

# ROTATIONAL SPECTROSCOPY OF $\text{CF}_2\text{ClCCl}_3$ AND ANALYSIS OF HYPERFINE STRUCTURE FROM FOUR QUADRUPOLEAR NUCLEI

ZBIGNIEW KISIEL, EWA BIAŁKOWSKA-JAWORSKA, *ON2, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland*; ICIAR URIARTE, FRANCISCO J. BASTERRETXEA, EMILIO J. COCINERO, *Departamento de Química Física, Universidad del País Vasco (UPV-EHU), Bilbao, Spain*.

$\text{CF}_2\text{ClCCl}_3$  has recently been identified among several new ozone- depleting substances in the atmosphere.<sup>a</sup> There are no literature reports concerning rotational spectroscopy of this molecule, although we were recently able to report its first chirped pulse, supersonic expansion spectrum.<sup>b</sup>  $\text{CF}_2\text{ClCCl}_3$  has a rather small dipole moment so that the spectrum is weak and each transition displays very complex nuclear quadrupole hyperfine structure resulting from the presence of four chlorine nuclei.

We have presently been able to carry out a complete analysis of the hyperfine structure by combining the information from chirped pulse spectra with dedicated higher resolution measurements made with a cavity supersonic expansion instrument. The hyperfine analysis was carried out with Pickett's SPFIT/SPCAT package and the sizes of Hamiltonian matrices are sufficiently large to require the use of 64-bit compilation of these programs (made available for both Windows and Linux systems on the PROSPE website). The resulting fit is to within experimental accuracy and is supported by *ab initio* calculations. The precise values of off-diagonal hyperfine constants for all nuclei lead to useful angular information that is complementary to direct structural information from moments of inertia.<sup>c</sup>

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<sup>a</sup>J.C.Laube, M.J.Newland, C.Hogan, et al., *Nature Geoscience* **7**, 266 (2014).

<sup>b</sup>Z.Kisiel, E.Białkowska-Jaworska, L.Pszczółkowski, I.Uriarte, P.Ejica, F.J.Basterretxea, E.J.Cocinero, 70<sup>th</sup> ISMS, Champaign-Urbana, Illinois, RF-11 (2015).

<sup>c</sup>Z.Kisiel, E.Białkowska-Jaworska, L.Pszczółkowski, *J.Chem.Phys.* **109**, 10263 (1998).