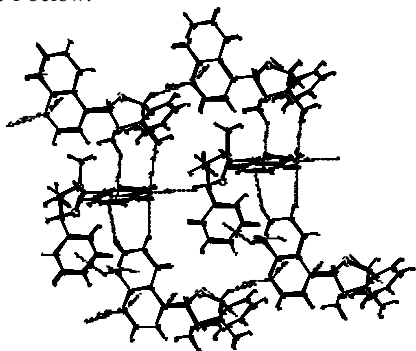


s9.m3.o3 Weak interactions in oxazolidine derivatives.

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Keywords: hydrogen bonding, weak interactions, 4-quinolinyl.

We are currently studying oxazolidine derivatives derived from (-)-ephedrine and several crystal structures will be discussed including the 4-quinolinyl derivative depicted in Figure 1 below.



(1a) $C_{20}H_{20}N_2O$, monoclinic, $P2_1$, $a = 9.0541(7)$, $b = 9.6253(7)$, $c = 9.6475(7)$ Å, $\beta = 100.969(7)^\circ$, $V = 825.40(11)$ Å³, $Z = 2$, $T = 294$ K, $D_x = 1.225$ Mg.m⁻³, $R = 0.032$ for 3692 reflections $> 2\sigma(I)$. Data were collected on an Enraf-Nonius CAD4 diffractometer.

Compound **1** crystallises with an interesting relay of C-H...N and C-H... π interactions utilising the phenyl and 4-quinolinyl groups as donors and acceptors in the solid state (Fig. 1 above). Data were also collected at 150K (using X-ray radiation) on a kappa-CCD diffractometer, **1b** and by neutron diffraction at the ISIS facility, Rutherford Appleton laboratory, **1c** in order to probe the nature of the relay of weak interactions in greater detail and for comparison with *ab initio* calculations.

These results will be compared with the crystal structure determinations of related oxazolidine derivatives¹⁻³ especially fluoro and alkoxy derivatives.

s9.m3.o4 Crystal structures and intermolecular interactions in new fullerene derivatives. I.S. Neretin,

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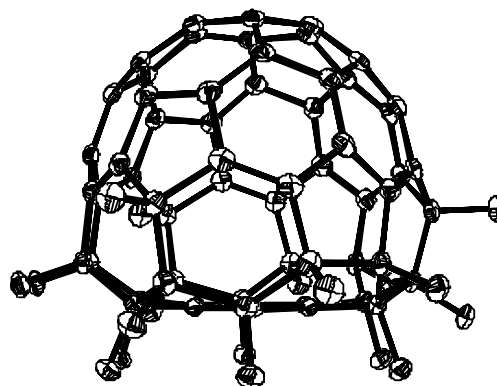
Keywords: fullerenes, disorder, molecular complexes.

Single crystal X-ray data for the six new derivatives of C_{60} and C_{70} were collected at 100-110K on SMART diffractometer in order to reveal correlations of a carbon cage disorder with intermolecular interactions.

Monoclinic structure of $C_{60} \cdot 2C_6H_5I$ with unusually short distance between C_{60} centres (9.89 Å) shows a fully ordered C_{60} moiety, whilst the previously studied $C_{60} \cdot 2C_6H_5Br$ ¹ with similar molecular packing motif have longer distances (10.00 Å) and rotationally disordered C_{60} molecules.

In a series of molecular complexes with metal tetraphenylporphyrinates (MTPP), fullerene molecules are rotationally disordered in $C_{60} \cdot 2CuTPP$, $C_{60} \cdot 2(PyZnTPP) \cdot Cp_2Fe \cdot C_6H_5CH_3$ (where Py is pyridine) and $C_{70} \cdot 2(PyZnTPP) \cdot C_6H_5CH_3$ with the normal van der Waals contacts, whereas C_{70} molecules are ordered in $C_{70} \cdot CuTPP \cdot (C_6H_5Me, C_2HCl_3)_2$ with a weak secondary $Cu \cdots C$ bonding at 2.88-3.03 Å. Notable is the disappearance of ferrocene molecule on a replacement of C_{60} by C_{70} in two related PyZnTPP derivatives.

In the fully ordered crystal structure of $C_{60}F_{18} \cdot C_6H_5CH_3$, carbon cage of $C_{60}F_{18}$ is strongly distorted (see Figure). C-C bond lengths vary from 1.372 Å in aromatic ring surrounded by $C(sp^3)-F$ vertices to 1.672 Å in a fluorinated belt. A high value of dipole moment (12.3 D at 3-21G* level) and strong electrostatic interactions in the crystal explain short forced $C \cdots F$ contacts (down to 2.75Å).



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