LINE LIST FOR THE LOWEST FOUR STATES OF NO

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We computed an accurate line list, called XABC, for nitric oxide (NO) which covers its pure rotational, vibrational and rovibronic spectra belonging to the lowest four electronic states of NO, i.e. X $^2\Pi$, A $^2\Sigma^+$, B $^2\Pi$ and C $^2\Pi$. XABC is a major extension and update of the ExoMol NOname line list which was calculated within the X $^2\Pi$ state of NO.

As first step we built a spectroscopic model which represents the rovibronic structure of A $^2\Sigma^+$, B $^2\Pi$, C $^2\Pi$ states of NO. Empirical energy levels for the three electronic states are determined using the a combination of the MARVEL procedure and *ab initio* calculations, and the available experimental data are critically evaluated. *Ab inito* methods which deal simultaneously with the Rydberg-like A $^2\Sigma^+$ and C $^2\Pi$, and the valence B $^2\Pi$ state are tested. Methods of modeling the sharp avoided crossing between the B $^2\Pi$ and C $^2\Pi$states are tested. A rovibronic Hamiltonian matrix is constructed using variational nuclear motion program DUO whose eigenvalues are fitted to the MARVEL energy levels. The matrix also includes coupling terms obtained from the refinement of the *ab initio* potential energy and spin-orbit coupling curves. Calculated and observed energy levels agree well with each other, validating the applicability of our method and providing a useful model for this open shell system. This part has been published in *J. Chem. Phys.* https://doi.org/10.1063/5.0038527.

A mixture of empirical and theoretical electronic transition dipole moments are used for the final calculation of NO rovibronic transitions belong to the A $^2\Sigma^+$ – X $^2\Pi$, B $^2\Pi$ – X $^2\Pi$ and C $^2\Pi$ – X $^2\Pi$ which correspond to the γ, β and δ band systems, respectively, as well as minor improvements to transitions within the X $^2\Pi$ ground state. Our model generates a high-accuracy NO ultraviolet line list covering the complicated regions where the B $^2\Pi$ -C $^2\Pi$ states interact. Technical details of this part are given in the XABC line list paper submitted to *Mon. Not. Roy. Astron. Soc.*.

XABC provides comprehensive data for $\lambda > 160$ nm ($\tilde{\nu} < 63000$ cm^{-1}) for the analysis of atmospheric NO on Earth, Venus or Mars, other astronomical observations and applications. It is available via www.exomol.com.

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