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

A. L. KALEDIN, M. C. HEAVEN, and K. MOROKUMA, *Cherry L. Emerson Center for Scientific Computation and Department of Chemistry Emory University, Atlanta, GA 30322*.

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

I($^2P_{3/2}$)+$O_2(a^1\Delta_g)$↔I($^2P_{1/2}$)+$O_2(X^3\Sigma^-{}_g)$

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.