

EXTENSIVE AND HIGHLY ACCURATE LINE LISTS FOR HYDROGEN HALIDES

G. LI and P.F. BERNATH, *Department of Chemistry, University of York, Heslington, York YO10 5DD, UK*; I.E. GORDON, L.S. ROTHMAN, C. RICHARD, *Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, Cambridge MA 02138, USA*; R.J. LE ROY, *Department of Chemistry, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada*; J.A. COXON, *Department of Chemistry, Dalhousie University, Halifax, Nova Scotia B3H 4J3, Canada*; P. HAJIGEORGIOU, *Department of Life and Health Sciences, University of Nicosia, 46 Makedonitissas Ave., P.O. Box 24005, Nicosia 1700, Cyprus*.

New dipole moment functions (DMF) for the ground $X^1\Sigma^+$ electronic states of the hydrogen halides (HF, HCl, HBr, HI) have been obtained using a direct fit approach that fits the best available and appropriately weighted experimental line intensity data for individual ro-vibrational transitions. Combining the newly developed (taking into account the most recent experiments) empirical potential energy functions and the DMFs, line positions and line intensities of the hydrogen halides and their isotopologues have been calculated numerically using program LEVEL^a. In addition, new semi-empirical algorithms for assigning line-shape parameters for these species have been developed. Using these improvements, new line lists for hydrogen halides were created to update the HITRAN spectroscopic database. These new lists are more accurate and significantly more extensive than those included in the current version of the database (HITRAN2008)^b.

^aR.J. Le Roy, "LEVEL 8.0, 2007", University of Waterloo Chemical Physics Research Report CP-663 (2007); see <http://leroy.uwaterloo.ca/programs/>.

^bL.S. Rothman, I.E. Gordon, A. Barbe, D.C. Benner, P.F. Bernath, *et al.*, "The HITRAN 2008 Molecular Spectroscopic Database," JQSRT 110, 532-572 (2009).