

Photoemission chronoscopy of the iodoalkanes

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(Received 4 April 2025; accepted 8 October 2025; published 18 November 2025)

Time delays in photoemission are on the order of attoseconds and have been experimentally determined in atoms, molecules, and solids. Their magnitude and energy dependence are expected to yield fundamental insights into the properties of the systems in which they are measured. In a recent study Biswas *et al.* [*Nat. Phys.* **16**, 778 (2020)] determined the absolute photoemission time of the $I4d$ level in iodoethane via attosecond streaking spectroscopy, finding the presence of a functional group to increase the photoemission time delay, suggesting a correlation between the size of the functional group and time delay based on a semiclassical calculation. Here we experimentally study the dependence of the $I4d$ photoemission time on the functional group in the iodoalkanes from iodomethane up to 2-iodobutane at three photon energies across the giant resonance in the $I4d \rightarrow \varepsilon f$ photoemission channel, finding that the presence alone of a functional group does not necessarily increase the photoemission delay, and that overall no clear correlation between its size and the photoemission time delay can be established.

DOI: [10.1103/vxnp-42jr](https://doi.org/10.1103/vxnp-42jr)

Introduction. Photoemission chronoscopy, i.e., the measurement of the absolute time delay between the interaction of one (typically) XUV photon with an atom, molecule, or condensed matter sample and the appearance of the ejected photoelectron in vacuum, has recently been demonstrated as a viable experimental technique in a landmark experiment [1]. Experimentally this scheme relies on the attosecond streak camera technique [2] and measures the photoemission time of the system under study relative to a chronoscope species in which the photoemission time delay is known, e.g., from *ab initio* calculation. Osslander *et al.* [1] established this scheme with the ultimate goal to determine the photoemission time of the $4f$ and valence states of a W(110) surface at an excitation energy of 105 eV, by constructing a chain of references involving the $I4d$ photoemission in small iodoalkanes as an important chain link. Iodine and its compounds are especially suited for this purpose due to the giant dipole resonance in the $I4d \rightarrow \varepsilon f$ (a transition from the $I4d$ into a continuum f wave with energy ε) channel in this energy range, which greatly enhances the photoemission cross section (cf. [3]), permitting their use even at very low concentrations or when XUV photons are scarce. Furthermore, the $d \rightarrow f$ photoemission channel strongly dominates the photoelectron signal when compared with the $d \rightarrow p$ channel, vastly simplifying the interpretation of the results. Following the experiment by Osslander *et al.* [1], Biswas *et al.* [4] aimed at uncovering

molecular effects in the observed time delay, finding that the $I4d$ photoemission time in iodoethane may be raised significantly by the presence of a functional group when compared to the atomic case, and they present a calculation that predicts that this increase should continue as the size of the functional group grows. Here we expand upon this experiment and explicitly test whether this prediction can be generalized by measuring the $I4d$ photoemission time in primary and secondary iodoalkanes from iodomethane up to 2-iodobutane at photon energies of 90, 105, and 118 eV. We compare our experimental results to those of Biswas *et al.* [4], a published calculation for atomic iodine as well as a scattering calculation on the Hartree-Fock level of theory.

Experiment. We apply attosecond streaking spectroscopy (cf. [5–7]) to measure the $I4d$ photoemission time delay in iodomethane, iodoethane, 1- and 2-iodopropane, as well as 1- and 2-iodobutane in a mixture with Helium, using the known He $1s$ photoemission time delay as our reference [8,9]. Briefly, high harmonics of a waveform-controlled near-infrared–visible (NIR–VIS) few-femtosecond laser pulse centered around $\lambda_c = 790$ nm are generated in a short gas cell (500 μm) backed with ~ 100 mbar of Neon. The harmonic radiation is spatially separated from the NIR–VIS light via a thin Zr foil (0.15 μm thickness) placed at the center of the two coaxial beams after multiple meters of propagation. The spatially separated beams are then reflected off an interferometric double-mirror assembly consisting of an annular silver focusing mirror that reflects the NIR–VIS light and a focusing XUV multilayer reflector acting as a bandpass filter, which is inset into the annular silver mirror. Via this bandpass filter, XUV attosecond pulses centered at 90, 105, or 118 eV and 5–6 eV bandwidth [~ 300 attosecond (as) duration] are isolated from the spectrally unmodulated cut-off portion of the high-harmonic spectrum, where the photon energy is set

