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Shapes of optical molecular resonances from first principles: calculations for atmosphere-relevant molecular systems HUBERT JOZWIAK, Nicolaus Copernicus University Torun, Poland, FRANCK THIBAULT, Universite de Rennes 1, Rennes, France, HUBERT CYBULSKI, Kazimierz Wielki University, Bydgoszcz, Poland, MACIEJ GANCEWSKI, PIOTR WCISLO, Nicolaus Copernicus University Torun, Poland — We present the results of the investigation of the line-shape parameters for two atmospheric systems based on ab initio quantum-scattering calculations. The first one is the N2-perturbed CO molecule, for which we investigated the R(0) purely rotational line. We use three recently reported potential energy surfaces (PESs), calculated by means of the state-of-the-art quantum chemistry methods, to determine the pressure broadening coefficient. We obtain reasonable agreement with the experimental data. The second system is the N2-perturbed O2 molecule. We employ the same methodology, generalized for the case of the active molecule in the $^3\Sigma$ electronic ground state. This is the first ab initio investigation of the line-shape parameters in the O2-N2 system. The data provided through the investigation of both systems is important for terrestrial atmospheric measurements, and can be used for populating the HITRAN database.

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