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He-perturbed H_2 spectra: unprecedented agreement between ab initio theory and experimental data HUBERT JOZWIAK, MICHAL SLOWIN-SKI, Nicolaus Copernicus University, Torun, Poland, FRANCK THIBAULT, Universite de Rennes 1, Rennes, France, YAN TAN, JIN WANG, AN-WEN LIU, SHUI-MING HU, University of Science and Technology of China, Hefei, China, SAMIR KASSI, ALAIN CAMPARGUE, University of Grenoble Alpes, Grenoble, France, MAGDALENA KONEFAL, Nicolaus Copernicus University, Torun, Poland, KONRAD PATKOWSKI, Aubrun University, PIOTR ZUCHOWSKI, ROMAN CIURYLO, DANIEL LISAK, PIOTR WCISLO, Nicolaus Copernicus University, Torun, Poland — Hydrogen molecule perturbed by the helium atom constitutes the simplest benchmark system for performing the tests of the ab initio quantum scattering theory on the ultra-accurate experimental spectra. Here, we report a full description of the collision-perturbed shapes of rovibrational lines for this particular system. We demonstrate, for the first time, agreement between measured and ab initio computed collision-perturbed shapes of molecular lines at the subpercent level: the root-mean-square difference between experimental and theoretical profiles is smaller than one-hundredth of the profile amplitude. In the analysis described here, we employed the state-of-the-art statistical model of the collision-perturbed shape of molecular lines, we obtained all the parameters of this model from quantum scattering calculations, and the dynamical calculations were performed on the most accurate potential energy surface to date.

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