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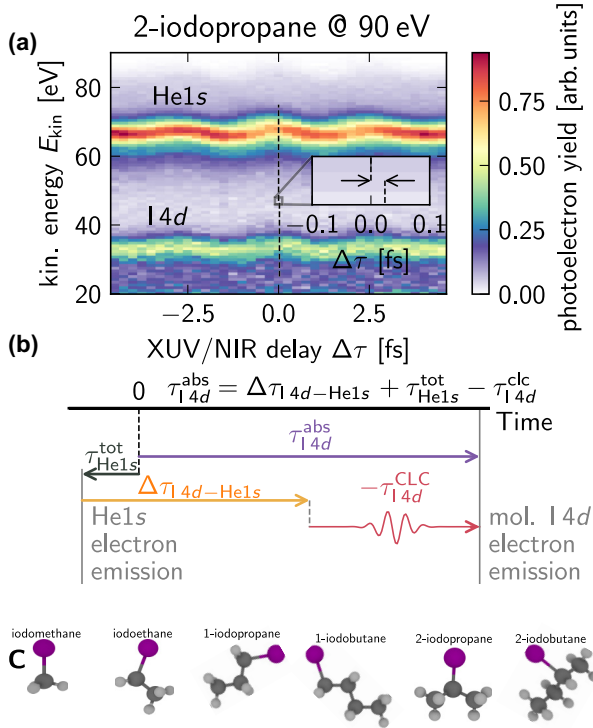


FIG. 1. Experimental determination of the absolute time delay of the I4d photoemission in the iodoalkanes. (a) Exemplary spectrogram recorded in a mixture of 2-iodopropane and Helium at 90 eV photon energy. The relative photoemission time $\Delta\tau_{I4d-He1s}$ is the lateral shift of the two streaking features with respect to each other and is extracted from the spectrogram via a multivariate fitting procedure. (b) With $\Delta\tau_{I4d-He1s}$ experimentally determined the absolute photoemission time of the I4d level τ_{I4d}^{abs} can be determined via the illustrated timing scheme. The photoemission time of the He 1s photoemission is known [8] and can be calculated with great precision, and the measurement-induced τ_{I4d}^{CLC} can be calculated analytically [10]. (c) Ball-and-stick models of the iodoalkanes under study. Iodine atoms are rendered in violet, Carbon atoms in dark gray, and Hydrogen atoms in light gray.

by the design of the XUV reflector in use. The interferometric time delay between the XUV and NIR pulse is controlled by axial translation of the XUV reflector with respect to the outer NIR mirror via a piezo actuator. The double mirror delay assembly focuses both beams near the exit of an effusive nozzle through which the mixture of Helium and the molecule is injected into the vacuum experimental apparatus. In the interaction region the attosecond XUV pulse initiates photoemission, ejecting a photoelectron wave packet from a molecule or Helium atom, which is then modulated in its kinetic energy by the action of the temporally offset NIR-VIS laser field. This modulation maps the temporal properties of the ejected photoelectron wave packet onto spectral information (cf. [5,7]). Photoelectron spectra are recorded with a time-of-flight electron spectrometer with an acceptance cone half-angle of $\sim 20^\circ$, and a sequence of spectra recorded as a function of XUV-NIR delay in this configuration constitutes a photoelectron spectrogram. Figure 1(a) shows an exemplary spectrogram, recorded at a photon energy of 90 eV on a gas mixture of Helium and 2-iodopropane. In a spectrogram the

TABLE I. Absolute photoemission time delays of the I4d $\rightarrow$ ϵf transition in the different molecules as determined by the experiment as well as the τ_{I4d}^{CLC} contribution and the absolute time delay τ_{He1s}^{tot} of the He 1s photoemission (see Supplemental Material [11]). The atomic I4d EWS time delay, extracted from the publication of Pi and Landsman [12] is given for reference.

