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THE VACUUM UV PHOTOABSORPTION SPECTRUM OF METHYL FLUORIDE (CH_3F). A VIBRATIONAL ANALYSIS.

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In the systematic investigation of the methyl monohalides by photoabsorption spectroscopy, threshold photoelectron spectroscopy and CIS spectroscopy [1,2], we concluded our work with the study of the photoabsorption spectrum of CH_3F. The dissociative ionization study of this molecule by electron impact [3] and by photoionization [4,5] has already been published earlier.

For this purpose, a M225-McPherson 1m-NIM monochromator (beamline: 1m-NIM - 2) modified to 1.5m-NIM has been used, equipped with a 1 200 ℓ/mm gold coated grating. The width of entrance and exit slits is l00 μm. A resolution of about 0.1 nm is obtained. A 1 mm thick stainless steel microchannel plate allows differential pumping of the monochromator. The absorption cell is a 30 cm long stainless steel cylinder where the pressure is measured by a capacitor manometer. The light is detected by a sodium salicylate sensitized multiplier. The recording of an absorption spectrum requires one scan with gas in the cell and one scan with empty cell.

The photoabsorption spectrum as recorded in this experiment is shown in fig. 1 where the molar extinction coefficient ε_{hv} is plotted as a function of the photon energy. Clearly the spectrum is made of strong broad peaks underlying weak but well defined fine structures extending over a broad photon energy range. For a detailed analysis, a background has been subtracted from the original spectrum. The result of this subtraction procedure is shown in fig. 2 where the point to point difference Δ between the original spectrum and the background is plotted against the photon energy in the range of 10-14 eV.

The broad components have successively all been assigned to 2e→3s at 9.4 eV, 2e→4s/3d at 11.3 eV, $5a_1$/le→3s, 3p at 13.6 eV, $5a_1$/le→4s/3d at 15.7 eV and $4a_1$→3s and 4s/3d at 19.9 eV and 22.0 eV [4].

The sharp and weak structures observed between 10-14 eV photon energy have been ascribed to two Rydberg transitions, i.e. the 2e→3p transition characterized by an effective quantum number n*=2.333 ± 0.010 at 10-12 eV and the 2e→6s/5d transition with an effective quantum number n*=5.010 ± 0.020 at 12-14 eV successively.

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***FIG. 1**: VUV photoabsorption spectrum of CH_3F between 7.5-24.0 eV photon energy.*

