Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Ab initio study on the electronic excited states and photodissociation mechanism of bromocarbene molecule

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Contents

1 Fig. S1-S3.

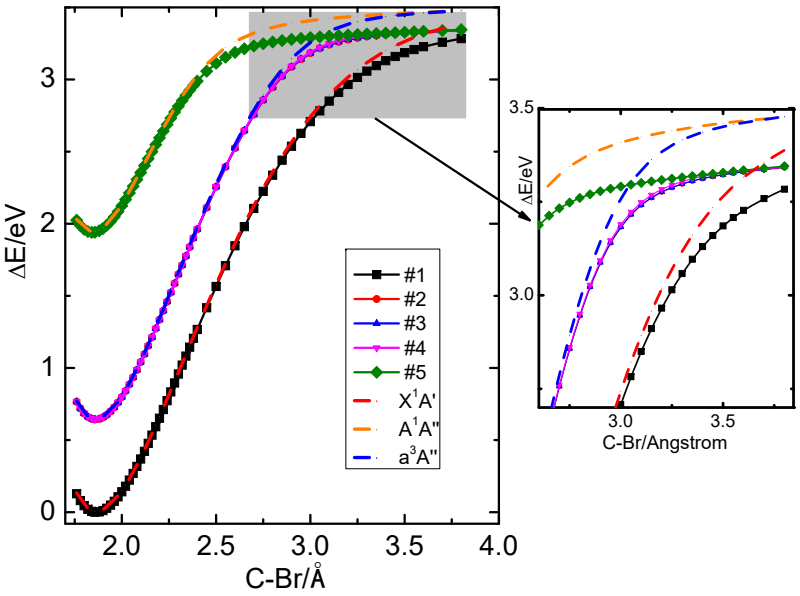

Fig. 1 Potential energy curves of the lowest three states of CHBr with the spin– orbit coupling (full lines) and without it (dotted lines) calculated at the MRCI-F12/cc-pVTZ-F12 level along the CBr bond length, with the other two geometric parameters fixed at their respective equilibrium values of the ground state.

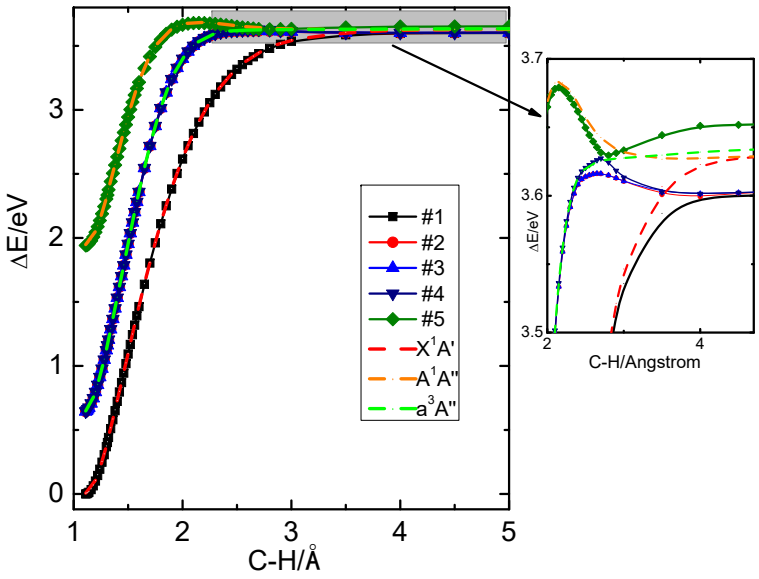

Fig. 2 Potential energy curves of the lowest three states of CHBr with the spin– orbit coupling (full lines) and without it (dotted lines) calculated at the MRCI-F12/cc-pVTZ-F12 level along the CH bond length, with the other two geometric parameters fixed at their respective equilibrium values of the ground state..

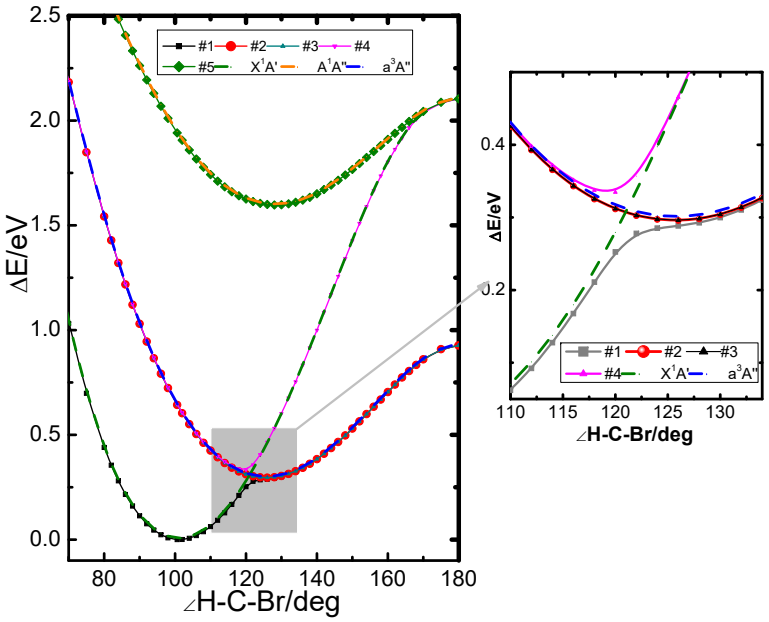

Fig. 3 Potential energy curves of the lowest three states of CHBr with the spin– orbit coupling (full lines) and without it (dotted lines) calculated at the MRCI-F12/cc-pVTZ-F12 level along the H-C-Br bond angle, with the other two geometric parameters fixed at their respective equilibrium values of the ground state.

