04. ATOMIC SCALE MECHANISM AND CHEMICAL PROPERTIES

04.5-10 'POLAR FLATTENING': THE EFFECTIVE VAN DER WAALS SHAPES OF ATOMS BONDED TO A CARBON ATOM. By S. C. Nyburg and C. H. Faerhlan, Department of Chemistry, University of Toronto, Toronto, Canada, MS8 lAL.

Using a fairly small number of crystal structures, it was shown (Nyburg and Szymanski, J. Chem. Soc. Chem. Commun., 1968, p.669) that the non-bonding effective shape of a fluorine atom bound to another halogen atom was flattened at the pole. More recently, similar flattening was demonstrated for C2, Br and I and for N in RCN (Nyburg, Acta Cryst. (1979) A35, 641).

We have now used the Cambridge Structure Data Base to retrieve all the non-bonded structures, it

04.6-1 THE CRYSTAL STRUCTURE OF TETRAHYDRATE, NICKEL(II) BY M.P. Gupta, A.T.A. Lenstra and H.I. Gelis, Department of Chemistry (U.I.A.), Universiteitplein 1, B-601 WlirleLk, Belgium.

The crystal structure of title compound has been re-determined (earlier unpublished work of Gupta, M.P. and, Sahn, H.I., 1980) using 1360 reflections among 60 (1)

04.6-2 HYDROGEN BONDING BETWEEN NITRO AND ACETATE GROUPS IN NORBORNYL SYSTEMS

By J.C.A. Boeyens, L.Denner and J.P. Michael, Department of Chemistry, University of the Witwatersrand, Johannesburg, South Africa.

Nitro and hydroxy groups on the 2 and 6 positions of the norbornyl system adopt conformations which are determined by hydrogen bonding interaction between them. The hydrogen bonds in 1, 11 and 111 have been studied by means of X-ray crystallography and spectroscopy.

An interesting intramolecular hydrogen bond exists in 1. The general case for the nitroalcohols is probably one in which the functional groups are too remote for interaction. However, in the case of 1, the nitro and hydroxy groups are restricted to close proximity by the norbornyl skeleton, allowing for sufficient interaction. This hydrogen bond is not bifurcated and persists in solution. A normal intermolecular hydrogen bond is present in the structure of 11, whereas a bifurcated hydrogen bond is found in the structure of 111. The orientations of both the hydroxy and nitro groups differ considerably, but this has been rationalised by structure analysis and force-field calculations.

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