

High Resolution Infrared Detection of O=PF in the Gas Phase

P. Paplewski, H. Bürger, and H. Beckers

Anorganische Chemie, FB 9, Universität-GH, D-42097 Wuppertal

Reprint requests to Prof. Dr. H. Bürger; Fax: +49 202 439 2901;

E-mail: buerger1@uni-wuppertal.de

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Dedicated to Prof. Dr. Reinhard Schmutzler on the occasion of his 65th birthday

Short-lived phosphinous fluoride, O=PF, has been made by flash pyrolysis of F_2POPF_2 in Ar at 1200°C and detected by gas phase IR spectroscopy. The ν_1 band, $\nu_0 = 1297.5372 \text{ cm}^{-1}$, has been studied with a resolution of $8 \times 10^{-3} \text{ cm}^{-1}$, and about 1500 transitions have been assigned. These were fitted using a Watson-type Hamiltonian, $\sigma = 1.5 \times 10^{-3} \text{ cm}^{-1}$, to excited state parameters up to quartic centrifugal distortion constants. The ν_2 band was located at 819.58 cm^{-1} . An extended set of ground state parameters was obtained by combining recently measured microwave transitions with ground state combination differences formed from ν_1 transitions.

The experimental results are in perfect agreement with the matrix IR spectra, mw measurements and *ab initio* calculations but disagree with a recently claimed low resolution detection of OPF in the gas phase.

Key words: High Resolution; Infrared Spectrum; Pyrolysis; Phosphinous Fluoride.