Studies of Hydrogen Bonding. Part XXXIII.* Dipole Moments of Phosphoryl Compounds and their Hydrogen-Bonded Complexes with Phenol

Thor Gramstad

Department of Chemistry, University of Bergen, Allégt. 41, N-5007 Bergen, Norway

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The dipole moments of 33 phosphoryl compounds and of their hydrogen-bonded complexes with phenol have been determined in carbon tetrachloride at 20 °C. In general there is no correlation between the dipole moments and the O–H stretching frequency shift accompanying the complexation of phenol with the phosphoryl compounds. A smooth correlation is observed, however, for some series of closely related phosphoryl compounds. The influence of the various substituents on the dipole moment is discussed.

The vectorially calculated dipole moments of the complexes were found to be smaller than the corresponding dipole moments obtained experimentally. The vectorial difference, $\Delta\mu$, is greatest for phosphoryl compounds containing the N–P=O and C_6H_5–P=O groups.

We have previously[2] studied phosphoryl compounds containing O–P, N–P and S–P bonds. It was shown that there is a fundamental difference between an RS and an R_2N group in the way in which they affect the P=O bond. Replacement of one or two RS groups in $(RS)_3PO$ or ArS in $(ArS)_3PO$ with Et_2N groups caused a great change in the hydrogen-bonding ability and in the dipole moment, whereas the P=O stretching frequency remained almost unaltered. We then found it of interest to extend our research in this field by increasing the number of phosphoryl compounds and by measuring the dipole moments of their hydrogen-bonded complexes with phenol. The main purpose of the present work was to make a comparison between experimental and vectorially calculated dipole moments.

Experimental

Materials. Phenol was purified by several recrystallizations from light petroleum ether and the white needles obtained were dried over phosphorus pentaoxide in a desiccator. Carbon tetrachloride was purified chromatographically by using molecular sieves Type 4 Å and basic aluminium oxide. The phosphoryl compounds, not commercially available, were synthesized by literature methods.[2] They were purified by redistillation or recrystallization immediately before use, and the purity was checked spectroscopically and by refractive index measurements.

Experimental dipole moments. The dipole moment measurements were carried out on carbon tetrachloride solutions at 20 °C. The instruments and methods of evaluation of the dipole moments were the same as reported elsewhere.[3] The mass fraction range of phenol was 4×10^{-4}–30×10^{-4} and of the phosphoryl compounds 1.2×10^{-3}–1.6×10^{-2}. The experimental polarization data α, β, γ, and the corresponding dipole moments of the phenols, μ_D^{exp}, and of the phosphoryl compounds, μ_A^{exp}, are tabulated in Table 1. Our data are, when a comparison is possible, in good agreement with literature values.[4]

To evaluate the experimental dipole moments of the hydrogen-bonded complexes, the concentration of the proton acceptor was kept 3–5 times greater than the concentration of the donor to minimize the formation of complexes other than the 1:1 hydrogen-bonded complex.[5] Otherwise the procedure was the same as reported elsewhere.[1,3] The results are listed in Table 2. The μ_D^{exp} and μ_A^{exp} values were estimated to be accurate to within ±0.05 D and μ_{DA}^{exp} to within ±0.10 D.

Calculated dipole moments. The stumbling block in our calculation of the dipole moments of the hydrogen-bonded complexes, μ_{DA}^{calc}, is that we do not know the dipole moments of the donor and acceptor molecules as they occur in the complex. However, by using the experimental dipole

* For Part XXXII see Ref. 1.

Table 1. Experimental dipole moment, μ_A^{exp}, and the corresponding total polarization, P_∞, molar refraction, R_D, the parameters α, β, γ and IR data of various phosphoryl compounds at 20 °C. Solvent: carbon tetrachloride.