	90 eV	105 eV	118 eV
I-methane	$(76.9^{+5.3}_{-11.6})$ as	(40.9 ± 4.1) as	(40.1 ± 4.0) as
I-ethane	$(62.8^{+6.2}_{-12.5})$ as	(39.6 ± 7.1) as	(25.1 ± 3.3) as
1-I-propane	$(36.6^{+4.1}_{-10.5})$ as	(23.1 ± 7.2) as	(10.3 ± 5.6) as
2-I-propane	$(78.5^{+6.7}_{-13.0})$ as	(63.9 ± 7.1) as	(20.0 ± 5.7) as
1-I-butane	$(33.0^{+6.8}_{-13.1})$ as	(31.7 ± 6.4) as	(35.4 ± 7.0) as
2-I-butane	$(28.8^{+4.4}_{-10.7})$ as	(35.3 ± 6.2) as	(32.0 ± 6.0) as
τ_{He1s}^{tot}	-6.5 as	-5.1 as	-4.3 as
τ_{I4d}^{CLC}	-19.2 as	-12.2 as	-9.1 as
$\tau_{I4d}^{at.}$ [12]	32.0 as	29.2 as	25.8 as

photoemission time $\Delta\tau_{I4d-He1s}$ of the I4d level relative to that of the He 1s photoemission is encoded as a small lateral shift of the I4d streaking feature with respect to He 1s feature [cf. [10,13], inset in Fig. 1(a)]. No less than 30 spectrograms per photon energy and molecule are taken. For extracting $\tau_{I4d-He1s}$ we apply a multivariate fitting procedure, which models the streaking process based on the strong-field approximation of the time-dependent Schrödinger equation (cf. [6,8,14–16] and Supplemental Material [11]) to each recorded spectrogram to determine this time shift at the central photon energy of the XUV pulse. The entire delay extraction procedure and statistical evaluation is detailed in the Supplemental Material [11].

Results and Discussion. Following Refs. [1,4], we take the total delay

$$\tau_{tot} = \tau_{abs} + \tau_{CLC} \quad (1)$$

of direct photoemission as measured by attosecond streaking spectroscopy as a sum of an absolute time delay τ_{abs} and the Coulomb-Laser-Coupling (CLC) contribution τ_{CLC} , which is introduced due to the interaction of the ejected photoelectron wave packet with the streaking laser field [10,13] in the long-ranged coulombic part of the photoion's potential. The CLC contribution is independent of the system under study and only depends on the kinetic energy of the photoelectron and the streaking pulse's wavelength. In the above expression, we identify the absolute delay τ_{abs} as the Eisenbud-Wigner-Smith (EWS) time delay due to the scattering of the outgoing photoelectron wave packet off the potential of the photoion (cf. [1,4]).

The relative I4d–He 1s time delay as measured in the experiment is then

$$\Delta\tau_{I4d-He1s} = (\tau_{I4d}^{abs} + \tau_{I4d}^{CLC}) - \tau_{He1s}^{tot}. \quad (2)$$

For the direct Helium 1s photoemission, the total photoemission time τ_{He1s}^{tot} is known with great precision from *ab initio* calculations in excellent agreement with experimental observation [8,9], and therefore Eq. (2) can be used to calculate absolute photoemission times τ_{I4d}^{abs} from the experimentally

