

SEMI-EMPIRICAL DIPOLE MOMENT FUNCTION OF $X^1\Sigma^+$ CO^a

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A new dipole moment function (DMF) for the ground $X^1\Sigma^+$ electronic states of carbon monoxide (CO) has been obtained using a direct fit approach that fits the best available and appropriately weighted experimental line intensity data for individual ro-vibrational transitions. This method was recently successfully applied to HF, HCl, HBr and HI molecules^a. The new dipole moment function benefits from the use of new accurate and extensive experimental data. Also our method allows proper weighting of the data as well as not being dependent on the amount of measured transitions within a band. Combining the newly developed (taking into account the most recent experiments) empirical potential energy functions and the DMF, line positions and line intensities of CO and their isotopologues have been calculated numerically using program LEVEL^b. In addition, new semi-empirical algorithms for assigning line-shape parameters and line shifts for these species have been developed. Using these improvements, new line lists for CO were created to update the HITRAN^c and HITEMP^d spectroscopic database.

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^aG. Li, I.E. Gordon, R.J. Le Roy, P.G. Hajigeorgiou, J.A. Coxon, P.F. Bernath, and L.S. Rothman, "Reference spectroscopic data for Hydrogen Halides. Part I: Construction and Validation of the Ro-vibrational Dipole Moment Functions," JQSRT 2013 (In Press).

^bR. Le Roy, "LEVEL. 8.0 ed2007" University of Waterloo Chemical Physics Research Report CP-663 (2007).

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

^dL.S. Rothman, I.E. Gordon, R.J. Barber, H. Dothe, R.R. Gamache, A. Goldman, V. Perevalov, S.A. Tashkun, and J. Tennyson, "HITEMP, the high-temperature molecular spectroscopic database," JQSRT 111, 2139-2150 (2010).