Proton acceptor	ν_{PO} / cm^{-1}	α	β	γ	P_∞	R_D	μ_A^{exp} / D
1 $(C_6H_5S)_3PO$	1221	3.4091	0.2188	0.9914	226.979	128.076	2.18
2 $(C_6H_5S)_2P(O)N(C_2H_5)_2$	1226	6.6617	0.3810	0.5556	335.189	113.889	3.26
3 $C_6H_5SP(O)[N(C_2H_5)_2]_2$	1225	9.9001	0.2778	0.3809	392.906	87.389	3.83
4 $(C_6H_5S)_2P(O)i\text{-}C_3H_7$	1205	4.3750	0.3684	0.7567	231.577	110.037	2.42
5 $C_6H_5SP(O)(C_3H_7)_2$	1187	10.2127	0.1400	0.8077	314.774	72.696	3.41
6 $(C_2H_5S)_3PO$	1200	3.8889	0.3095	0.3103	157.285	67.125	2.08
7 $(C_2H_5S)_2P(O)N(C_2H_5)_2$	1214 1190	5.7895	0.7000	0.3750	240.059	97.727	2.62
8 $C_2H_5SP(O)[N(C_2H_5)_2]_2$	1217 1186	8.8889	0.6667	0.4286	330.550	101.376	3.32
9 $(C_2H_5S)_2P(O)i\text{-}C_3H_7$	1192	4.6154	0.4595	0.3889	170.302	72.358	2.17
10 $C_2H_5SP(O)(C_3H_7)_2$	1183	9.7902	0.2955	0.2507	252.098	51.348	3.16
11 $(C_6H_5O)_3PO$	1314 1298	5.3333	0.2568	0.4583	267.019	95.597	2.87
12 $(C_6H_5O)_2P(O)N(C_2H_5)_2$	1271	7.4235	0.5769	0.9677	345.221	133.424	3.19
13 $C_6H_5OP(O)[N(C_2H_5)_2]_2$	1238	10.5582	0.2800	0.4186	391.031	83.768	3.84
14 $(C_6H_5O)_2P(O)i\text{-}C_3H_7$	1273 1298	5.6250	0.4038	0.2333	246.107	85.148	2.78
15 $C_5H_5OP(O)(C_3H_7)_2$	1152 1261	12.3077	0.2813	0.4286	353.124	67.154	3.71
16 $(C_2H_5O)_3PO$	1272 1255	19.4444	0.4000	0.6470	235.023	38.272	3.07
17 $(C_2H_5O)_2P(O)N(C_2H_5)_2$	1252	9.7826	0.4483	−0.0417	280.495	62.644	3.24
18 $C_2H_5OP(O)[N(C_2H_5)_2]_2$	1234	10.6667	0.0476	0.0462	310.829	44.897	3.58
19 $(C_2H_5O)_2P(O)i\text{-}C_3H_7$	1231	8.2051	0.4390	−0.4146	211.378	44.416	2.83
20 $C_2H_5OP(O)(C_3H_7)_2$	1198	13.4483	0.7692	−0.8966	324.369	50.595	3.63
21 $(C_2H_5O)_2P(O)CH_3$	1245	9.4388	0.3333	−0.1364	193.529	37.912	2.74
22 $(C_2H_5O)_2P(O)CH_2Cl$	1667	9.4827	0.2286	−0.2258	232.416	39.112	3.05
23 $(C_2H_5O)_2P(O)CHCl_2$	1272	9.1667	0.2692	0.1402	270.627	57.749	3.20
24 $(C_2H_5O)_2P(O)CCl_3$	1278	7.6316	0.2368	−0.4667	268.904	47.294	3.26
25 $(CH_3O)_3PO$	1289 1270	12.5000	0.2000	−0.3293	217.726	26.435	3.03
26 $(CH_3O)_2P(O)H$	1261	15.5556	0.2353	−0.6963	207.498	22.428	2.98
27 $(C_2H_5O)_2P(O)H$	1258	13.3333	0.7500	−0.3333	248.597	47.039	3.11
28 $(i\text{-}C_3H_7O)_2P(O)H$	1254	11.3281	0.4043	−0.2548	274.534	42.288	3.14
29 $(C_6H_5)_3PO$	1202	15.5555	0.3429	0.5405	533.407	90.580	4.61
30 $[(CH_3)_2N]_3PO$	1207	22.0588	0.4091	0.1667	469.334	54.205	4.47
31 $(CH_3)_3PO$	1196	42.0000	0.5116	−0.3750	436.754	44.913	4.45
32 $(C_2H_5)_3PO$	1178	29.8077	0.3000	−0.2500	455.903	30.387	4.52
33 $(C_3H_7)_3PO$	1170	21.4286	0.3182	0.1136	446.522	48.166	4.38
C_6H_5OH		4.6154	0.4762	0.3125	75.853	31.637	1.47[a]
C_6F_5OH		4.5238	0.2473	−0.0682	107.579	20.579	2.05[a]

