

## HIGH LEVEL *AB INITIO* INVESTIGATION OF INTERCOMBINATION BANDS OF C<sub>2</sub>

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High level *ab initio* calculations were carried out on the  $X^1\Sigma_g^+$ ,  $A^1\Pi_u$ ,  $a^3\Pi_u$ ,  $b^3\Sigma_g^-$ ,  $c^3\Sigma_u^+$  and  $d^3\Pi_g$  levels of the C<sub>2</sub> radical. Calculations were carried out at the MRCI level with full-valence CASSCF reference wavefunctions and basis sets up to aug-cc-pv6z. The resulting wavefunctions and potential energy surfaces were employed to calculate Einstein coefficients for allowed transitions and intercombination bands. These values were used to model the behaviour of the C<sub>2</sub> system in interstellar and circumstellar environments, paying particular attention to the Red Rectangle (HD 44179).