〔Bunseki Kagaku, **41**, T103-T108 (1992)〕 [Lab. of Pharm. Analytical Chemistry]

A Round Robin Test for the Total Cyanide Determination of Complicated Wastewater.

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A round robin test between seven universities was carried out for the determination of total cyanide in complicated wastewater samples by Japanease Industrial Standards and other analytical methods. Six kinds of waste samples obtained from university laboratories and a tap water sample were prepared. Relative standard deviation of the analytical data for these samples by the Japanease official method were within ±10 %.

〔Chem. Lett., **1992**, 1017-1020〕 [Lab. of Pharm. Analytical Chemistry]

How Active *p*-Quinone Dianions Are as Proton Acceptors!

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Formation constants ($K^{=}$) of two-point hydrogen-bonded complexes of *p*-quinone dianions ($PQ^{=}$) with CH_3OH (1 : 2) have been successfully determined to be of the order of 10^4 dm^6 mol^{-2}. The quite large values of $K^{=}$ indicate that $PQ^{=}$ strongly attracts the weak proton-donors such as alcohols. The hydrogen-bond distance calculated by the HF energy gradient method with 4-31G basis sets is very short and the atomic bond population is large enough to be considered as a value of a weak covalent bond. These calculations have revealed that the bond of $PQ^{=}$ with CH_3OH is remarkably strong compared to usual hydrogen bonds involving O···H−O, and clearly explain the origin of the quite large observed $K^{=}$ values, considering enthalpy driven stabilization of a hydrogen bonding.

〔Bull. Chem. Soc. Jpn., **65**, 2697-2703 (1992)〕 [Lab. of Pharm. Analytical Chemistry]

Spectroscopic Analysis and Geometry Assignment of the Minimum Energy Conformations of 2-Phenoxypyridines and Diphenyl Ethers.

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The conformational preferences of 2-phenoxypyridines and diphenyl ethers have been determined by the spectral measurements and their analyses based on CNDO/S-CI calculations, and by the minimum energy optimization using the method of ab initio molecular orbital calculations with STO-3G basis sets. The conformation of diphenyl ether is non-rigid with the dihedral angles, around 90°, of two phenyl rings at room temperature. The spectral observation at 77K have provided evidence for this conclusion. 2-Phenoxypyridine is, however, found to possess sufficient internal barriers to stabilize the two aromatic rings in a skew form.