[a] Means the μ_D^{exp} value.

moments of the uncomplexed proton donor and acceptor we obtained calculated dipole moments of the complexes which, when compared with the corresponding experimental values, gave us important information about the polarization within the hydrogen-bonded complex. In our calculations we have assumed that the direction of μ_A^{exp} in the phosphoryl molecules of the type X_3PO which possess C_3 symmetry, lies along the C_3 axis, i.e., is coincident with the P=O direction. The direction of μ_D^{exp} in the pentafluorophenol molecule was calculated[6] by taking the angle between the group moments Ph−F (μ_F = 1.45 D) and Ph−OH (μ_{OH} = 1.47 D) to be 90° (the C−F bond moments at C2, C3, C5 and C6 compensate one another). The angle between μ_{OH} and μ_D^{exp} was then determined to be 45° (see Fig. 1). The molecular dipole moment, μ_D^{exp}, of phenol coincides with the O−H bond moment.[6] Furthermore, to calculate μ_{DA}^{calc} we also need to know the structure of the hydrogen-bonded complex. As a geometrical model for the complexes between phenol and the various phosphoryl compounds, we have used the crystal structure[7] of a stable hydrogen-bonded complex between pentafluorophenol and triphenylphosphine oxide. The P=O···H and C−O−H angles were found to be 141° and 112° (the C−O−H angle in phenol has been estimated[6] to be 110°). The angle between the direction in which μ_A^{exp} and μ_D^{exp} are acting in the complex was then calculated to be 16° for the pentafluoro-

Table 2. Experimental dipole moment μ_{DA}^{exp}, the corresponding total polarization, P_∞, molar refraction, R_D, the parameters α, β, γ and IR data of hydrogen-bonded complexes formed between various phosphoryl compounds and phenol at 20 °C. Solvent: carbon tetrachloride.

