

NOTE

Improved Molecular Constants for the Ground State of DO₂

Molecular constants for the ground state of DO₂ are redetermined using a combined analysis of previously published microwave measurements (1) and combination differences from a rotational analysis of the 000–000 band of the $\tilde{A}^2A' \rightarrow \tilde{X}^2A''$ electronic transition in the 7000 cm⁻¹ region (2). The analysis method follows on that used previously for HO₂ (3), and employs the parameterized Hamiltonian given in Ref. (4). The microwave measurements include 58 lines, from 51 to 196 GHz, with rotational levels up to $N = 7$, $K_a = 2$. The line at 74.579170 GHz was omitted from the fitting, as in Ref. (1). The line at 114.657274 GHz is reassigned as an unresolved combination of $F' - F'' = 5/2 - 7/2$ and $3/2 - 5/2$; the line at 143.160834 GHz is reassigned as $F' - F'' = 15/2 - 13/2$; 174 combination differences for rotational levels up to $N = 31$, $K_a = 9$ from the $\tilde{A}^2A' \rightarrow \tilde{X}^2A''$ band are used in the analysis.

A revised set of molecular constants is obtained by combining both sets of data with appropriate weightings, where the combination differences are assigned uncertainties of 0.003 cm⁻¹ and the microwave measurement uncertainties are taken from Ref. (1), and refitting to the parameterized Hamiltonian. Since the combination differences do not resolve the hyperfine structure, the hyperfine terms a_F , T_0^2 , T_1^2 , and T_2^2 in the parameterized Hamiltonian were first determined using only the microwave lines, and then fixed to these values in the final fitting analysis. The weighted RMS of the fit is 1.15. The molecular constants are given in Table 1.

An attempt was made to also include the millimeter-wave (field-free) measurements from Ref. (5) in the combined analysis. It was found that significantly

worse fitting results were obtained with this combination of data, and with the combination of microwave and millimeter-wave measurements, than with those from the microwave and combination difference measurements.

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TABLE 1

Revised Molecular Constants for the DO₂ Ground State (MHz)^a

Constant	Value	σ	Constant	Value	σ
$A - (B + C)/2$	305 366.141	0.035	a_0	9176.555	0.020
$(B + C)/2$	30 233.649 53	0.000 94	a_s	8984.205	0.018
$(B - C)/4$	711.402	0.031	b_s	199.321	0.014
$\Delta_N \times 10^2$	9.4191	0.0083	d_s	-44.9	1.4
Δ_{NK}	2.258 32	0.000 89	Δ_K^s	6.653	0.046
Δ_K	40.065	0.034	$\Delta_{NK}^s + \Delta_{KN}^s$	0.2783	0.0062
$\delta_N \times 10^3$	8.486	0.021	a_F	-4.212	0.013
δ_K	1.443	0.031	T_0^2	-0.4808	0.0083
$\Phi_{KN} \times 10^4$	3.33	0.25	T_1^2	12.4	1.9
$\Phi_K \times 10^2$	1.808	0.035	T_2^2	0.9091	0.0076

^a For definition of the constants, see (4).

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