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

Supporting Information for Dynamics and Quantum Yields for $CHBrCl_2$ Photodissociation from 215–265 nm

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A. Fits for beta parameter at each wavelength for both channels

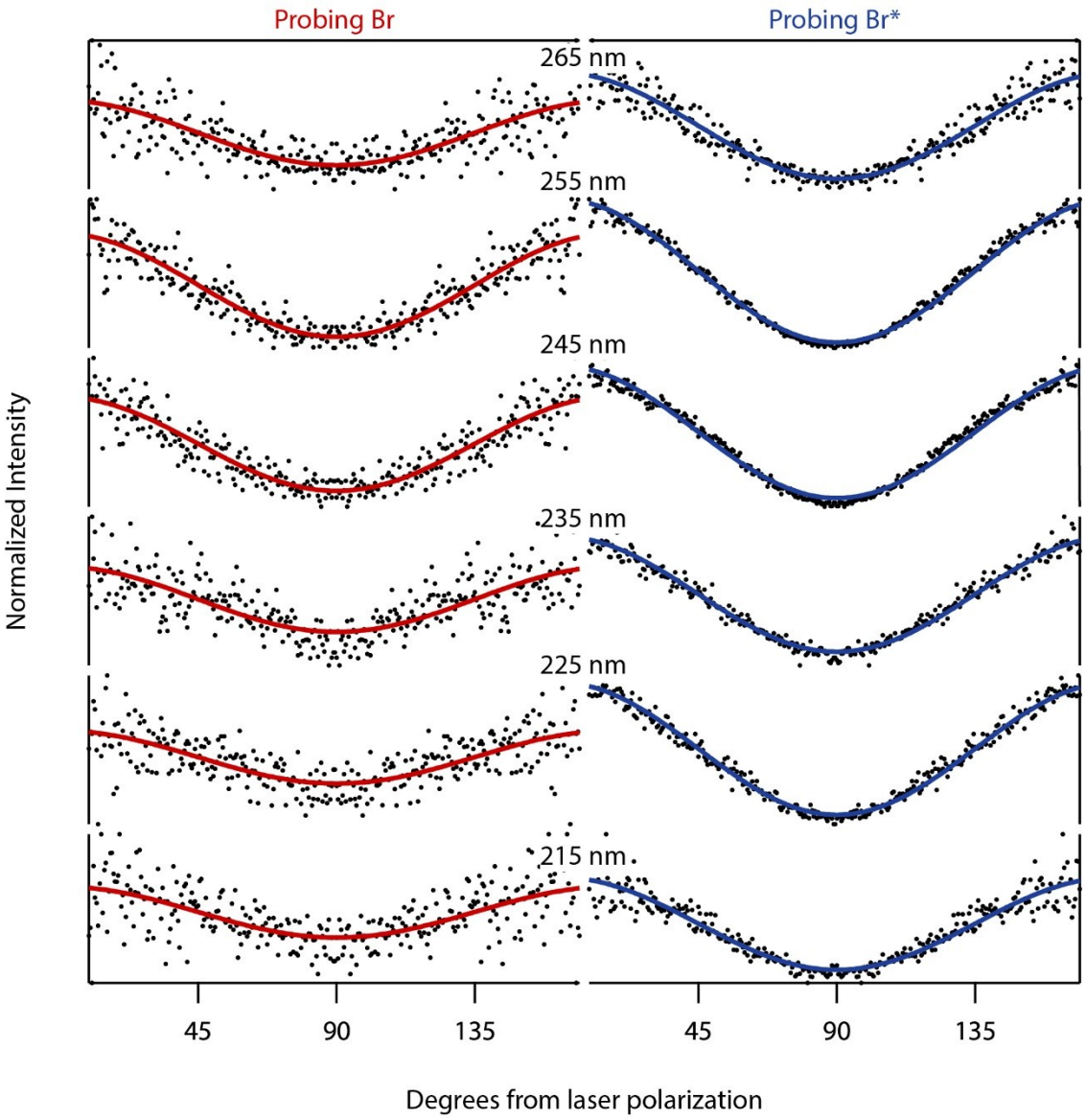

Figure S1 Angular distributions of intensity from VMI data at most probable translational energy for each photolysis wavelength employed. The vertical axis gives image intensity as a function of the angle away from the electric field polarization of the photolysis laser. All data was fit with equation 6 (red line) and beta parameters were extracted from the individual fits.