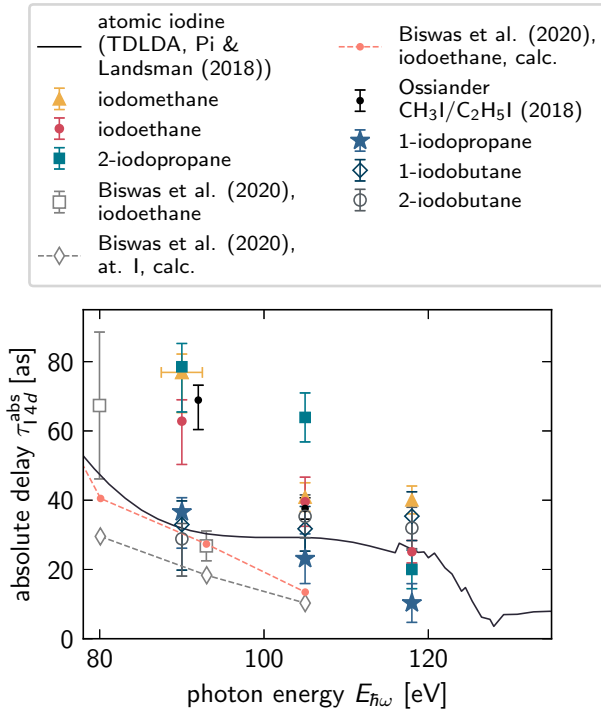


FIG. 2. Absolute photoemission time delays of the I4d photoelectrons in the iodoalkanes in comparison with the results of other experiments [1,4,17]. The black curve represents the atomic calculation by Pi and Landsman [12], gray diamonds are the semiclassical calculation for atomic iodine, and salmon points are the molecular calculation from [4]. Horizontal error bars for our data are given by the XUV reflector's bandwidth and are only plotted once for clarity.

determined relative time delays. This procedure is illustrated in panel (b) of Fig. 1.

Absolute photoemission times. Turning first to iodomethane and iodoethane, we compare our experimentally determined τ_{I4d}^{abs} with those determined for iodomethane and iodoethane by Ossiander *et al.* [1] and in [17] and those by Biswas *et al.* [4]. Our experimentally determined delays are listed in Table 1. We find excellent agreement of our data for iodomethane and iodoethane at 105 eV with the results of Ossiander *et al.* [1] and at 90 eV with those from [17] at 92.5 eV (see Fig. 2). Our data at 90 eV, however, does not reproduce the experimental result of Biswas *et al.* [4] at 93 eV, who use the $2p$ photoemission of Neon as their chronoscopy reference for which they calculate the absolute delay. It is possible that the difference in reference species and/or data analysis method is the reason for the disagreement between their results and ours.

Overall we find the photoemission times to decrease with energy in all molecules except for 1-iodobutane and 2-iodobutane where it is almost constant within the uncertainties. The decrease with energy is expected as it is a general property of the EWS delay time [18]. Compared to a calculation for atomic iodine by Pi and Landsman [12] we find the photoemission time delays in iodomethane, iodoethane, and 2-iodopropane to be significantly elevated at 90 and 105 eV. The delay in 1-iodopropane exceeds the atomic calculation at 90 eV but is lower at the higher energies. In 1- and

2-iodobutane the atomic prediction is only exceeded significantly at 118 eV. At no photon energy does the calculation for iodoethane of Biswas *et al.* [4] (salmon points in Fig. 2) agree with our experimental data or that of Ossiander *et al.* [1]. Of note is the comparison between the atomic calculation of [12] based on the time-dependent local density approximation (TDLDA) and the semiclassical calculation for atomic iodine of [4]: the semiclassical calculation is tens of attoseconds below the TDLDA prediction (which can be expected to be quite accurate, as it produces a photoemission cross section in accord with spectroscopic data, e.g., [3,19,20]) for all photon energies, raising the question of whether it is actually capable of accurately describing the I4d photoemission in this energy range, in particular the giant resonance.

