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Ultracold Scattering of ArNO in Three Dimensions[1] ALEXANDER TEPLUKHIN, BRIAN KENDRICK, Los Alamos National Laboratory — Until now, the scattering of Ar and NO has been treated in two dimensions, with the internuclear NO distance held fixed at the equilibrium geometry. In the present study we go beyond that limitation and describe the Ar–NO ($\tilde{X}\,^2\Pi$) complex using all three dimensions. The calculations are based on new potential energy surfaces (A' and A''), computed using the coupled-cluster CCSD(T) method in the complete basis set limit and coupled by the spin-orbit interaction. Both $^2\Pi_{3/2} \rightarrow {}^2\Pi_{1/2}$ and $^2\Pi_{3/2} \rightarrow {}^2\Pi_{3/2}$ transitions are studied, with the former "downhill" (exoergic) transition being the main focus. The rate coefficients are computed using the coupled-channel APH3D code and are analyzed for a wide range of ultracold and cold temperatures, from 1 nK to 10 K. The calculations are carried out in Delves hyperspherical coordinates and the channels are propagated using a log-derivative method. This is the first-ever theoretical treatment of Ar–NO scattering in full dimensionality and also for the ultracold energy regime.

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