THE ROTATIONAL SPECTRUM OF THE H_2-OCS VAN DER WAALS COMPLEX

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The microwave spectrum of the H_2-OCS complex has been studied using molecular beam electric resonance optothermal spectrometer with 20% 40:1 H_2/OCS gas mixture in 5 atm He. This investigation is stimulated by the recent He droplet study of this species[a]. The H_2-OCS complex has T-shaped global minimum according to a high-level *ab initio* potential surface calculation. We have performed bound state calculations with bound program[b] to obtain the rotational transitions of the ground state for *para*-H_2-OCS complex. Several spectral transitions of ^{32}S and ^{34}S isomers have been measured at frequencies close to the prediction in the frequency region of 9-31 GHz. For example, two observed peaks at 10218.3 and 20385.7 MHz from H_2-OC^{32}S complex have been compared with the predicted $1_{01}\leftarrow 0_{00}$ and $2_{02}\leftarrow 1_{01}$ transitions at 10594.7 and 21110.2 MHz, respectively. However a number of transitions predicted were not observed although the analogous transitions in the He-OCS complex have been readily seen[c]. In addition, small doublet splitting of near 50 KHz is observed. Since *ortho*-H_2 contributes to about 75 percent abundance of normal H_2 at room temperature and might bind stronger with OCS molecule than *para*-H_2, we believe that what we observed in this study may belongs to *ortho*-H_2-OCS complex. Our current experimental measurement with pure *para*-H_2 would provide detailed results for rotational transitions of the ground state for H_2-OCS complex in the near future.

[a] S. Grebenev, B. G. Sartakov, J. P. Toennies and A. F. Vilesov, *J. Chem. Phys.* **114**(2), 617, 2001.
[b] J. M. Hutson, Bound Computer Program, Version5, 1993 .
[c] Kelly Higgins and William Klemperer, *J. Chem. Phys.* **110**(3), 1383, 1999.