AB INITIO STUDY OF THE EXCITED STATES OF O_2

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O_2 is important for spectroscopic applications in the IR, Visible and UV regions. In this work eight lowest electronic states were studied using the CASSCF and MRCI methods and the AV5Z basis sets with the D_2h point group symmetry, namely $X\ ^3\Sigma_g^-$, $A\ ^3\Sigma_u^+$, $A'\ ^3\Delta_u$, $a\ ^1\Delta_g$, $b\ ^1\Sigma_g^+$, $c\ ^1\Sigma_u^-$ (bound), $C\ ^3\Pi_g$, $d\ ^1\Pi_g$ (unbound). Potential energy curves (PECs) for 8 electronic states and spin-orbit coupling, electronic angular moment and transition quadrupole moment curves for the five states $X\ ^3\Sigma_g^-$, $a\ ^1\Delta_g$, $b\ ^1\Sigma_g^+$, $d\ ^1\Pi_g$ and $C\ ^3\Pi_g$, were computed and used to predict rovibronic spectra and lifetimes of O_2. Our aim is to construct an accurate ro-vibronic molecular line list for O_2. This will require an empirical refinement of the *ab initio* curves and will be considered in our future work.