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Spectroscopic and *ab initio* study of the open-shell Xe-O_2 van der Waals Complex QING WEN, WOLFGANG JÄGER, Department of Chemistry, University of Alberta — Rotational spectra of the open-shell Xe-O_2 van der Waals complex were recorded using a pulsed-nozzle Fourier transform microwave spectrometer. Magnetic hyperfine structure arising from the earth's magnetic field was observed and reduced by mounting Helmholtz coils on to the sample chamber. Several spectral lines measured in the in the 4-18 GHz region were assigned to transitions within the $\Omega = 0$ spin component of the $^3\Sigma^-$electronic ground state. Transitions within the $\Omega = \pm 1$ spin components were not observed because of the small population in these levels. The hyperfine structures due to Fermi contact coupling between the electron spin of $O_2(S = \mathrm{l})$ and the ^{129}Xe nuclear spin (I= 1/2) were detected and analyzed. The determined spectroscopic constants, including the Fermi contact coupling constant, were used to derive information about the electronic and geometric structure of the complex. The experimental data were complemented by the construction of an *ab initio* potential energy surface at the RCCSD(T) level of theory. The results provide detailed insight into the intermolecular interaction between Xe and paramagnetic oxygen. This may help to understand the relaxation mechanism of hyperpolarized ^{129}Xe in human blood in *in vivo* magnetic resonance imaging experiments.

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