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Agnes M. Modro^a; Tom A. Modro^a ^a University of Pretoria, South Africa

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THE PHOSPHORYL AND THE CARBONYL GROUP AS HYDROGEN BOND ACCEPTORS

Agnes M. Modro and Tom A. Modro University of Pretoria, South Africa

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The hydrogen bonding acceptor abilities of the phosphoryl and the carbonyl groups were compared by determining the formation constants for the complexes between a selected donor (phenol) and selected phosphoryl or carbonyl compounds from the IR $\Delta \nu$ shifts.¹

$$Y=O \xrightarrow{PhOH} Y O H-OPh$$

$$(Y=C, P)$$

For simple carbonyl compounds the K_{assoc} values were determined from the $\Delta\nu_{OH}$ for the donor. The obtained values are in the range 7–12, and agree well with the literature data. For selected phosphoryl compounds two sets of K_{assoc} values were determined—from the $\Delta\nu_{OH}$, and the $\Delta\nu_{P=O}$ shift. The former were in the range 300–600 and agree well with the literature data, indicating that the P=O group is about two orders of magnitude stronger acceptor than the C=O group. The values of K_{assoc} determined from the $\Delta\nu_{P=O}$ shifts were much lower and scattered, indicating that the IR absorption band of the P=O group shows weak response to the involvement in the hydrogen bonding.

For the β -diphosphoryl, or for the 1,3-ketophosphoryl systems, no evidence for the enolization involving the P=O function was found.

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Address correspondence to Tom A. Modro, Centre for Heteroatom Chemistry, Department of Chemistry, University of Pretoria, Pretoria 0002, South Africa. E-mail: tamodro@scientia.up.ac.za