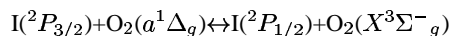


AB INITIO POTENTIAL ENERGY SURFACES FOR THE $I(^2P_{3/2}) + O_2(a^1\Delta_g) \leftrightarrow I(^2P_{1/2}) + O_2(X^3\Sigma^-_g)$ ENERGY TRANSFER PROCESS

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Ab initio electronic structure calculations have been used to investigate the electronic energy transfer process:



Potential energy surfaces for all states associated with the reactants and products were obtained using CASSCF and CASPT2 methods, including the effective one-electron spin-orbit Hamiltonian. Surfaces correlating with the reactants and products were all found to be non-bonding. Shallow van der Waals minima were predicted at long range. Surface crossings were found at energies below the $I(^2P_{3/2}) + O_2(a^1\Delta_g)$ asymptote. It is probable that these crossings are responsible for the efficient transfer of electronic energy in this system.