUCTURES OF FIVE RELATED IMINIUM SALTS. By T.G.D. van Schalkwyk, Physics Department, University of the Western Cape, Bellville, 7530 Republic of South Africa.

Crystal and molecular structures of the secondary amine salt bis-(3,5,5-trimethyl-pyrazolinium)hexachlorostanate and five of its condensation products containing an iminium moiety, which up to now has been only rarely described, is fully discussed. Secondary interactions are considered.

04.1-06 CONFORMATIONS OF SEVEN-MEMBERED RINGS : A FOURIER TRANSFORM ANALYSIS. By F.H. Cano, C. Foces-Foces and S. García-Blanco, Departamento de Rayos-X, Instituto "Rocasolano", C.S.I.C., Serrano 119, Madrid-6. Spain.

There are several models for dealing with these rings (W.M.J. Flapper & C. Romers, Tetrahedron (1975) 31, 1705; D.F. Bocian et al., J. Am. Chem. Soc. (1975) 97, 687; (1977) 99, 2876; D. Cremer & J.A. Pople, J. Am. Chem. Soc. (1975) 97, 1354; J.B. Hendrickson, J. Am. Chem. Soc. (1967) 89, 7036 and 7047) but we have found some queries in the description and in the assignment of types when using those models, namely:

- Two different sequences of torsion angles are called boats (W. Henske & R.E. Davis, Acta Cryst. (1975) B31, 1511; G. Bandoli & D.A. Clemente, J. Chem. Soc. Perkin II (1967) 413; P. Chananont et al., Acta Cryst. (1980) B36, 2115 among other).
- Some types of rings with sequences not having been described, have been spotted (L. Párkányi & G. Argay, Acta Cryst. (1976) B32, 3316; P.M. Warner et al., J. Am. Chem. Soc. (1977) 99, 5102; H.L. Ammon et al., J. Am. Chem. Soc. (1973) 95, 1968. See table nos. 12 and 13 respectively).

We have studied these discrepancies with the two component description given at the top of the table (F.H. Cano et al., Acta Cryst. (1978) A34, S91), and we have found some points:

- There is a relationship between our pseudorotation parameters and those of Bocian.
- We think the sequence no. 8 should be called boat-chair (vs. boat-sofa of Flapper et al.) leaving the name boat-sofa for sequence no. 10.
- Sequence no. 12 could be considered a transition between no. 2 (TB) and no. 11 (TS).
- Sequences no. 13 and 14 seem to be different from those of chair or twist-chair (nos. 3 and 4); this is reflected by the lack of the second component, q_3.

Table

We are studying the rings through the following expression for the torsion angles ϕ_j.

$$\phi_j \equiv Q.\tau_j = q_2 \cos(S_2 + 2\pi\tfrac{2j}{7}) + q_3 \cos(S_3 + 2\pi\tfrac{3j}{7})$$

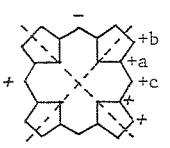
N	Type	τ_0	τ_1	τ_2	τ_3	τ_4	τ_5	τ_6	S_2	S_3	q_2/q_3
1	B	0	-1	0.4	0.8	-0.8	-0.4	1	90	-	∞
2	TB	-1	0.2	0.9	-0.6	0.6	0.9	0.2	180	-	∞
3	C	0	-1	1.3	-0.9	0.9	-1.3	1	90	90	0.3
4	TC	1	-1.3	1.6	-0.7	-0.7	1.6	-1.3	180	0	0.4
5	TC/TB	-1	0	1.5	-0.9	-0.9	1.5	0	180	0	3.8
6	TC/TB	-1	-1.9	6.2	-3.3	-3.3	6.2	-1.9	180	0	1.3
7	TC/TB	0	-1	2.4	-1.2	-1.2	2.4	1	180	0	1.0
8	BC	0	-1	0.8	0	0	-0.8	1	90	90	1.3
9	S	0	0	-1	2.3	-2.3	1	0	90	270	0.5
10	BS	0	-1	0	1.8	-1.8	0	1	90	270	1.8
11	TS	-1	0.7	-0.2	0	0	-0.2	0.7	180	180	0.4
12	TB/TS	-1	0.7	0	-0.2	-0.2	0	0.7	180	180	0.7
13		0	-1	1.8	-2.3	2.3	-1.8	1	-	90	0
14		1	-0.9	0.6	-0.2	-0.2	0.6	-0.9	-	0	0

B stands for boat, C for chair, S for sofa and T for twist. Q is a proportionality constant.

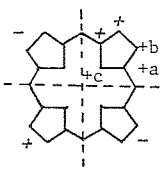
04.1-07 FLEXIBILITY OF THE PORPHYRIN RING. By Peter Murray-Rust and Christoph Kratky, Department of Chemistry, University of Stirling, Scotland and Institut für physikalische Chemie, Universität Graz, Austria.

The Cambridge Data File was used to prepare a file of all metalloporphyrins (90 unique molecular fragments). The deviations of atoms from the mean plane through the 24 ring atoms were calculated (GEOM). These were analysed by factor analysis after the 16 possible permutations of labels (in D_{4h}) had been included.

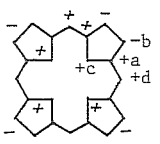
For this 22 dimensional problem, 98% of the observed oop deviation is accounted for by the first 6 factors, which have B_{1u}, B_{2u}, A_{2u}, E_g and B_{2u} symmetry.



$B_{1u}(D_{2d})$
a:b:c=1:0.7:1.7



$B_{2u}(D_{2d}')$
a:b:c=1:2.4:0.4



$A_{2u}(C_{4v})$
a:b:c:d=
1:3:3.6:0.5

All 6 deformation modes leave the pyrrole rings essentially planar, but involve non-planar α-atoms.

The two largest factors (B_{1u} and B_{2u}), which together account for 76% of the observed deformation, correspond very closely to