High resolution spectrum of D_2O-CO_2 van der Waals complex around the 3OD vibrational excitation

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Water and CO_2 are the most important greenhouse gases of our atmosphere. The solvation of CO_2 is a decisive process in the chemistry of clouds and oceans. A precise characterization of the interaction of these two molecules is thus of prime importance. In the present work, we recorded the rotationally resolved spectrum associated to the triple excitation of the OD stretch in the D_2O-CO_2 molecular complex. This represents a further step in our longstanding effort to characterize better the dynamics of interaction of CO_2 and H_2O notably through a systematic increase of the vibrational excitation [1–3]. All the measurements were performed using the FANTASIO experimental setup [4,5]. The complexes were formed from 8 cm long pulsed slit supersonic jet and probed using CRDS technique in the spectral range of the second OD overtone of D_2O. The recorded spectrum was vibrationally assigned to the $(v_1,v_2,v_3) \leftarrow (v_1',v_2',v_3') = (2,0,1) \leftarrow (0,0,0)$ and $(1,1,1) \leftarrow (0,0,0)$ where v_1,v_2,v_3 are the vibrational quantum numbers of the isolated D_2O molecule. In this talk, I will present the experimental spectrum and the improvements of the experimental set-up which allowed the recording of this spectral signature. I am going to present our progress in the analysis of this spectrum using group theory and effective Hamiltonian.

[1] C. Lauzin, A.C. Imbreckx, T. Foldes, T. Vanfleteren, N. Moazzen-Ahmadi, and M. Herman, Mol. Phys. 118, e1706776 (2020).
[2] A.S. Bogomolov, A. Roucou, R. Bejjani, M. Herman, N. Moazzen-Ahmadi, and C. Lauzin, Chem. Phys. Lett. 774, 138606 (2021).
[3] T. Gartner, C. Lauzin, A.R.W. McKellar, and N. Moazzen-Ahmadi, J. Phys. Chem. A 127, 3668 (2023).
[4] M. Herman, K. Didriche, D. Hurtmans, B. Kizil, P. Macko, A. Rizopoulos, and P.V. Poucke, Mol. Phys. 105, 815 (2007).
[5] A.S. Bogomolov, R. Glorieux, M. Herman, T. Corbo, S. Collignon, B.M. Hays, D. Lederer, N. Moazzen-Ahmadi, A. Libert, B. Tomasetti, J. Fréreux, and C. Lauzin, Mol.Phys., doi: 10.1080/00268976.2024.2413417.