2 Fig.S4-S6.

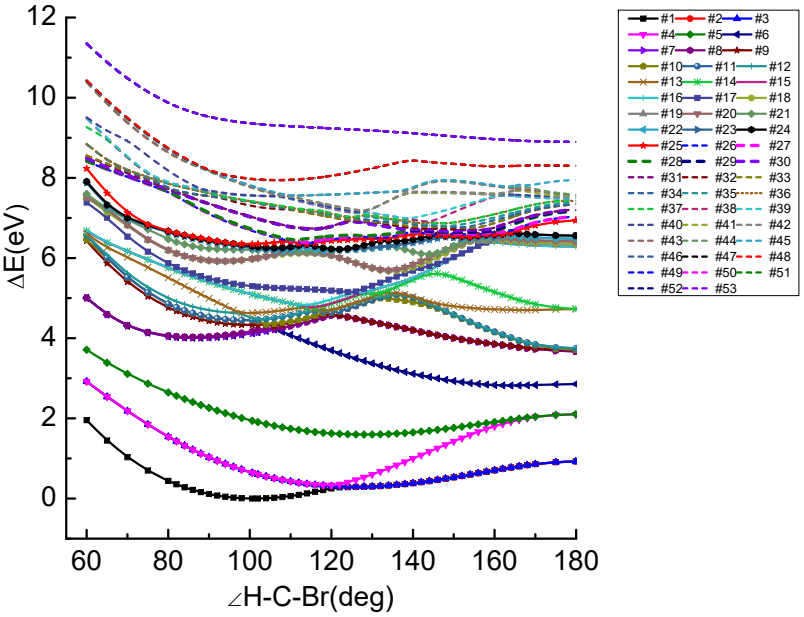

Fig. 4 Potential energy curves of the spin-coupled states of CHBr calculated at the MRCI-F12/cc-pVTZ-F12 level along the H-C-Br bond angle with the other two geometric parameters fixed at their respective equilibrium values of the ground state.

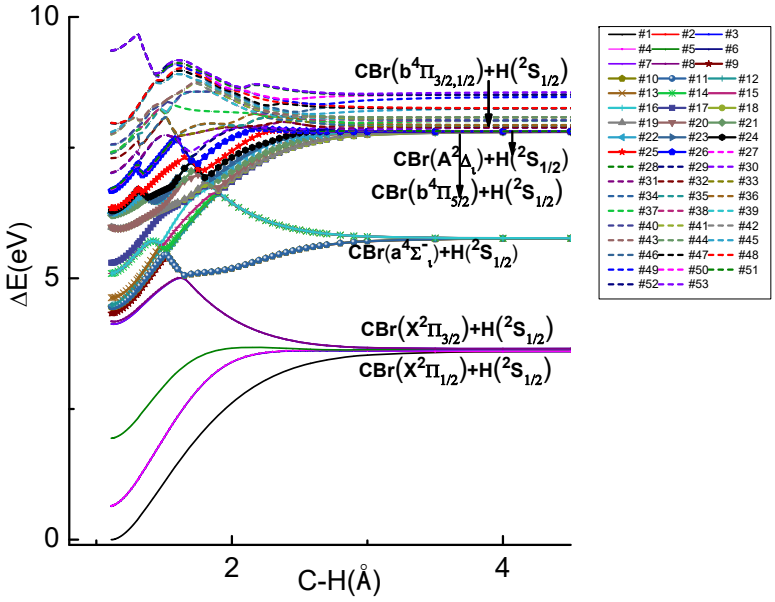

Fig. 5 Potential energy curves of the spin-coupled states of CHBr calculated at the MRCI-F12/cc-pVTZ-F12 level along the CH bond length with the other two geometric parameters fixed at their respective equilibrium values of the ground state.

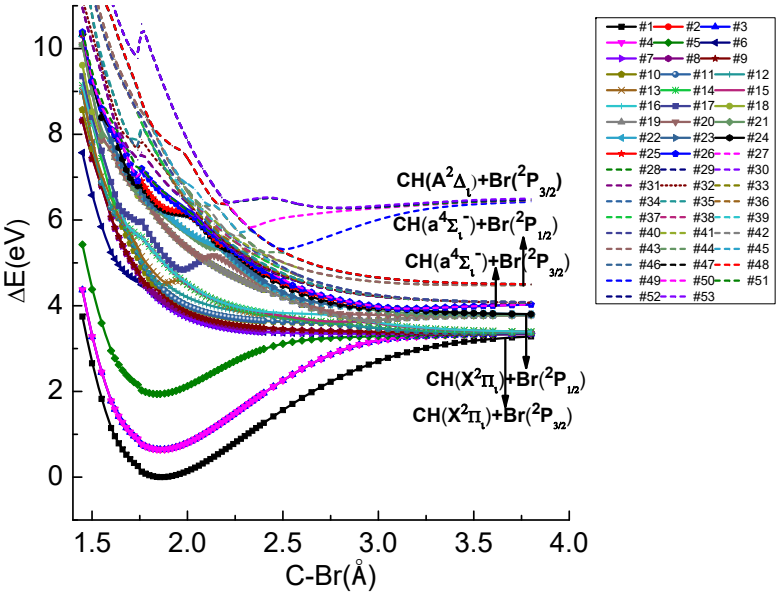

Fig. 6 Potential energy curves of the spin-coupled states of CHBr calculated at the MRCI-F12/cc-pVTZ-F12 level along the CBr bond length with the other two geometric parameters fixed at their respective equilibrium values of the ground state.