B. Wavelength-dependent data for various alkyl halides

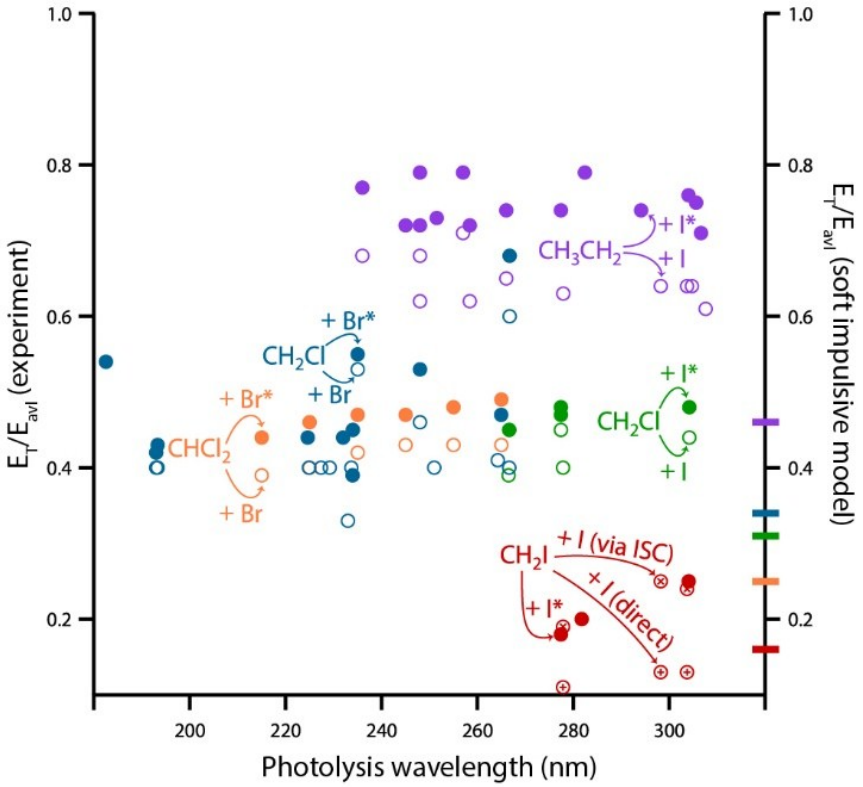

Figure S2 Wavelength dependence of data averaged for Figure 6. Experimental data taken from various other studies on similar alkyl halides: CH_3CH_2I[18,48,61-63] (purple), CH_2ClBr[25,26,29,33,36] (blue), ICH_2Cl[31,34] (green), $CHCl_2Br$ (this work, orange), and CH_2I_2[28] (red). Open markers denote dissociations leading to spin-excited halogen fragments, and closed markers denote ground-state halogen fragments. Predictions of translational energy partitioning from the soft impulsive model[63] are shown with hash marks on the right-hand vertical axis.

C. Measured internal energy and modeled rotational energy for $CHCl_2$

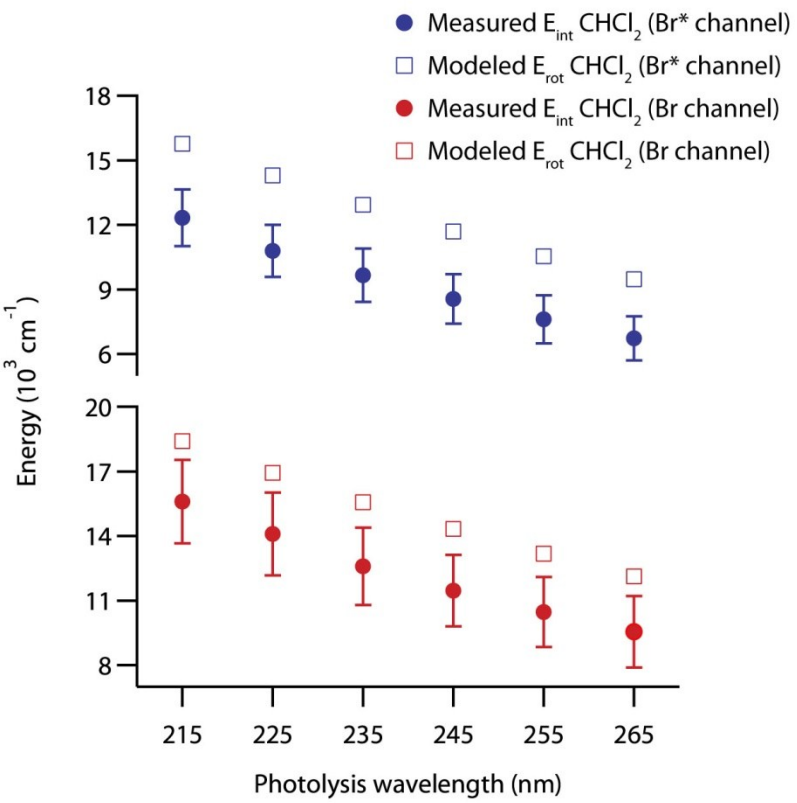

Figure S3 Wavelength dependence of measured internal energy (closed circles) and modeled rotational energy (open squares). Bars on measured data indicate the full-width, half-maximum spread of the internal energy. Modeled data assumes no vibrational excitation (rigid model).

D. Geometry optimizations used for impulsive modeling

The $CHBrCl_2$ geometry was optimized at the B3LYP level of theory with an aug-cc-pVTZ basis. The xyz coordinates (in Angstroms) are:

C	0.00000000	0.00000000	0.00000000
H	0.90340200	0.59060400	0.00000000
Cl	0.00000000	-1.00026400	1.46858200
Cl	0.00000000	-1.00026400	-1.46858200
Br	-1.48869400	1.26896000	0.00000000

The ICH_2Cl geometry was optimized at the B3LYP level of theory with 6-311++G(3df,3pd) basis for the C, H, and Cl atoms and a LanL2DZ basis for the I atom (as is consistent with Cheng and coworkers). The xyz coordinates (in Angstroms) are:

C	-1.0516232795	0.8916619626	0.0000005149
I	0.9087821748	-0.0509807772	-0.0000013228
H	-1.0960169952	1.4897122106	-0.8986818834
H	-1.0960198857	1.4897141230	0.8986826823
Cl	-2.4021719577	-0.2511362588	0.0000000091