Proton acceptor	$\Delta\nu_{OH}$	K_{ass}^{a}	α	β	γ	P_∞	R_D	μ_{DA}^{exp}
	cm^{-1}	M^{-1}						D
1 $(C_6H_5S)_3PO$	260	69	5.4545	0.0565	0.9821	326.603	138.939	3.28
2 $(C_6H_5S)_2P(O)N(C_2H_5)_2$	318	114	9.7959	0.0870	0.8235	533.236	123.598	4.44
3 $C_6H_5SP(O)[N(C_2H_5)_2]_2$	382	445	13.6364	−0.2188	0.3589	614.149	60.125	5.16
	412							
4 $(C_6H_5S)_2P(O)i\text{-}C_3H_7$	316	152	7.6595	0.3125	0.7059	434.711	135.203	3.74
5 $C_6H_5SP(O)(C_3H_7)_2$	370	360	19.2000	0.2065	0.6667	596.975	101.803	4.88
6 $(C_2H_5S)_3PO$	307	75	8.5714	−0.3077	0.5313	322.622	47.569	3.64
7 $(C_2H_5S)_2P(O)N(C_2H_5)_2$	343	148	11.0526	0.1528	0.5454	465.234	91.818	4.23
8 $C_2H_5SP(O)[N(C_2H_5)_2]_2$	404	631	14.2857	0.5106	0.3056	634.157	119.673	4.97
	424							
9 $(C_2H_5S)_2P(O)i\text{-}C_3H_7$	335	166	9.7674	0.2647	0.5000	394.161	91.868	3.81
10 $C_2H_5SP(O)(C_3H_7)_2$	402	386	16.6667	0.2143	0.4000	575.655	79.307	4.89
11 $(C_6H_5O)_3PO$	230	41	9.2307	0.3488	0.4440	527.325	133.134	4.35
12 $(C_6H_5O)_2P(O)N(C_2H_5)_2$	298	109	11.7647	0.0833	0.4667	576.575	98.419	4.79
13 $C_6H_5OP(O)[N(C_2H_5)_2]_2$	395	360	15.8537	0.1500	0.4583	715.091	99.625	5.44
14 $(C_6H_5O)_2P(O)i\text{-}C_3H_7$	296	101	10.2941	0.2500	0.4762	494.679	108.447	4.31
15 $C_5H_5OP(O)(C_3H_7)_2$	355	166	15.0000	0.2100	0.2978	584.066	84.193	4.90
16 $(C_2H_5O)_3PO$	330	257	13.1579	0.2500	0.1364	451.752	70.532	4.28
17 $(C_2H_5O)_2P(O)N(C_2H_5)_2$	374	491	14.7059	0.2069	0.1956	541.676	75.749	4.73
18 $C_2H_5OP(O)[N(C_2H_5)_2]_2$	444	1248	16.1290	0.1429	0.3214	633.066	81.413	5.15
19 $(C_2H_5O)_2P(O)i\text{-}C_3H_7$	371	457	12.1212	0.3529	0.2073	427.658	80.013	4.09
20 $C_2H_5OP(O)(C_3H_7)_2$	400	824	17.6471	0.8077	0.1111	618.777	110.455	4.94
21 $(C_2H_5O)_2P(O)CH_3$	363	381	13.7096	0.5600	0.1276	439.988	83.649	4.14
22 $(C_2H_5O)_2P(O)CH_2Cl$	305	239	11.2903	0.2209	0.2037	402.312	71.542	3.99
23 $(C_2H_5O)_2P(O)CHCl_2$	270	133	10.4166	0.3000	0.1363	470.644	84.830	4.07
24 $(C_2H_5O)_2P(O)CCl_3$	244	73	9.0909	0.1316	0.1400	410.743	78.038	3.99
25 $(CH_3O)_3PO$	305	183	15.1515	0.2308	0.1379	431.753	58.665	4.24
26 $(CH_3O)_2P(O)H$	280	123	16.1765	0.2549	0.1538	399.419	52.837	4.08
27 $(C_2H_5O)_2P(O)H$	298	162	15.2940	0.2780	0.0682	433.781	59.448	3.98
28 $(i\text{-}C_3H_7O)_2P(O)H$	313	237	15.7407	0.3636	0.1094	505.269	74.139	4.55
29 $(C_6H_5)_3PO$	410	1055	21.8750	0.2895	0.8372	955.143	125.721	6.31
30 $[(CH_3)_2N]_3PO$	460	1874	29.4117	0.2667	0.1613	915.424	71.852	6.37
31 $(CH_3)_3PO$	450	1836	30.0000	0.3125	0.2954	676.711	54.053	5.45
32 $(C_2H_5)_3PO$	468	2522	28.3333	0.2857	0.0313	739.442	57.891	5.72
33 $(C_3H_7)_3PO$	466	2341	23.5294	0.0426	0.4127	723.052	62.253	5.64
$(C_6H_5)_3PO^{b}$	–	6000	23.8095	0.1250	0.4286	1257.641	117.253	7.40

[a] K_{ass} data from Ref. 2. [b] Hydrogen-bonded complex with pentafluorophenol.

phenol/triphenylphosphine oxide complex (see Fig. 1) and 59° for the phenol/phosphoryl compound complexes. The vectorially calculated dipole moments, μ_{DA}^{calc}, of the various complexes are presented in Table 3. The vectorial difference between the experimental dipole moment and the vectorial sum of the components can be expressed in terms of a dipole increment, Δμ, defined by the equation $\Delta\vec{\mu} = \vec{\mu}_{DA}^{exp} - \vec{\mu}_{DA}^{calc} = \vec{\mu}_{DA}^{exp} - (\vec{\mu}_{D}^{exp} + \vec{\mu}_{A}^{exp})$ as shown in Fig. 1. In this calculation the additional dipole moment, Δμ, is directed along the H-bond,[1,8] from the proton acceptor towards the proton donor, i.e., it has not been taken into account the electronic redistribution in other parts of the hydrogen-bonded complex. The Δμ values are tabulated in Table 3.

