Photodissociation dynamics of bromoiodomethane from the first and second absorption bands. A combined velocity map and slice imaging study

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Supplementary Material

Table S1 Energy at the Franck-Condon (FC) geometry of CH_2BrI, symmetry in C_s, as well as total dipole moment (TDM) and for each axis of the computed electronic states. X axis is located in the I-C-Br plane, perpendicular to the C-I bond, Y axis in the I-C-Br plane, along the C-I bond, and the Z axis is perpendicular to the I-C-Br plane. The correlated symmetry in C_{3v} and the notation by North *et al.* [1] are also listed.

State number	Franck-Condon energy (eV)	Symmetry (C_s)	Correlated symmetry (C_{3v})	North *et al.*'s notation [1]	TDM	X	Y	Z
1	0	$1A'$	–	$1A'$	0.48635	0.439920	0.207390	0.000000
2	3.83	$1A''$	$^3Q_2$	–	0.00241	0.000000	0.000000	0.002411
3	3.83	$2A'$	$^3Q_2$	–	0.0033	0.003140	0.001030	0.000000
4	3.96	$2A''$	$^3Q_1$	$2A'$	0.01134	0.000000	0.000000	0.011340
5	4.00	$3A'$	$^3Q_1$	$1A''$	0.11854	0.068830	0.096510	0.000000
6	4.28	$3A''$	$^3Q_{0-}$	–	0.00054	0.000000	0.000000	0.000540
7	4.39	$4A'$	$^3Q_{0+}$	$3A'$	0.13841	0.052570	0.128040	0.000000
8	4.60	$4A''$	$^1Q_1$	$2A''$	0.03196	0.000000	0.000000	0.031960
9	4.62	$5A'$	$^1Q_1$	$4A'$	0.34889	0.188250	0.293740	0.000000
10	5.01	$5A''$	$2A_2$	–	0.00498	0.000000	0.000000	0.004976
11	5.05	$6A'$	$4E$	–	0.10490	0.061870	0.084710	0.000000
12	5.10	$6A''$	–	–	0.00884	0.000000	0.000000	0.008831
13	5.17	$7A'$	–	–	0.08522	0.013610	0.084130	0.000000
14	5.25	$7A''$	–	–	0.00077	0.000000	0.000000	0.000770
15	5.27	$8A'$	–	–	0.02185	0.004100	0.021460	0.000000
16	5.65	$8A''$	–	–	0.06935	0.000000	0.000000	0.069351
17	5.70	$9A'$	–	–	0.55903	0.162310	0.534950	0.000000
18	5.99	$9A''$	–	–	0.00753	0.000000	0.000000	0.007533
19	5.99	$10A''$	–	–	0.01055	0.000000	0.000000	0.010555
20	6.01	$10A'$	–	–	0.09662	0.043860	0.086090	0.000000
21	6.29	$11A'$	–	–	0.05822	0.056740	0.013060	0.000000
22	6.43	$11A''$	–	–	0.00003	0.000000	0.000000	0.000030
23	6.43	$12A'$	–	–	0.07150	0.014690	0.069970	0.000000
24	6.45	$12A''$	–	–	0.01837	0.000000	0.000000	0.018362
25	6.67	$13A'$	–	–	0.31790	0.158010	0.275840	0.000000
26	6.84	$13A''$	–	–	0.00971	0.000000	0.000000	0.009710
27	6.86	$14A'$	–	–	0.04988	0.000500	0.049880	0.000000
28	6.89	$14A''$	–	–	0.01800	0.000000	0.000000	0.018003
29	7.03	$15A'$	–	–	0.13242	0.057720	0.119170	0.000000
30	7.03	$15A''$	–	–	0.01041	0.000000	0.000000	0.010406
31	7.06	$16A'$	–	–	0.05829	0.056530	0.014230	0.000000
32	7.22	$16A''$	–	–	0.13694	0.000000	0.000000	0.136932
33	7.45	$17A'$	–	–	0.83620	0.395750	0.736620	0.000000
34	7.70	$17A''$	–	–	0.00659	0.000000	0.000000	0.006587
35	7.70	$18A''$	–	–	0.02174	0.000000	0.000000	0.021744
36	7.70	$18A'$	–	–	0.15985	0.076880	0.140150	0.000000

References

1 W. S. McGivern, R. Li, P. Zou and S. W. North, *The Journal of Chemical Physics*, 1999, **111**, 5771–5779.