Selenourea Inclusion Compounds

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ADDUCTS of urea and of thiourea are well known[1] and used for the separation[1,2] and configurational analysis[3,4] of organic compounds. Owing to the difference in diameter of the channel, the fields of applications of urea and thiourea adducts are different. We now report on inclusion compounds of selenourea.

Adducts of selenourea have been prepared with the compounds listed in the Table by treating them with a saturated methanolic solution of selenourea (stabilised by a trace of hydroquinone) and cooling to 0°. Many related compounds could not be included in selenourea in this way.

These adducts crystallise as needles and are outwardly indistinguishable from selenourea for which two modifications have been described;[5] they are identified by elemental analysis or i.r. spectroscopy. Characteristic shifts appear at *ca.* 3200 (NH_2 str.), 1610 (NH_2 bend.), and 1480 cm.$^{-1}$ (C–N str.), similar to those observed for thiourea and its adducts.[6] The density of the adducts of selenourea was found to vary between 1·60 and 1·65 g./cm.^{3}, distinctly lower than that of selenourea (2·08 g./cm.^{3}). The densities[1] of urea and its adducts (1·30 and 1·20 g./cm.^{3}) and of thiourea and its adducts (1·40 and 1·10 g./cm.^{3}) differ in the same way.

Crystals of selenourea adducts are rhombohedral as are

TABLE

Crystallographic data for selenourea adducts

Compound	a (Å)	c (Å)	l (Å)	
4-t-Butyl-1-neopentylbenzene	16·28	12·87	12·9	(R)
1,4-Dineopentylbenzene	16·38	12·81	12·8	(R)
trans-1,4-Di-isopropylcyclohexane	16·21	12·91	11·4	
trans-1-t-Butyl-4-isopropylcyclohexane	16·32	12·91	11·5	
trans-1,4-Di-t-butylcyclohexane	16·41	12·95	11·8	
cis-1,4-Di-t-butylcyclohexane	16·46	12·88	11·5	
trans-1-t-Butyl-4-neopentylcyclohexane	16·36	12·87	12·9	(R)
cis-1-Bromo-4-t-butylcyclohexane	16·39	12·89	9·5	
Bicyclo[3.3.1]nonane	16·49	12·87	6·4	(R)
Adamantane	16·56	12·82	6 4	(R)
Camphor	16·71	12·97	6·5	(R)

those of the thiourea adducts.[7] The Table lists the unit-cell dimensions as determined from X-ray powder photographs and the period of the guest [the length of channel occupied by one included molecule·(l)] as determined from rotation diagrams. In some cases the guest has its own period, in other cases one or two molecules just have the same length as the c axis [rational adducts (R)].

There are more striking differences in the unit-cell dimensions of the selenourea adducts than are observed for thiourea adducts.[3,6] Apparently, adaption of the selenourea lattice to the shape and size of the included molecules is relatively easy. It is interesting that a reasonably linear relation exists between the number of carbon atoms per channel-period and the a axis.

All compounds listed could also be included in thiourea. Though the difference in channel-diameter between thiourea and selenourea adducts is small, selenourea seems to be much more selective in the choice of its guest compounds. For example trans-1-t-butyl-4-neopentylcyclohexane formed an adduct with selenourea whereas the cis-isomer was not included, thus enabling separation of these isomers. Thiourea showed no observable preference in this case.

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