ROTATIONALLY RESOLVED IR SPECTRA OF LiD_2^+ AND LiH_2^+

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Photodissociation infrared spectra of mass selected LiD_2^+ and LiH_2^+ have been obtained in the D-D and H-H stretch region respectively, using a tandem mass spectrometer and detecting the Li^+ loss channel. For the first time rotationally resolved spectra of these complexes are available providing structural parameters and allowing direct comparison with theoretical data [a]. For LiD_2^+ around 100 lines of the K_a=0←K_a=0, K_a=1←K_a=1, and K_a=2←K_a=2 parallel transitions were fitted to a Watson A-reduced Hamiltonian. The analysis of the spectrum was supported by quantum chemical calculations using the program TRIATOM [b] and the potential from Gianturco *et al.* [c]. The LiD_2^+ complex was found to have T-shaped structure in agreement with theoretical predictions. An analogous analysis has been performed for the LiH_2^+ spectrum which differs from the LiD_2^+ spectrum due to larger rotational constants and an altered ortho:para ratio.

[a] V. P. Bulychev, K. M. Bulanin, and M. O. Bulanin, *Mol. Spec.* **96**, 2004, 205-216
[b] J. Tennyson, S. Miller, and C. R. Le Sueur, *Comp. Phys. Comm.* **75**, 1993, 339-364.
[c] R. Martinazzo, G. F. Tantardini, E. Bodo, and F. A. Gianturco, *J. Chem. Phys.* **119**, 2003, 11241-11248