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Calculation of Molecular Shape Resonances Using Grid Based Exterior Complex Scaling and N^2-Term Separable Potentials[1] BRANT ABELN, University of California, Davis, THOMAS N. RESCIGNO, Lawrence Berkeley National Laboratory, C. WILLIAM MCCURDY, Lawrence Berkeley National Laboratory, University of California, Davis — A novel approach employing Exterior Complex Scaling (ECS) and discrete grid methods is used to calculate molecular resonance energies and widths for the $^2\Pi_g$ shape resonance state of N_2^- and $^2\Pi_u$ shape resonance of CO_2^-. These calculations are performed using a Finite Element Discrete Variable Representation (FE-DVR) in prolate spheroidal coordinates with an atomic center placed at each of the foci of the coordinate system, thereby preserving the cusp condition at those sites. A separable approximation to the interaction potential is made from the matrices of the nuclear attraction, direct and exchange operators generated by an existing quantum chemistry structure code in a Gaussian basis. These potentials are then represented on our ECS FE-DVR grid allowing the calculation of complex-valued resonance energies. The method is demonstrated here in the static-exchange approximation.

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