Variation of the photoemission time with the size of the functional group. Biswas *et al.* [4] also use their semiclassical calculations to predict how the I4d photoemission time should behave as the attached functional group is varied, and find that the total I4d photoemission time nearly doubles when moving from iodoethane to 2-iodo-2,3,3-trimethylbutane $[(\text{CH}_3)_5\text{C}_2\text{I}]$; see Fig. 4(e) in [4], assuming an intermediate value for the fluorinated analog of iodoethane. Although the authors do not state at which excitation energy specifically this result is obtained, they predict a streaking time shift of ~ 12 as for iodoethane in this calculation, which is close to their calculated data point at 105 eV in Fig. 3(a) of Ref. [4]. Their calculated EWS time delay reported at this energy is ~ 14 as [Fig. 3(b) of [4]]. They attribute the predicted increase from iodoethane to $(\text{CH}_3)_5\text{C}_2\text{I}$ to the difference in molecular environment the leaving photoelectron experiences, which manifests as “an increase of the overall delay with the size of the ligand” [[4], p. 783]. While our study does not address $(\text{CH}_3)_5\text{C}_2\text{I}$ specifically, our results generally do not consistently show the photoemission time delay increasing as the ligand size increases. We also do not find iodoethane to have an EWS delay of 14 as at 105 eV, or any other photon energy our experiment is conducted at. As Fig. 3 shows, we find that the I4d photoemission delay rather tends to *decrease* as the size of the functional group (as measured by its mass) increases. At 90 eV this decrease occurs consistently across iodomethane, iodoethane, and 1-propane, as well as between 2-iodopropane and 2-iodobutane. For the higher photon energies and the primary iodoalkanes τ_{I4d}^{abs} goes through a minimum for 1-iodopropane, while for the secondary iodoalkanes we find the delay to decrease with ligand mass at 105 eV and increase at 118 eV. Overall, no meaningful and consistent correlation can be established. Now, the question of whether the decrease of the I4d photoemission time observed here will continue towards 2-iodo-2,3,3-trimethylbutane or whether one will find it to rise again, in line with the prediction in [4] can only be answered by performing the experiment on the difficult to obtain molecule. However, taking all available data (Fig. 2) into account, it stands to reason that the semiclassical calculation of Biswas *et al.* [4] is incorrect: their own experiment agrees with this calculation only at a single photon energy (93 eV) within uncertainties, and this result is replicated neither by Ossiander [p. 65, [17]], nor by us. Furthermore, the calculation by Pi and Landsman [12] for atomic iodine (the accuracy of which can be verified by comparison of the predicted cross section with experimental data; e.g.,

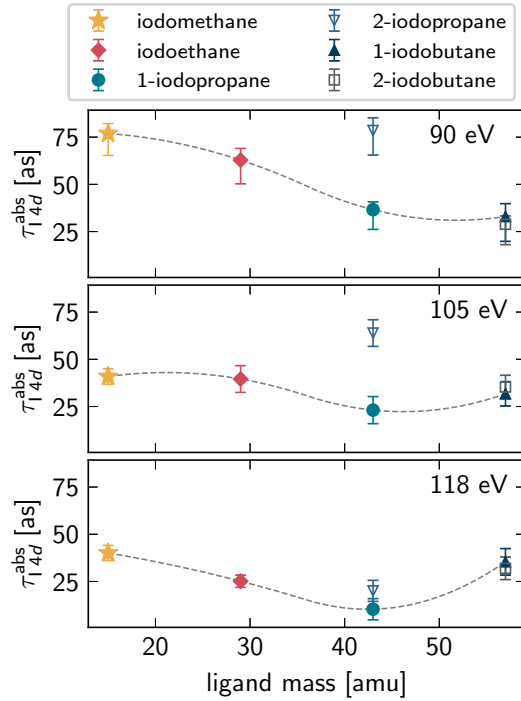


FIG. 3. Correlating the absolute I4d photoemission time delay with the ligand size as measured by its mass. While Ref. [4] predicts an increase of the I4d photoemission delay with ligand mass we find that τ_{I4d}^{abs} tends to *decrease* (primary and secondary iodoalkanes at 90 eV, secondary iodoalkanes at 105 eV) or to initially decrease and go through a shallow minimum for 1-iodopropane as seen for the primary iodoalkanes at 105 and 118 eV. The gray dashed lines have been added as a guide to the eye.

[3,19]) gives much larger values than what Biswas *et al.* [4] find for the isolated atom, corroborating our assessment. We must therefore conclude that the predicted correlation of the photoemission time delay with the size of the molecule in [4] is simply an artifact of their calculation, and it is therefore not observed in our experiment.

