THE SALT MOLECULE $LiKF_2$

JENS-UWE GRABOW, *Gottfried-Wilhelm-Leibniz-Universität, Institut für Physikalische Chemie, Callinstraße 3A, 30167 Hannover, Germany*; RICHARD J. MAWHORTER, *Pomona College, Department of Physics and Astronomie, 610 North College Avenue, Claremont, CA 91711*.

The mixed alkali halide dimer $LiKF_2$ has been observed and characterized using LASER-ablation supersonic-jet Fourier transform microwave spectroscopy. This is the first step in extending the earlier successful studies[ab] of $LiNaF_2$ to heavier mixed dimers. Fifteen transitions of 3 isotopologues of $LiKF_2$, $^6Li^{39}KF_2$, $^6Li^{41}KF_2$, and $^7Li^{39}KF_2$, have been observed. This allows a determination of the kite-shaped $LiKF_2$-structure as well as the leading centrifugal distortion constants, which in turn provide more insight into the nature of these ionic bonds. Measurements of the hyperfine splitting of these spectral lines provides another constraint on molecular charge density, i.e. a further detailed check of theoretical calculations.

[a] S. Biermann, et al., J. Chem. Phys. 105, 9754-9761 (1996).
[b] R.J. Mawhorter, et al., J. Mol. Struct. 413-414, 415-422 (1997).