

Supplemental Material

Influence of the Emission Site on the Photoelectron Circular Dichroism in Trifluoromethyloxirane

K. Fehre,¹ F. Trinter,^{1,2} N. M. Novikovskiy,^{3,4} S. Grundmann,¹ D. Tsitsonis,¹ S. Eckart,¹
L. Bauer,¹ M. Hilzinger,¹ T. Jahnke,⁵ R. Dörner,¹ Ph. V. Demekhin,³ and M. S. Schöffler¹

¹*Institut für Kernphysik, Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany*

²*Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany*

³*Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany*

⁴*Institute of Physics, Southern Federal University, 344090 Rostov-on-Don, Russia*

⁵*European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany*

In order to retrieve sufficient statistics for all cases of different emitter sites we integrated over a set of four breakup channels as stated in the main text. Here, we provide corresponding photoelectron circular dichroism (PECD) maps by integrating only over three of the four channels. Figure S1 depicts these maps for the different combinations of breakup channels and emitter sites. Table S1 provides information on the experimental statistics of the different breakup channels. The consistency of the different PECD maps suggest that our findings are robust against integration over the breakup channels. The PECD map for the case of the 3F-emitter neglecting the strongest channel (4) (second column, second row) suggest a lack of statistics resulting in PECD values on the order of the respective statistical uncertainty.

TABLE S1: The number of valid events in each fragmentation channel and for each considered emitter used in the present analysis of the PECD in Fig. S1.

Channel/Emitter	O	3F	2C	1C
(1) CF_3^+ (m/q=69) – COH^+ (m/q=29)	7 226 977	139 756	739 480	150 461
(2) CF_2^+ (m/q=50) – COH^+ (m/q=29)	209 014	377 690	337 811	112 926
(3) CF_3^+ (m/q=69) – C_2H_2^+ (m/q=26)	996 796	260 559	739 347	211 477
(4) CF_2^+ (m/q=50) – C_2H_2^+ (m/q=26)	495 061	1 268 206	578 840	248 731

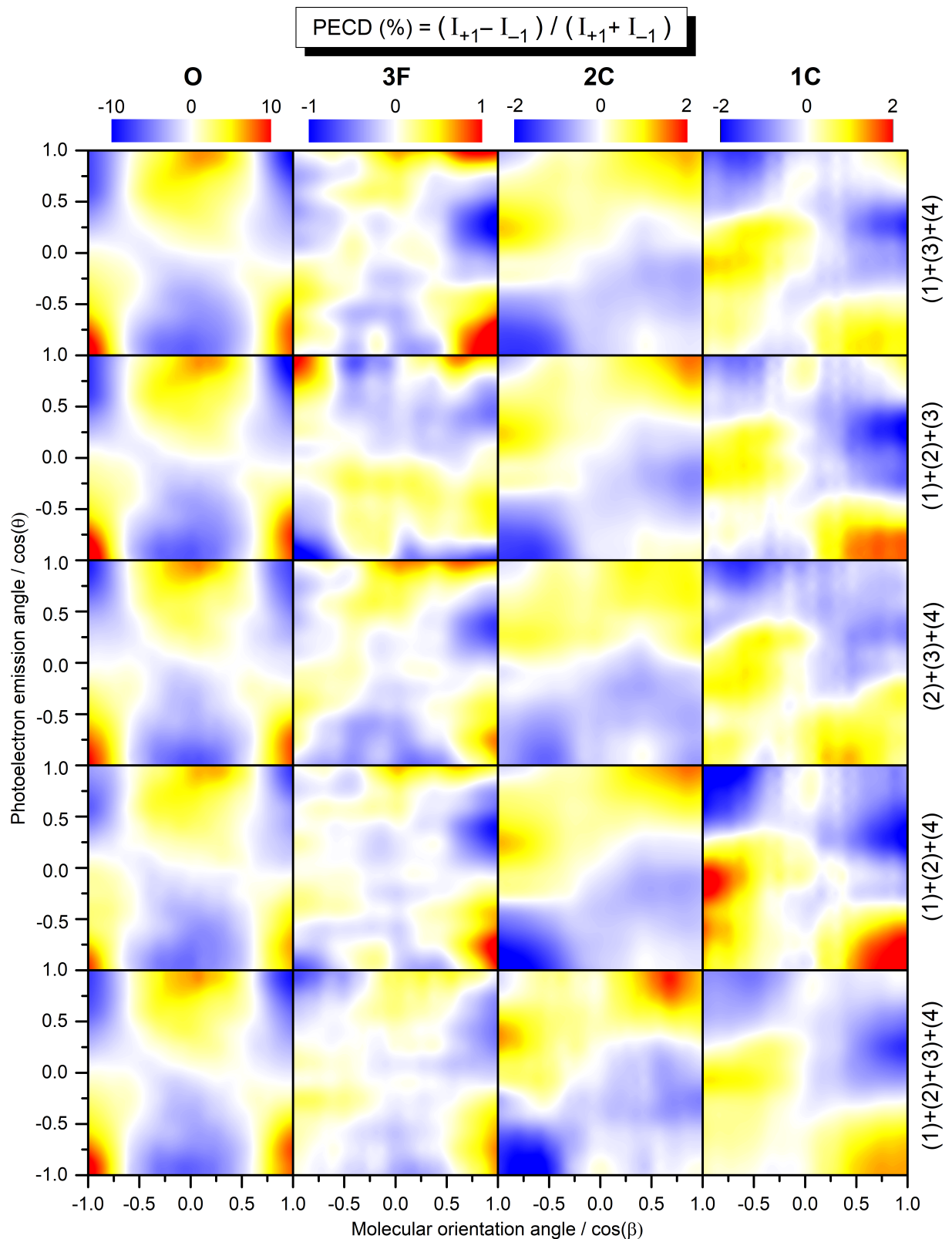


FIG. S1: Experimental PECD of R-TFMOx represented as the normalized difference of the electron emission probabilities, obtained for $1s$ -photoelectrons of 11 eV kinetic energy of the oxygen atom (first column, O), all three fluorine atoms (second column, 3F), the two carbon atoms from the oxirane ring (third column, 2C), and the carbon atom in the trifluoromethyl group (fourth column, 1C). The following four fragmentation channels (1) CF_3^+ ($m/q=69$) – COH^+ ($m/q=29$), (2) CF_2^+ ($m/q=50$) – COH^+ ($m/q=29$), (3) CF_3^+ ($m/q=69$) – C_2H_2^+ ($m/q=26$), and (4) CF_2^+ ($m/q=50$) – C_2H_2^+ ($m/q=26$) were used in the data analysis in different combinations (see Table S1 for the total number of events for each channel and emitter). First row: (1)+(3)+(4) channels. Second row: (1)+(2)+(3) channels. Third row: (2)+(3)+(4) channels. Fourth row: (1)+(2)+(4). Fifth row: all (1)+(2)+(3)+(4) channels (the same as in Fig. 2 of the manuscript).