Results and discussion

μ_A^{exp}. The experimental dipole moments, μ_A^{exp}, of the phosphoryl compounds do not in general form a monotonic correlation with the P=O stretching frequency (see Table 1) or, as can be seen in Fig. 2, with the O−H stretching frequency shift, $\Delta\nu_{OH}$, accompanying the formation of a hydrogen bond with phenol ($\Delta\nu_{OH}$ = IR stretching frequency of free phenol O−H bond minus the frequency of the hydrogen-bonded O−H). The plot μ_A^{exp} vs. $\Delta\nu_{OH}$ is virtually a scatter diagram. There is, however, for some selected series of compounds a smooth correlation, e.g. for the series $(C_6H_5S)_3PO$ (**1**), $(C_6H_5S)_2P(O)i\text{-}C_3H_7$ (**4**), $C_6H_5SP(O)(C_3H_7)_2$ (**5**), $(C_3H_7)_3PO$ (**33**) and the series $(C_2H_5S)_3PO$ (**6**), $(C_2H_5S)_2P(O)i\text{-}C_3H_7$ (**9**), $C_2H_5SP(O)(C_3H_7)_2$ (**10**), $(C_3H_7)_3PO$ (**33**). On replacing the sulfur atoms in

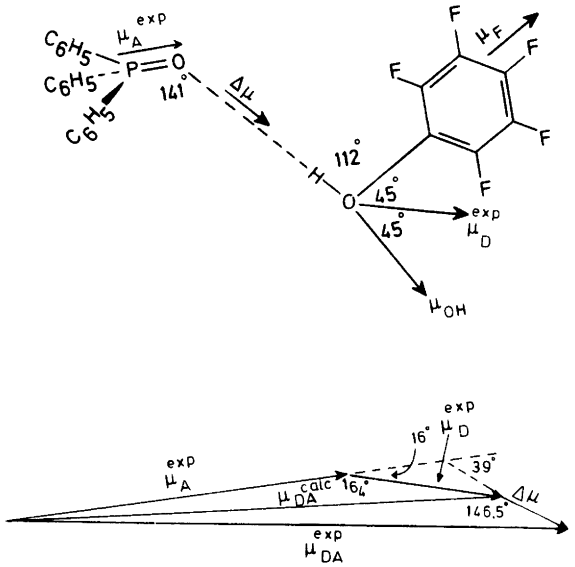

Fig. 1. The hydrogen-bonded complex between pentafluorophenol and triphenylphosphine oxide.

these series with oxygen, the smooth correlation falls (see compounds **11**, **14**, **15**, **33** and **16**, **19**, **20**, **33** in Fig. 2).

