## ANHARMONIC AND CORIOLIS INTERACTIONS IN THE $v_3 = 2/v_2 = 1/v_5 = 1/v_3 = v_6 = 1$ LEVEL SYSTEM OF CH<sub>3</sub>Br

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The  $\nu_2/\nu_5$  band system of CH<sub>3</sub>Br, a methyl halide playing an important role in the catalytic destruction of stratospheric ozone, already constituted the subject of several medium and high-resolution studies.

The novelty of the present study consists in considering, besides the strong Coriolis and  $\alpha$ -interactions coupling the  $v_2 = 1$  and  $v_5 = 1$  levels, a large variety of anharmonic and rovibrational interactions involving also the  $v_3 = 2$  and  $v_3 = v_6 = 1$  levels. Thousands of new data, belonging either to high J and K values in the  $\nu_2$  and  $\nu_5$  bands or to the, very weak,  $\nu_3 + \nu_6$  combination band, were included in the least-squares calculations.



Thanks to the large set of data, including more than 6300 experimental wavenumbers of the  $\nu_2$ ,  $\nu_5$ ,  $2\nu_3$  and  $\nu_3 + \nu_6$  rovibrational bands, with  $J \le 74$  and  $K \le 18$ , combined to the completeness of the theoretical model, the global standard deviation,

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of  $2.34 \times 10^{-4}$  cm<sup>-1</sup>, represents a great improvement with respect to the previous high-resolution study of the  $\nu_2/\nu_5$  band system<sup>1</sup>. Moreover, the present study explores also the reductions' issue, in the spirit of the work of Střiteská *et al*<sup>2</sup> and Sarka et  $al^3$ . Two different reductions schemes were thus applied and were proved to be equally successful.

CH3 <sup>79</sup> Br:	Parameter	QQ	QC
	$(\eta_J^5 + \eta_K^5) \times 10^5$	-20.9766(47)	-20.9704(47)
	$\alpha_2^A \times 10^3$	-21.8459(36)	-21.8479(36)
	$\alpha_5^A \times 10^3$	46.7461(36)	46.7461(36)
	$(\alpha_2^B + 4q_{22}) \times 10^3$	1.02914(10)	1.02865(11)
	$(\alpha_5^B - 2q_{22}) \times 10^3$	-0.032513(23)	-0.031836(69)
	$(\alpha_2^B + 2\alpha_5^B) \times 10^3$	0.96412(11)	0.964981(95)
CH3 <sup>81</sup> Br:	Parameter	QQ	QC
	$(\eta_{J}^{5} + \eta_{K}^{5}) \times 10^{5}$	-21.0762(71)	-21.0639(71)
	$\alpha_2^A \times 10^3$	-21.8565(43)	-21.8587(44)
	$\alpha_5^A \times 10^3$	46.7752(43)	46.7840(43)
	$(\alpha_2^B + 4q_{22}) \times 10^3$	1.02346(22)	1.02285(22)
	$(\alpha_5^B - 2q_{22}) \times 10^3$	-0.03028(13)	-0.02952(13)
	$(B, \alpha, B) = 10^3$	0.0(000(0.4)	0.0(202(1.4)

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<sup>&</sup>lt;sup>1</sup>F. Kwabia Tchana, I. Kleiner, J. Orphal, N. Lacome, O. Bouba, J. Mol. Spectrosc. 228 (2004) 441-452.

<sup>&</sup>lt;sup>2</sup>L. Nová Střiteská, K. Sarka, Š Urban, J. Mol. Spectrosc. 256 (2009) 135-140.

<sup>&</sup>lt;sup>3</sup>K. Sarka, L. Nová Střiteská, A. Ceausu-Velcescu, J. Mol. Spectrosc. 311 (2015) 84-99.