

## On the molecular geometry of the $\text{FCO}_2^{\cdot}$ radical

J. Koucký<sup>a</sup>, P. Kania<sup>b</sup>, T. Uhlíková<sup>c</sup>, H. Beckers<sup>d</sup>, H. Willner<sup>e</sup>, and Š. Urban<sup>f</sup>

<sup>a</sup> Institute of Chemical Technology, Department of Analytical Chemistry, Technická 5, 166 28, Prague 6, Czech Republic, Tel.: +420 220 444 274 , E-mail: jan.koucky@vscht.cz

<sup>b</sup> Institute of Chemical Technology, Department of Analytical Chemistry, Technická 5, 166 28, Prague 6, Czech Republic, Tel.: +420 220 444 274 , E-mail: patrik.kania@vscht.cz

<sup>c</sup> Institute of Chemical Technology, Department of Analytical Chemistry, Technická 5, 166 28, Prague 6, Czech Republic, Tel.: +420 220 444 274 , E-mail: tereza.uhlikova@vscht.cz

<sup>d</sup> Bergische Universität Wuppertal, FB C - Anorganische Chemie, Gaußstr. 20, 42097 Wuppertal, Germany, Tel.: +49 202 439 2504, E-mail: beckers@uni-wuppertal.de

<sup>e</sup> Bergische Universität Wuppertal, FB C - Anorganische Chemie, Gaußstr. 20, 42097 Wuppertal, Germany, Tel.: +49 202 439 2517, E-mail: willner@uni-wuppertal.de

<sup>f</sup> Institute of Chemical Technology, Department of Analytical Chemistry, Technická 5, 166 28, Prague 6, Czech Republic, Tel.: +420 220 444 267 , E-mail: stepan.urban@vscht.cz

The rotational spectra of the three isotopologues of the fluoroformyloxyl radical have been measured and analysed. Together with the experimental work, detailed *ab initio* calculations were performed to stand as a theoretical base for transition assignments. Analyses of all the spectra provided three sets of accurate molecular constants. These parameter sets were used to get various types of radical geometries – the combination of effective and substitution geometry, semiempirical equilibrium geometry, and, in the case of  $\text{FC}^{16}\text{O}^{18}\text{O}$ , even the different bond lengths of C- $^{16}\text{O}$  and C- $^{18}\text{O}$  were evaluated in vibrational ground state.