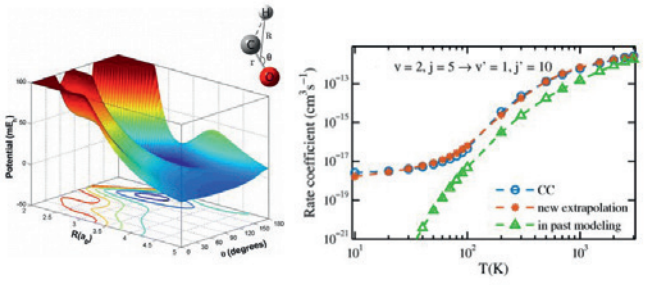
Colloquium

SFB 956

Conditions and Impact of Star Formation

02.11.2015
Monday 4:00 pm

Physikalische Institute Köln
Lecture Hall III
Zülpicher Straße 77 | 50937 Köln



Ad van der Avoird
Theoretical Chemistry, Radboud University Nijmegen, The Netherlands

From the Spectra of Molecular Complexes and Scattering Resonances to Rate Coefficients for Astrophysical Modeling

Rate coefficients for ro-vibrational transitions in small molecules, such as CO, H_2O, NH_3, and CH_4, induced by collisions with other molecules or atoms are an essential ingredient in the astrophysical modeling of star-forming regions, protoplanetary disks, planetary atmospheres, etc. Such rate coefficients can be reliably obtained from quantum scattering calculations, if the corresponding intermolecular interaction potentials are accurately known. These potentials can be obtained from *ab initio* electronic structure calculations. I will describe how the accuracy of the potentials can be sensitively tested through calculations of the ro-vibrational levels of Van der Waals complexes and of molecular collision cross sections and comparison with high-quality experimental data. Then I will show results for collisions of CO, the second most abundant molecule in the interstellar medium, with hydrogen atoms and their application in astrophysical models.