Spectroscopic and computational studies of the laser photolysis of matrix isolated 1,2-dibromoethanes: Formation and fate of the bromoethyl radicals

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Supporting Information

Table 1S. Orbital configurations associated with the transitions reported in Table 2.

	B3LYP/ aug-cc-pvdz aug-cc-pvtz aug-cc-pvqz	CAM-B3LYP/ aug-cc-pvdz aug-cc-pvtz aug-cc-pvqz	M06/ aug-cc-pvdz aug-cc-pvtz aug-cc-pvqz	M062x/ aug-cc-pvdz aug-cc-pvtz aug-cc-pvqz
S_1	$43 \rightarrow 44$ $43 \rightarrow 44$ $43 \rightarrow 44$	$43 \rightarrow 44$ $43 \rightarrow 44$ $43 \rightarrow 44$	$43 \rightarrow 44$ $43 \rightarrow 44$ $43 \rightarrow 44$	$43 \rightarrow 44$ $43 \rightarrow 44$ $43 \rightarrow 44$
S_2	$42 \rightarrow 44$ $42 \rightarrow 44$ $42 \rightarrow 44$	$42 \rightarrow 44$ $42 \rightarrow 44$ $42 \rightarrow 44$	$42 \rightarrow 44$ $42 \rightarrow 44$ $42 \rightarrow 44$	$42 \rightarrow 44$ $42 \rightarrow 44$ $42 \rightarrow 44$
S_3	$40 \rightarrow 44$ $41 \rightarrow 44$ $41 \rightarrow 44$	$40 \rightarrow 44$ $40 \rightarrow 44$ $40 \rightarrow 44$	$40 \rightarrow 44$ $41 \rightarrow 44$ $41 \rightarrow 44$	$40 \rightarrow 44$ $40 \rightarrow 44$ $40 \rightarrow 44$
S_4	$39 \rightarrow 44$ $40 \rightarrow 44$ $40 \rightarrow 44$	$39 \rightarrow 44$ $39 \rightarrow 44$ $39 \rightarrow 44$	$39 \rightarrow 44$ $40 \rightarrow 44$ $40 \rightarrow 44$	$39 \rightarrow 44$ $39 \rightarrow 44$ $39 \rightarrow 44$
S_5	$41 \rightarrow 44$ $39 \rightarrow 44$ $39 \rightarrow 44$	$41 \rightarrow 44$ $41 \rightarrow 44$ $41 \rightarrow 44$	$41 \rightarrow 44$ $39 \rightarrow 44$ $39 \rightarrow 44$	$41 \rightarrow 44$ $41 \rightarrow 44$ $41 \rightarrow 44$

Figure 1S. The B3LYP/aug-cc-pvqz orbitals calculated for the C_2H_4—Br_2 complex (shown for the ground state configuration).