s9.m3.p27 **The Simple Structure Of [Co(ostaH)₃]**. R.A. Coxall[1], D.K. Henderson[1], S. Parsons[1], R.E.P. Winpenny[1], *University of Edinburgh, Department of Chemistry, King's Building's, West Mains Road, Edinburgh, EH9 3JJ.*
Keywords: intermolecular interactions, heterocyclic ligands, hydrogen bonding.

S-Substituted heterocyclic ligands have potential applications in such diverse areas as solvent extraction, controlled engineering of metal surfaces and in the synthesis of high spin complexes. Therefore , as part of an ongoing investigation into the co-ordination of S-substituted heterocyclic ligands towards metal centres, the complex [Co(ostaH)₃] was synthesised and structurally characterised (where ostaH = 4-hydroxo-6-(diethylamino)-2-mercapto-1,3,5,-triazine). Despite the apparently simple co-ordination around the metal atom in the [Co(ostaH)₃] molecule, the complexity of the structure increases considerably when intermolecular interactions are examined. A discussion of the intermolecular interactions will be given.

s9.m3.p28 **Stability conditions for Quasi-Racemates of Coordination Compounds** R. Härter, U. Englert, C. Hu, I. Kalf, X. Zheng *Arbeitsgemeinschaft für Kristallographie und Strukturchemie, Institut für anorganische Chemie der RWTH Aachen, Germany.*
Keywords: quasi-racemates, crystal engineering, cobalt-(III)-complexes.

We recently presented an introduction to the use of quasi-racemates in the field of crystal engineering together with some first results[1].

Our model system relies on cobalt-(III)-complexes of the general formula [Co(dmgH)₂(L)X], X = anionic ligand, dmgH = dimethylglyoximato, L = chiral ligand, enantiopure or racemic. These coordination compounds offer the following advantages: cobalt-(III) is inert, it generally undergoes ligand exchange only at a low reaction rate; the complexes are stable to air and moisture; they are diamagnetic and therefore easy to investigate in spectroscopy.

In first attempts we found that in complexes with halogenes as anionic ligands, i.e. X=Cl,Br, ligand exchange occurs on the time scale of crystallization.

In consequence we prepared and fully characterized the compounds **1-4**.

X=NO₂	L=R-Phenethylamine	**1**
X=NO₂	L=*rac*-Phenethylamine	**2**
X=CN	L=S-Phenethylamine	**3**
X=CN	L=*rac*-Phenethylamine	**4**

1 and **3** are sufficiently inert to allow for the preparation of a 1:1 quasi-racemate **5**.

The following crystal data have been obtained:

	SpGr	T[°C]	λ	a	b	c	β	V	Z
1	P2₁	20	Cu	12,64	12,61	12,77	99,1	2009,4	4
2	P2₁/c	20	Cu	12,75	12,35	12,86	101,0	1986.2	4
3	P2₁	20	Cu	12,54	12,44	13,17	98,5	2032,3	4
4	P2₁/c	20	Cu	12,53	12,27	13,26	100,6	2004,5	4
5	P2₁	-30	Mo	12,60	12,24	13,03	100,9	1972,5	4

The molecular volume as defined by may serve as a crude measure for the stability of enantiopure versus racemic compounds. Brock, Schweizer and Dunitz[2] investigated the validity of Wallach's rule. In the case of in solution not interconverting enantiomers they found that the racemic crystals are about 1% more tightly packed than their chiral counterparts.

The calculated center of gravity between the two molecule's cores (Co,N,X) of **5** lies only 0.145Å from the corresponding center of inversion in P2₁/c. Due to Kitaigorodsky a center of inversion is a good packing element. To gain further insights about packing, intra- and intermolecular interaction or H-bridging of these compounds, we are carrying out lattice energy calculations.

[1] Härter, R. "About Quasi-Racemates", Z. Krist. Suppl., (2000), 17:59.
[2] Brock, C.P. "On the validity of Wallach's rule:...", J. Am. Chem. Soc., (1991), 113:9811.