

Abstract Submitted
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Mechanisms of Dissociative Electron Attachment to CO₂ and NH₃¹ WILLIAM MCCURDY², Department of Chemistry, University of California, Davis, DANIEL HAXTON, Chemical Sciences Division, Lawrence Berkeley National Laboratory, SPIRIDOULA MATSIKA, Department of Chemistry, Temple University, THOMAS RESCIGNO, Chemical Sciences Division, Lawrence Berkeley National Laboratory — Recent experiments at LBNL on the angular dependence of dissociative electron attachment (DEA) to CO₂ and NH₃ have raised new questions about the mechanism of DEA in both cases. In the case of CO₂, for attachment via the shape resonance at 4 eV, the angular distribution of O⁻ is peaked along the axis of the incident direction of the electron, even though the resonance through which the electron is attached is of ²Π symmetry. We present an explanation based on both the attachment amplitude from *ab initio* complex Kohn scattering calculations and the identification of two conical intersections, one involving a Σ/Π intersection, that may both be involved in the surprisingly complicated mechanism for this low energy DEA process. In NH₃, complex Kohn scattering calculations identify the ²A' Feshbach resonance near 5 eV that produces both H⁻ and NH₂⁻ fragments in the experiment, also involving at least one conical intersection.

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