Invited Lecture

SPECTRA OF DIATOMIC MOLECULES: FROM COLD TO HOT

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Diatomic molecules have been an object of very intensive investigation for different physical conditions. We shall discuss theoretical aspects of some investigations in a wide range of temperatures. At ultra-cold conditions (100 μK) in a magneto-optical trap (MOT) cold molecules can be produced by two-photon photoassociation of colliding atom pairs. The produced molecules are translationally and rotationally cold because only low partial-wave collisions (s-wave and p-wave) of cold atoms contribute to the process. We shall describe one of the scenarios for the formation of cold Cs_2 molecules by photoassociation. Cold helium nanodroplets act as a low-temperature cryostat (0.4 K) for the adsorbed Cs_2 molecules, which "skate" around on the surface, internally cold in the lowest vibrational and rotational state. Excitation spectra of Cs_2 molecules were probed by laser-induced fluorescence between 560 and 690 nm. All observed spectral features are identified by comparison with theoretical spectra simulations based on the simple reflection formula. CO molecules are very important in atmosphere investigation, especially the greenhouse gas remediation. We calculated the quantum-mechanical absorption and emission spectra for the Angstrom transition of CO molecule at room temperature (300 K). We studied absorption and thermal emission of cesium vapor superheated in the all-sapphire cell at very high temperatures (1000 - 1200 K). The measured spectra of the Cs2 diffuse band around 710 nm were compared with theoretical simulations. Because of the small rotational energy splitting in the Cs_2 molecule, in our calculations we used the semiquantum approach. In the case of an alkali-helium dimer, the free-free transitions dominate the optical spectra, so the semiclassical approximation of spectra simulation is acceptable. We compare the fully quantum-mechanical and the semiclassical approach in the case of K-He spectra in the wide range of temperatures (300 – 3000 K) typical for the atmospheres of brown dwarfs and giant exoplanets.