IMPROVED CO_2 IR LINE LIST FOR 1500K - 3000K

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Previously published high temperature CO_2 IR line lists either do not cover the region >10,000 cm^{-1}, or lack convergence due to cutoffs, or have noticeable noises. We report a new CO_2 IR line list improved for applications in the range from 1500K to 3000K, denoted Ames-3000K.[a] With at least 7 billion lines of CO_2 626, 636, 628 and 627, it covers the whole range from 0 to 20,000 cm^{-1}. We estimate it is converged up to 20,000 cm^{-1}at 1000K, up to 10,000-15,000 cm^{-1}at 2000K, or up to 5000-8000 cm^{-1}at 3000K, but needs further PES and DMS improvements for 4000K and above. Compared to our earlier CO_2 line list work, e.g., Ames-296K/1000K and Ames-4000K, the Ames-3000K combines the advantages of two sets of IR line lists. The 1^{st} set focuses on the low energy region, with intensity computed using the best available Ames-2 PES, and the best available ab initio DMS, Ames-2021. The Ames-2021 DMS based IR intensity represents a major improvement for theoretical CO_2 intensity calculations. Our predictions for the CO_2 2001x and 3001x bands matched high accurate experiments to -0.1$\pm$0.1% (NIST) or 0.2$\pm$0.4% (DLR). But the Ames-2021 DMS was fit only up to 30,000 cm^{-1}. The 2^{nd} set of line lists provides reliable prediction for IR transitions with E′ up to 36,000 cm^{-1}. Related calculations were run on a different PES, X01d. To enhance the success rate of Ames vs. CDSD matches in the range of 15,000 - 22,000 cm^{-1}, the X01d PES was refined specifically using selected CDSD Effective Hamiltonian model levels up to 24,000 cm^{-1}, but at a price of the accuracy reduced for lower energy levels and transitions. The ab initio dipole dataset of Ames-2021 DMS was refitted with 40,000 cm^{-1}cutoff to generate an DMS suitable for the intensity calculation at higher energy, denoted Ames-2021-40K. The two sets of line lists are then combined and updated using the CDSD energy levels to get accurate line positions for E′ <15,000 $\mathrm{cm}^{-1}$and J<150 transitions. The accuracy, consistency, and issues of the Ames-3000K IR line list will be evaluated by comparing with high temperature experiments and databases.

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