Absorption coefficients data of lead iodine perovskites using 14 different organic cations

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ABSTRACT
This Data article presents the absorption coefficients of Lead Iodine perovskites using 14 different organic cations. In addition, the absorption coefficients have been split into inter-atomic species components in order to quantify all of the contributions. For more details on the methodology, interpretation and discussion, refer to the full length article entitled “Effect Of the organic cation on the optical properties of lead iodine perovskites”. https://doi.org/10.1016/j.solmat.2019.110022 Data may be useful for future research, and to identify the contribution of different species to the absorption.

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1. Data

The data and figures shown below represent the total and split absorption coefficients of 14 organic cations of lead iodine perovskites. The total absorption coefficients \( \alpha_{TOT} \) have been split into inter-atomic species components \( \alpha_{TOT} = A_{12} + A_{34} \). The first term \( A_{12} = \sum_{A=1}^{n} \sum_{B=1}^{n} \alpha_{AB} \) involves intra-species (\( A = B \)) and inter-species (\( A \neq B \)) contributions, and the \( A_{34} \) term involves 3-species (\( A \neq B \neq C \)) and 4-species (\( A \neq B \neq C \neq D \)) contributions. It allows to quantify and split into contributions other properties related to the absorption of radiation. In Figs. 1–14 \( \alpha_{pb-pb} \) and \( \alpha_{1-1} \) are intra-species, \( \alpha_{pb-i} \) is a...
Specifications Table

| Subject                      | Energy                                                                 |
|------------------------------|------------------------------------------------------------------------|
| Specific subject area        | Renewable Energy, Sustainability and the Environment                   |
| Type of data                 | Table and Figures                                                      |
| How data were acquired       | They have been obtained from first principles in two steps: (i) the electronic properties are obtained from first-principles calculations based on density-functional theory, and (ii) the optical properties were obtained from the imaginary part of the dielectric function. |
| Data format                  | Raw and analysed                                                       |
| Experimental factors         | The imaginary part of the dielectric function was calculated within the random phase approximation. The absorption coefficients and other optical properties were obtained from the imaginary part of the dielectric function using the Kramers-Kronig relationships. Later, they were split into inter-species, intra-species, 3-species and 4-species contributions |
| Experimental features        | The absorption coefficients of Lead Iodine perovskites using 14 different organic cations were obtained using first principles calculations. Later, they were split as a many-specie expansion. |
| Data source location         | Instituto de Energía Solar, E.T.S.I. de Telecomunicación,             |
|                             | Universidad Politécnica de Madrid, Ciudad Universitaria s/n, 28040 Madrid, SPAIN. |
| Data accessibility           | Repository name: zenodo                                                |
|                             | Data identification number: 10.5281/zenodo.3335833                      |
|                             | Direct URL to data: [https://doi.org/10.5281/zenodo.3335833](https://doi.org/10.5281/zenodo.3335833) |
| Related research article     | César Tablero Crespo,                                                  |
|                             | Effect Of the organic cation on the optical properties of lead iodine perovskites, Solar Energy Materials and Solar Cells, [https://doi.org/10.1016/j.solmat.2019.110022](https://doi.org/10.1016/j.solmat.2019.110022). |

**Value of the data**

- The total absorption coefficients can serve as reference for experimental results in perovskites with different organic cations.
- The inter-atomic species components of the absorption coefficients allows to analyze the optical characteristics that the substitution of Pb by another element should satisfy to maintain a high absorption capacity.
- The total absorption coefficients can be used to obtain efficiencies of solar cells.

Inter-species, and $A_{34}$ the 3- and 4-species contributions to the total absorption coefficient $a_{TOT}$. The datafiles were deposited at zenodo repository ([https://doi.org/10.5281/zenodo.3335833](https://doi.org/10.5281/zenodo.3335833)), and they contains the raw data corresponding to the total absorption coefficients for the 14 organic cations described in Table 1.

2. Experimental design, materials, and methods

The methodology, interpretation and discussion are described in reference [1]. In Table 1 are shown the 14 organic cations ($A$) for the lead iodine perovskites $APb\_2$, and in Figs. 1–14 the total and split absorption coefficients.

The data has been obtained according to the following process:

(i) The electronic properties were obtained from first-principles calculations based on density-functional theory.

(ii) Using the energies and the occupation of the states obtained previously, and additionally calculating the transition probabilities, the optical properties were obtained from the imaginary part of the dielectric function within the random phase approximation.

(iii) From the dielectric function, and using the Kramers-Kronig relationships, the total absorption coefficients were obtained.
**Fig. 1.** APb$_3$ total absorption coefficient $\alpha_{\text{TOT}}$ (right y axis) for $A =$ Me. The most important intra- and inter-species $\alpha_{\text{Pb-Pb}}, \alpha_{I-I}, \alpha_{\text{Pb-I}}$, and the 3 and 4-species contributions ($A_{34}$) are represented in the left y axis.

**Fig. 2.** Same legend as that in Fig. 1, but for $A =$ Di.

**Fig. 3.** Same legend as that in Fig. 1, but for $A =$ Tr.
Fig. 4. Same legend as that in Fig. 1, but for A = Te.

Fig. 5. Same legend as that in Fig. 1, but for A = Pr.

Fig. 6. Same legend as that in Fig. 1, but for A = Is.
Fig. 7. Same legend as that in Fig. 1, but for $A = Ac$.

Fig. 8. Same legend as that in Fig. 1, but for $A = Im$.

Fig. 9. Same legend as that in Fig. 1, but for $A = Az$. 
(iv) The total absorption coefficients were split into inter-species, intra-species, 3-species and 4-species contributions according to the process described in the previous section.

A remarkable feature of the previous figures is that almost all organic lead iodine perovskites absorption coefficients are qualitatively similar. For energies close to the bandgaps, the main contribution to the absorption coefficient is from the Pb–Pb intra-species transitions. With the increase in the photon energy above the energy bandgaps, the I–I and Pb–I contributions, and the contributions of 3 and 4 species begin to be as important as the Pb–Pb contribution. The exception is for the H2I cation with a larger energy bandgap than the rest of the perovskites. Note that the organic cation atoms almost do not contribute to the intra- and inter-species terms. In the 3 and 4 species terms are included the organic cation contributions. Therefore, summarizing the data: (i) the absorption properties do not vary considerably, except for the H2I cation; (ii) the organic cations do not directly contribute to the optical properties via intra- and inter-species terms, but indirectly through of the 3 and 4 species terms for energies above the energy bandgap.

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Conflict of Interest

The author declare that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

[1] C. Tablero Crespo, Effect of the organic cation on the optical properties of Lead Iodine perovskites, Sol. Energy Mater. Sol. Cells 200 (2019) 110022, https://doi.org/10.1016/j.solmat.2019.110022.