DIRECT POTENTIAL FITTING FOR THE $A\,^3\Pi_{1u}$ and $X\,^1\Sigma_g^+$ STATES OF Br_2

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Bromine dimer has been studied by many researchers in various wavelength regions. The $A\,^3\Pi_{1u}$ and $X\,^1\Sigma_g^+$ states have been well observed using magnetic rotation spectroscopy,[a] by laser-induced fluorescence,[b,c] by laser absorption,[d] by Fourier transform absorption,[e] and by UV emission.[f] This yields a data set consisting of 16916 transitions in which the observed vibrational levels for the $X\,^1\Sigma_g^+$ and $A\,^3\Pi_{1u}$ states span 83% and 99% of the potential well depths, respectively, with the highest observed vibrational level of the $A\,^3\Pi_{1u}$ state lying only 2 cm^{-1} below the dissociation limit.[a] In order to provide the most compact and comprehensive description of these data, and the ability to make reliable predictions outside their range, we have chosen to perform a "direct potential fit" (DPF), rather than a conventional Dunham-expansion analysis. In particular, accurate analytic potential energy functions for the $A\,^3\Pi_{1u}$ and $X\,^1\Sigma_g^+$ states are determined from a combined-isotopologue DPF analysis that also yields the electronic isotope shift, the Ω-doubling radial strength function, and an experimental value for the long-range inverse-power C_5 constant of the $A\,^3\Pi_{1u}$ state, as well as centrifugal Born-Oppenheimer Breakdown (BOB) functions for both states. To reveal characteristics of the $A\,^3\Pi_{1u}$ state, band constants calculated from these potentials are compared with those determined from a conventional parameter-fitting analysis reported by Coxon.[g]

[a] C. D. Boone, PhD Thesis, University of British Columbia (1999).
[b] C. Focsa *et al.*, J. Mol. Spectrosc. 200, 104 (2000).
[c] D. J. Postell *et al.*, to be published.
[d] N. Nishimiya *el al.*, Columbus Meeting, paper WH02 (2005).
[e] S. Gerstenkorn *et al.*, J. Physique, 48, 1685 (1987).
[f] P. Venkateswarlu *et al.*, J. Mol. Spectrosc. 96, 247 (1982).
[g] J. A. Coxon, J. Mol. Spectrosc. 41, 548 (1972).