The introduction of one alkyl group into triethyl or triphenyl phosphate causes an increase in $\Delta\nu_{OH}$, but a lowering of the μ_A^{exp} values as compared with the corresponding phosphate (compounds **14** and **19**). In these compounds the C_{3v} symmetry is broken and the resultant of the bond moments happens to be less than the dipole moment of the corresponding phosphate. Introduction of two alkyl groups, however, results in a large enhancement in both the μ_A^{exp} and the $\Delta\nu_{OH}$ values, and in the polarity of the P=O bond, as expected from the inductive effect of two alkyl groups. Furthermore, there exists for the closely related compounds, $(C_2H_5O)_2P(O)CH_3$ (**21**), $(C_2H_5O)_2P(O)CH_2Cl$ (**22**), $(C_2H_5O)_2P(O)CHCl_2$ (**23**) and $(C_2H_5O)_2P(O)CCl_3$ (**24**) a fairly good linear correlation between μ_A^{exp} and $\Delta\nu_{OH}$. Along this series there is a decrease in the K_{ass} values (from 382 to 73 M^{-1}) in the $\Delta\nu_{OH}$ (from 363 to 244 cm^{-1}) and in the P=O polarity (from 1245 to 1278 cm^{-1}), whereas an increase in the μ_A^{exp} values (from 2.78 to 3.26 D) is found, i.e., there is an increase in the molecular dipole moment, but a lowering of the proton accepting ability. These findings may easily be explained by the electron withdrawing power of the chlorine atoms. The effect of the chlorine atoms may also be demonstrated by comparison of $(C_2H_5O)_2P(O)CCl_3$ (**24**) with $C_2H_5SP(O)(C_3H_7)_2$ (**10**). The dipole moments are comparable, but the latter is a much stronger proton acceptor. The dipole moments of triphenyl phosphate (μ_A^{exp} = 2.87 D) and of triethyl phosphate (μ_A^{exp} = 3.07 D) are also comparable. There is, however, a big difference in the K_{ass} and $\Delta\nu_{OH}$ values on association with phenol (see Table 2). The reason for this behaviour is that the inductive and mesomeric effects of an RO group have a greater tendency than an ArO group to increase the electron density around the phosphoryl oxygen and hence to increase the K_{ass} and $\Delta\nu_{OH}$ values, whereas the contribution of bond moments making up the molecular dipole moment is nearly the same in both molecules. A similar conclusion might be drawn by comparison of $(C_6H_5O)_3PO$ with $(C_6H_5S)_3PO$. The latter is the strongest proton acceptor, but the dipole moment is greatest for triphenyl phosphate.

Table 3. Vectorially calculated dipole moments, μ_{DA}^{calc}, and additional dipole moments, $\Delta\mu$, of the hydrogen-bonded complexes, C_6H_5OH/X_3PO and $C_6F_5OH/(C_6H_5)_3PO$.

Proton acceptor	μ_{DA}^{calc}	$\Delta\mu$
	D	D
$(C_6H_5S)_3PO$	3.19	0.099
$(C_2H_5S)_3PO$	3.11	0.546
$(C_6H_5O)_3PO$	3.84	0.538
$(CH_3O)_3PO$	3.99	0.266
$(C_2H_5O)_3PO$	4.03	0.267
$(C_6H_5)_3PO$	5.51	0.877
$[(CH_3)_2N]_3PO$	5.38	1.077
$(CH_3)_3PO$	5.36	0.094
$(C_2H_5)_3PO$	5.42	0.331
$(C_3H_7)_3PO$	5.29	0.384
$(C_6H_5)_3PO^a$	6.61	0.926

[a]Hydrogen-bonded complex with pentafluorophenol.

μ_{DA}^{exp}, μ_{DA}^{calc} and $\Delta\mu$. There is in general no correlation between experimental dipole moments, μ_{DA}^{exp}, of hydrogen-bonded complexes and $\Delta\nu_{OH}$ (see Table 2). A smooth correlation is observed, however, for closely related complexes, i.e., we have found the same trend for the relationship μ_{DA}^{exp} vs. $\Delta\nu_{OH}$ as for μ_A^{exp} vs. $\Delta\nu_{OH}$.

The vectorially calculated dipole moments of the various hydrogen-bonded complexes of the type C_6H_5OH/X_3PO are less than those found experimentally (see Table 3). This finding demonstrates clearly that the formation of a hydrogen bond brings about displacement of electrons. Further strong support for this view is that the IR spectra of phosphoryl compounds are greatly perturbed on complex formation with iodine[2] and with pentafluorophenol.[9] In addition CNDO/2 calculations[10,11] have shown that considerable charge shift and charge transfer take place upon hydrogen-bond formation. Drift of electrons is also demonstrated in this work, particularly for compounds containing N−P=O and C_6H_5−P=O groups where unshared electron pairs and π-electrons may operate. The dipole moments of triphenylphosphine oxide, hexamethylphosphoramide, trimethylphosphine oxide, triethylphosphine oxide and tripropylphosphine oxide are almost the same, μ_A^{exp} = 4.49(±0.12) D. However, on complexation with phenol, differences in the μ_{DA}^{exp} values become evident. The μ_{DA}^{exp} values of the hydrogen-bonded complexes phenol/triphenylphosphine oxide and phenol/hexamethylphosphoramide are 6.34 (±0.03) D, whereas the values of the complexes phenol/trialkylphosphine oxide are 5.58(±0.14) D. Since the hydrogen bond strengths of these complexes are comparable, the differ-

