EXTRA HIGH ACCURACY FITTING OF THE PES FOR SUB-PERCENT CALCULATION OF INTENSITIES

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Calculation of rotation-vibration line intensities with sub-percent accuracy has recently become a standard requirement for the applications in retrieval and monitoring of gases in the Earth's atmosphere and potentially in the atmospheres of exoplanets. A major factor in the accurate calculation of intensities is the requirement for a high accuracy *ab initio* Dipole moment surface (DMS) (e.g. references [a] and [b]). We demonstrate here that the change from the "good" potential energy surface (PES) to "excellent" PES, used for the intensity calculations is also important. By "good" we mean here, for example, the PES a standard deviation of 0.025 $\mathrm{cm}^{-1}$and by "excellent" - the PES with the standard deviation 0.011 cm^{-1}. Details of studies on H_2O[c], O_3 [d], HCN and CO_2 molecules will be presented in the talk.

[a] L.Lodi, J. Tennyson and O.L. Polyansky, *Journal of Chemical Physics*, **135**, 034113, (2011)

[b] O.L. Polyansky, K. Bielska, M. Ghysels, L. Lodi, N.F.Zobov, J.T.Hodges, J. Tennyson *Physical Review Letters*, **114**, 243001, (2015)

[c] I.I Mizus, A.A. Kyuberis, N.F. Zobov, V.Y. Makhnev, O.L. Polyansky and J. Tennyson *Phil. Trans. R. Soc. A*, **376**, 20170149, (2018)

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