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Genetic based fitting techniques for potential energy curves of diatomic molecules IAN STEVENSON, JESUS PEREZ-RIOS, DAN ELLIOTT, Purdue University — We present development of a genetic algorithm for fitting potential energy curves of diatomic molecules to experimental data. Our program takes in a 'guess' potential, often from an *ab initio* calculation, along with experimental measurements of vibrational binding energies, rotational constants, and the experimental uncertainty. The fitting program is able modify the guess potential until it reproduces the experimental data with better than 1% uncertainty. We present the details of this technique along with a comparison of potentials calculated by the genetic algorithm and by an inverted perturbation approach for the $X\ ^1\Sigma^+$ potential of lithium-rubidium.

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