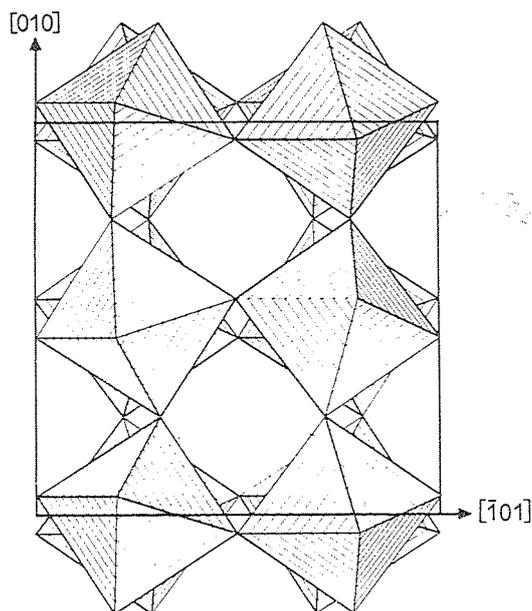


is presented by a STRUPLO-plot [R.X. Fischer, J. Appl. Cryst. 1985, 18, 258 - 262].



Arrangement of the corner-linked RuO_6 -octahedra in CaRuO_3 ; projection along [101]

04.2-2 SOLID STATE N-BROMOSUCCINIMIDE-BROMIDE COMPLEXES. By J. Albertsson and C. Svensson, Inorganic Chemistry 2, Chemical Center, University of Lund, P.O.Box 124, S-221 00 Lund, Sweden

N-Bromosuccinimide (SBr: 1-bromo-2,5-pyrrolidinedione) serves as a brominating agent in the presence of tetraalkylammonium bromides. There is strong evidence that 1:1 SBr/ Br^- complexes play a vital role in the mechanism by which addition products are formed by SBr and olefins. The SBr/ Br^- complex should slowly decompose into succinimide, polymaleimide and tribromide ions so the latter species could be responsible for the addition reaction. Bromide ion acts as a catalyst for the electron transfer oxidation of ferrocene to ferricinium ion by SBr, in all probability by forming the SBr/ Br^- complex which should be a strong oxidant.

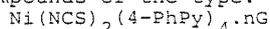
In order to study the possible formation of distinct SBr...Br bonds and their influence on the N-Br bond in SBr we are investigating the crystal structures of SBr· $(\text{C}_2\text{H}_5)_4\text{NBr}$ and SBr·1/3CsBr. The tetraethylammonium compound crystallizes in $\text{P2}_1/\text{n}$, $a=18.091(3)$, $b=8.925(2)$, $c=10.587(4)$ Å, $\beta=103.16(2)^\circ$, $V=1665(1)$ Å³, $Z=4$, $D_x=1.549(1)$ g cm⁻³, $\mu=12.30$ cm⁻¹ (MoK α). The caesium compound crystallizes in $\text{R}\bar{3}$, $a=14.013(2)$, $c=17.921(9)$ Å, $V=3047(1)$ Å³, $Z=18$, $D_x=2.441(1)$ g cm⁻³, $\mu=96.6$ cm⁻¹ (MoK α). While the former compound most probably contains a 1:1 complex the caesium ion, which is smaller than the tetraethylammonium ion, induces the formation of $[\text{Br}(\text{SBr})_3]^-$ complex in the solid state (Svensson et al, Acta Cryst. 1986, C42, 1502-1505).

The bonding situation around the N-Br bond in the SBr/ Br^- complexes should be comparable to that in recently prepared "hypervalent" halogen species (Farnham & Calabrese, J. Am. Chem. Soc. 1986, 108, 2449-2451). We are now working with salts of the complex $[\text{S}'\text{Br}\cdots\text{S}']^-$ where S' is tetramethyl substituted succinimide.

04.2-1 4-PHENYL PYRIDINE: A NEW LIGAND IN WERNER CLATHRATES.

L.R. Nassimbeni and M.W. Taylor. Physical Chemistry, University of Cape Town, Rondebosch 7700, South Africa.

We have elucidated the structures of a series of compounds of the type:



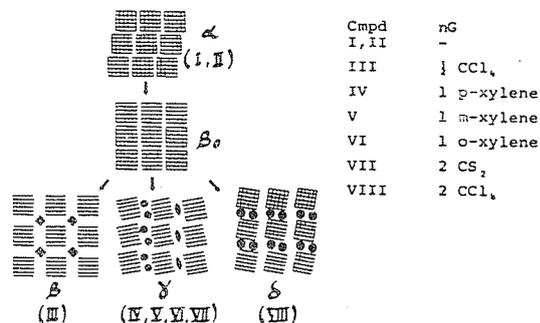
Cmpd.	n	G	Space Group
I	-	-	Pbca
II	2	o-xylene	Fdd2
III	2	m-xylene	C2/c
IV	1	p-xylene + DMSO	P1
V	1	4-PhPy+methyl cellosolve	$\text{P2}_1/\text{n}$

Rotational freedom of the substituted pyridine has been advanced as a possible reason for the host molecules, in Werner Clathrates, to adopt a suitable conformation to allow accommodation of a guest molecule. This host complex offers eight moieties each of which can independently rotate, thus offering many possible conformations.

We have undertaken a series of comparisons between the eight torsion angles in each compound to try and relate them to their structure and to the size and shape of the channel in which the guest molecules are accommodated.

04.2-3 HOST-GUEST INTERACTIONS IN WERNER CLATHRATES. L.R. Nassimbeni, M.H. Moore and M.L. Niven, Department of Physical Chemistry, University of Cape Town, Rondebosch 7700 South Africa.

We have synthesised and characterised the structures of a series of compounds of general formula $\text{Ni}(\text{NCS})_2(4\text{Et-Py})_4 \cdot n\text{G}$



The structures can be grouped into distinct phases α , β , γ , δ and their structural relations are discussed. The geometry of the channels was mapped in detail with the program OPEC (Gavezzotti 1984). Differential Thermal Analysis and Thermal Gravimetric Analysis of these compounds have allowed us to understand their thermal decomposition patterns and to estimate the enthalpy of the host-guest interactions.