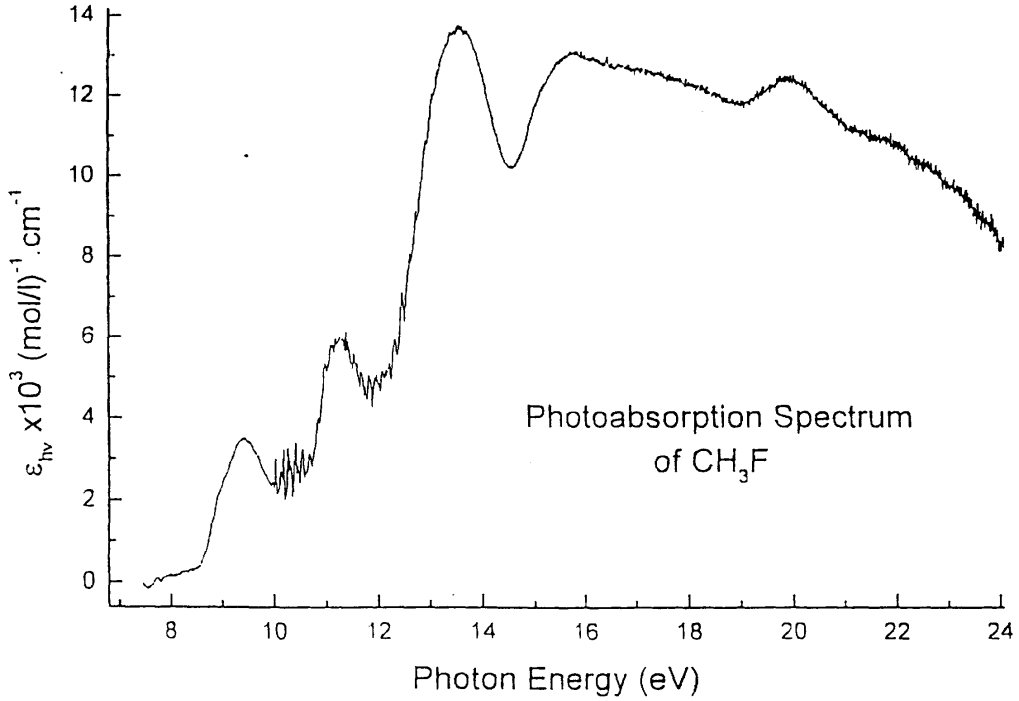
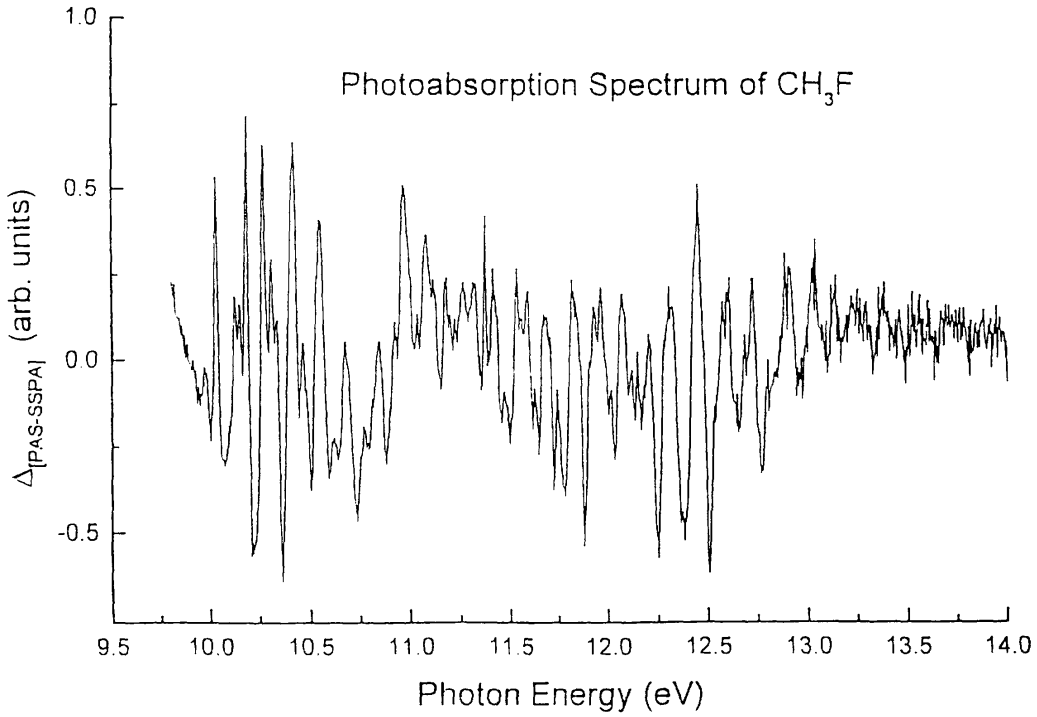


***FIG. 2**: Structured part between 10-14 eV of the photoabsorption spectrum of CH_3F enhanced by a continuum subtraction procedure.*



About 70 levels have been identified and assigned in this photon energy range. Both

states clearly show a Jahn-Teller splitting which has been measured. The vibrational assignments will be based on the results of *ab initio* calculations. These are still in progress.

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REFERENCES

[1]. R. Locht, B. Leyh, H. W. Jochims, K. Hottmann and H. Baumgärtel, BESSY Jahresber. (1996) 162.

[2]. R. Locht, A. Hoxha, B. Leyh, K. Hottmann, H. W. Jochims and H. Baumgärtel, BESSY Jahresber. (1997) 160.

[3]. R. Locht and J. Momigny, Intern. J.Mass SpectromJon Proc. 71(1986) 141.

[4]. R. Locht, E. Rühl, J. Momigny and H. Baumgartel, Chem.Phys. 117 (1987) 305.

[5]. K.M. Weitzel, F. Güthe, J. Mähnert, R. Locht and H. Baumgärtel, Chem.Phys. 201 (1995) 287.