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

Supporting Information for:

Tracking dissociation dynamics of strong-field ionized 1,2-dibromoethane with femtosecond XUV transient absorption spectroscopy

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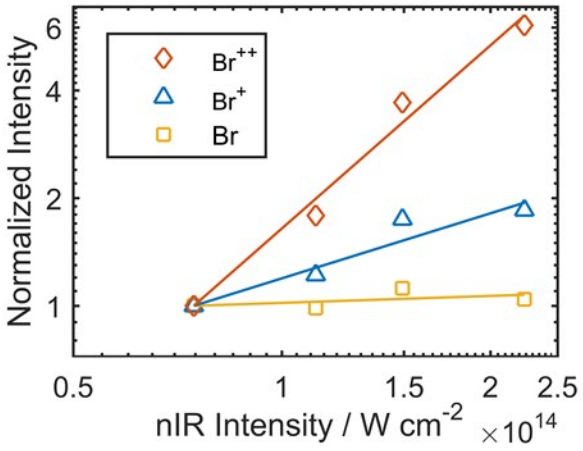

Figure S1 – Intensities of the strongest peaks of the three Br charge states as a function of the pump pulse intensity. Note the double logarithmic scale. All data have been shifted along the ordinate to a common first point at 1. Solid lines show least squares fits to linear functions, giving slopes of 0.06, 0.60 and 1.7 for charge states of 0, +1, and +2, respectively.

Table S1 – Assignments and fit results for the fit to Br· peaks in the 1 ps spectrum (Fig. 1c)

Assignment †	**Lit. Energy (eV)** †	**Fit Energy (eV)**	**Fit Intensity (arb.)**	**Fit FWHM (eV)** ‡
$^2P_{3/2} \rightarrow {}^2D_{5/2}$	64.38	64.40	0.37	0.20
$^2P_{1/2} \rightarrow {}^2D_{3/2}$	64.97	64.97	0.08	0.12

† From ref. 34.

‡ The fit was constrained to a maximum FWHM of 0.2 eV, to prevent the fit algorithm erroneously fitting multiple peaks with a single broad envelope.

Table S2 – Assignments and fit results for the fit to Br^+ peaks in the 1 ps spectrum (Fig. 1c)

Assignment †	Lit. Energy (eV) †	Fit Energy (eV)	Fit Intensity (arb.)	Fit FWHM (eV) ‡
$^3P_1 \rightarrow {}^1D_2$	65.59	65.62	0.07	0.20
$^3P_2 \rightarrow {}^1D_2$	66.00	66.05	0.15	0.11
$^3P_2 \rightarrow {}^3D_3$	66.21	66.24	0.81	0.14
$^1D_2 \rightarrow {}^3F_2$ $^1D_2 \rightarrow {}^1F_3$	66.45	66.42	0.55	0.13
$^3P_1 \rightarrow {}^3D_2$ $^3P_1 \rightarrow {}^3D_1$	66.52	66.57	0.46	0.19
$^3P_1 \rightarrow {}^3P_1$	67.07	67.10	0.15	0.17
$^3P_2 \rightarrow {}^3P_2$	67.30	67.35	0.24	0.18
$^3P_2 \rightarrow {}^3P_1$ $^3P_2 \rightarrow {}^3P_0$	67.44	67.49	0.11	0.20
$^3P_2 \rightarrow {}^3F_2$	67.86	67.87	0.04*	0.10
$^3P_0 \rightarrow {}^1P_1$	68.19	68.24	0.11	0.20

† From ref. 34.

‡ The fit was constrained to a maximum FWHM of 0.2 eV, to prevent the fit algorithm erroneously fitting multiple peaks with a single broad envelope.

* This peak is overlapping with a Br^{++} peak, so the fitted intensity is not conclusive.

Table S3 – Assignments and fit results for the fit to Br^{++} peaks in the 1 ps spectrum (Fig. 1c)

Assignment †	Lit. Energy (eV) †	Fit Energy (eV)	Fit Intensity (arb.)	Fit FWHM (eV) ‡
$^2P_{1/2} \rightarrow (^3P)\ ^2D_{3/2}$	67.86	67.87	0.05*	0.10
$^2P_{3/2} \rightarrow (^1D)\ ^2F_{5/2}$	68.00	68.02	0.13	0.20
$^2P_{3/2} \rightarrow (^1P)\ ^2D_{5/2}$	68.36	68.46	0.20	0.20
$^2D_{5/2} \rightarrow (^1D)\ ^2F_{7/2}$ $^4S_{3/2} \rightarrow (^3P)\ ^2P_{3/2}$	68.67	68.72	0.24	0.20
$^4S_{3/2} \rightarrow (^3P)\ ^4P_{5/2}$ $^2D_{3/2} \rightarrow (^1D)\ ^2D_{3/2}$ $^2D_{5/2} \rightarrow (^3P)\ ^2D_{5/2}$	68.90	68.92	0.29	0.20
$^4S_{3/2} \rightarrow (^3P)\ ^4P_{1/2}$ $^2D_{5/2} \rightarrow (^3P)\ ^2D_{5/2}$ $^4S_{3/2} \rightarrow (^3P)\ ^4P_{3/2}$	69.63	69.62	0.24	0.20
$^2D_{3/2} \rightarrow (^3P)\ ^2D_{5/2}$ $^2P_{3/2} \rightarrow (^1S)\ ^2D_{5/2}$	69.87	69.88	0.03	0.08
$^2D_{5/2} \rightarrow (^1D)\ ^2P_{3/2}$ $^4S_{3/2} \rightarrow (^3P)\ ^4D_{3/2}$	70.18	70.23	0.01	0.15
$^2P_{1/2} \rightarrow (^1S)\ ^2D_{3/2}$	71.08**	70.96	0.02	0.10
$^2D_{5/2} \rightarrow (^1S)\ ^2D_{5/2}$	71.52**	71.24	0.06	0.20

† From ref. 34.

‡ The fit was constrained to a maximum FWHM of 0.2 eV, to prevent the fit algorithm erroneously fitting multiple peaks with a single broad envelope.

* This peak is overlapping with a Br^{++} peak, so the fitted intensity is not conclusive.

** Predicted by theory, but not observed in ref. 34.