

## HAVING A BALL! MICROWAVE SPECTRUM OF THE (NEARLY) SPHERICAL TOP TEFLIC ACID

SVEN HERBERS, DANIEL A. OBENCHAIN, PETER KRAUS, JENS-UWE GRABOW, *Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität, Hannover, Germany.*

The microwave spectrum of teflic acid ( $\text{TeF}_5\text{OH}$ ) in the range of 3 to 25 GHz was analyzed. Though teflic acid is an asymmetric top in its equilibrium structure, it behaves like a symmetric top because of the OH group internal rotation. The strongest transitions in the spectrum originate from the  $^{130}\text{TeF}_5\text{OH}$ ,  $^{128}\text{TeF}_5\text{OH}$  and  $^{126}\text{TeF}_5\text{OH}$  species as shown in the figure below. The  $\text{TeF}_5^{18}\text{OH}$ ,  $\text{TeF}_5\text{OD}$  and  $\text{TeF}_5^{18}\text{OD}$  isotopologues were also analyzed. From the rotational constants of the different isotopologues and with help of quantum chemical calculations a semi empirical equilibrium structure of teflic acid was determined. The Te-O equilibrium bondlength was determined with accuracy to the hundredth of an angstrom.

