Rotational Spectra of Phosphorus Monosulfide up to 1 THz

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The submillimeter-wave rotational spectrum of the PS radical in the electronic and vibrational ground state ($X^2\Pi_{1/2}$, $X^2\Pi_{3/2}$) was recorded with the Cologne terahertz spectrometer in the frequency region between 540 GHz and 1.07 THz, covering rotational quantum numbers from J = 30.5 to 60.5. The PS radical has been produced by discharging $PSCl_3$ buffered with Ar. For all transitions the Λ-doubling was resolved for both the $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ states. For some transitions with $\Delta F = 0$ the hyperfine structure (hfs) caused by the P-atom could partially be resolved even for rather high J values. Analysis of the complete rotational data set of PS allows the derivation of a full set of molecular parameters, including the rotational constants B, D, H, the fine-structure constants A, γ, D_γ, the parameters for the Λ-doubling p, D_p, q, and the magnetic hyperfine constants a, b, c, d, C_I. All parameters have been determined, whereby a, c, and the nuclear spin rotation-constant C_I were obtained for the first time.

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