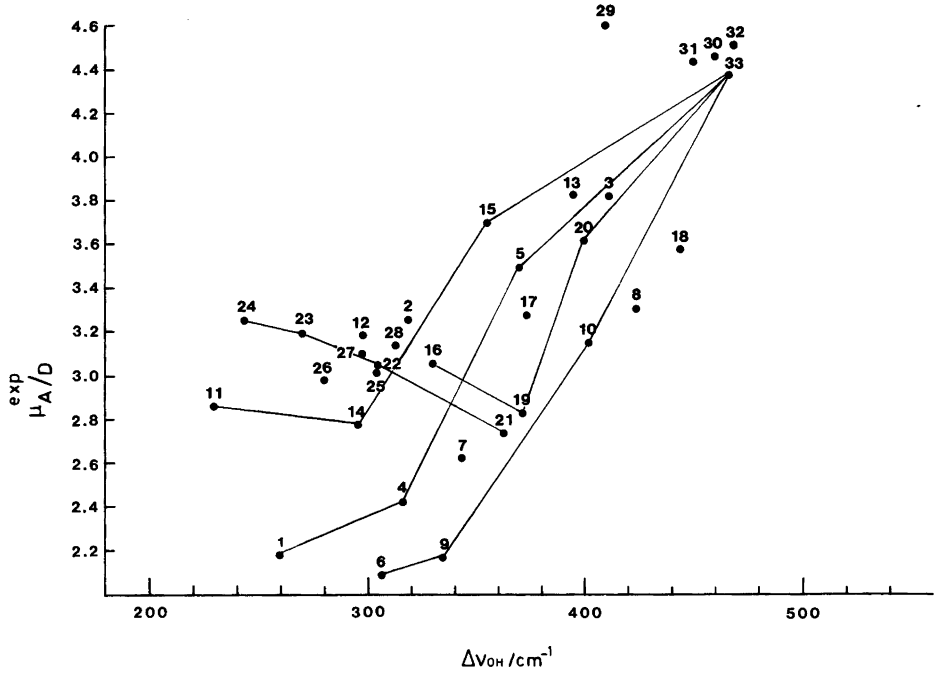

Fig. 2. Correlation between the dipole moments, μ_A^{exp}, of various phosphoryl compounds and the stretching frequency shift, $\Delta\nu_{OH}$, of the phenol O–H bond upon complexation with phosphoryl compounds.

ence in the dipole moments of 0.76 D may be attributed to resonance structures such as $N^{\delta+}\text{----}P^{\delta-}$ and $C_6H_5^{\delta+}\text{----}P^{\delta-}$ which contribute to the molecular dipole moment. Similar resonance structures are not likely for the trialkylphosphine oxide complexes. Since we have used the same proton donor and a series of phosphoryl compounds of the type X_3PO, we found it reasonable to assume similar geometry for all these complexes. Hence the difference in the μ_{DA}^{exp} values of the various complexes should depend only on the resultant of the individual vectors associated with each of the bonds within the complex, and not on different geometry. Accordingly, we believe that the vectorial difference between experimental and vectorially calculated dipole moments, $\Delta\mu$, does not arise entirely from an additional dipole along the H-bond, but also from changes in other bond moments. The change in the dipole moment of the phenol molecule due to polarization of the π-electrons on complex formation, has been shown by quantum mechanics calculations[12] to be small, of the order of 0.1 D, and hence has been neglected in our calculation.

The dipole moment of the hydrogen-bonded complex between pentafluorophenol and triphenylphosphine oxide (7.40 D) is much greater than that of the phenol/triphenylphosphine oxide complex (6.31 D). This is in accordance with the fact that pentafluorophenol forms a much stronger H-bond than does phenol with triphenylphosphine oxide.[9] What is surprising, however, is that the large difference in the dipole moments of the two complexes is not reflected in the $\Delta\mu$ values (see Table 3). The reason for this behaviour is not yet clear and more work needs to be done, for example by using more differentiated phenols, to reveal the full explanation.

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