How sensitive is the experiment to the molecular environment? Another noteworthy observation is that at all studied photon energies and within their respective uncertainties 1- and 2-iodobutane have equal delays, which are very close to the atomic prediction by Pi and Landsman [12]. This raises the question of whether the experiment may become insensitive to the position of the Iodine atom within the molecule for larger molecules, or even insensitive to the presence and shape of the ligand overall. Furthermore, this shows that the mere *presence* of a functional group does not necessarily raise the I4d photoemission delay when compared to the atomic case. Unfortunately, an accurate independent theoretical assessment of the photoemission time delay in the iodoalkanes is currently out of reach. Both Osslander *et al.* [1] and Biswas *et al.* [4] compare their experimental results with scattering calculations based on the Schwinger variational procedure and local density approximation (LDA) on the Hartree-Fock (HF) level of theory [21–23] using the EPOLYSCAT software package (see Supplemental Material for details [11]), but as Fig. 4 shows such calculations fail to produce photoionization cross sections in agreement with experimental data even for

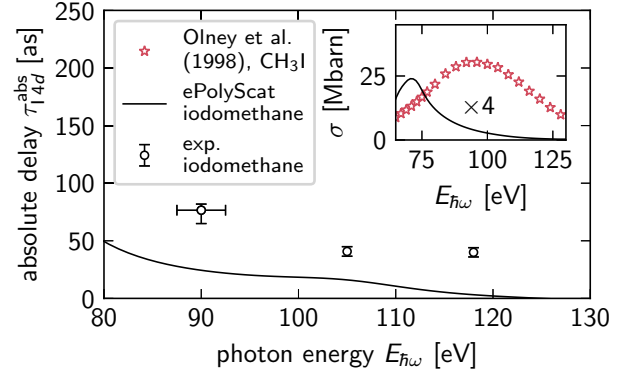


FIG. 4. Comparison of our experimental result for iodomethane with a quantum scattering calculation on the HF + LDA level of theory (EPOLYSCAT). The inset shows the calculated cross section in comparison to the experiment on iodomethane by Olney *et al.* [3]. It is easily seen that the giant resonance is not rendered adequately.

iodomethane, discouraging a comparison of calculations and our experiment. The primary reason for this failure lies in the inadequacy of the LDA as a description of the giant resonance in the $I4d \rightarrow \epsilon f$ photoemission, as it has also previously been shown for the giant resonance in both the I4d [20] and Xe 4d photoemission [24]. For the larger molecules these calculations quickly become infeasible overall as they rely on a single-center partial wave expansion, which requires prohibitively large values of ℓ to converge as the molecule grows in size. A promising candidate for the theoretical assessment of photoemission time delays in molecules at an appropriate level of theory, however, is the *R*-matrix method with time dependence as developed by Mařin *et al.* [25].

Conclusion. In this work we presented a systematic survey of the I4d photoemission time delay in the iodoalkanes from iodomethane to 2-iodobutane. We find that the presence of different functional groups modulates the delay in a unique manner for the smaller molecules under study, while we find very similar values in the larger iodoalkanes. Overall, our results indicate that the I4d photoemission time as determined via attosecond streaking spectroscopy in the gas phase does not increase with the size of the attached functional group as has been suggested by Biswas *et al.* [4]. Generally, no clear correlation between observed delay and any measure of size of the molecule can be established from the presented data, and it is evident that more experimental and especially theoretical work is needed to understand the origin and meaning of the variations observed in the time delays, for which we hope that our experimental results can serve as a useful benchmark.

Acknowledgments. The authors gratefully acknowledge valuable discussions with Andreas Westfahl and Michael Mittermair, and thank Alexander Guggenmoos, Yang Cui, and Ulf Kleineberg for providing the XUV multilayer reflectors. The authors acknowledge funding support from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germanys Excellence Strategy-EXC 2089/1-390776260 (e-Conversion).

C.A.S. conceived the study, performed the experiments and calculations, analyzed the data, and wrote the first draft of the manuscript. M.P., P.F., S.-J.P., and M.F. assisted with the

experiments. M.O. estimated the influence of the NVV Auger-Meitner emission on the delay retrieval. R.K. supervised the study. All authors reviewed the manuscript and contributed with valuable discussions.

Data availability. The data that support the findings of this article are openly available [26].

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