



Cite this: *Phys. Chem. Chem. Phys.*,  
2023, 25, 31514

## Correction: Optical absorption and shape transition in neutral $\text{Sn}_N$ clusters with $N \leq 40$ : a photodissociation spectroscopy and electric beam deflection study

Andreas Lehr,\* Filip Rivic, Marc Jäger, Martin Gleditsch and Rolf Schäfer

DOI: 10.1039/d3cp90218h

rsc.li/pccp

Correction for 'Optical absorption and shape transition in neutral  $\text{Sn}_N$  clusters with  $N \leq 40$ : a photodissociation spectroscopy and electric beam deflection study' by Andreas Lehr *et al.*, *Phys. Chem. Chem. Phys.*, 2022, **24**, 11616–11635, <https://doi.org/10.1039/D2CP01171A>.

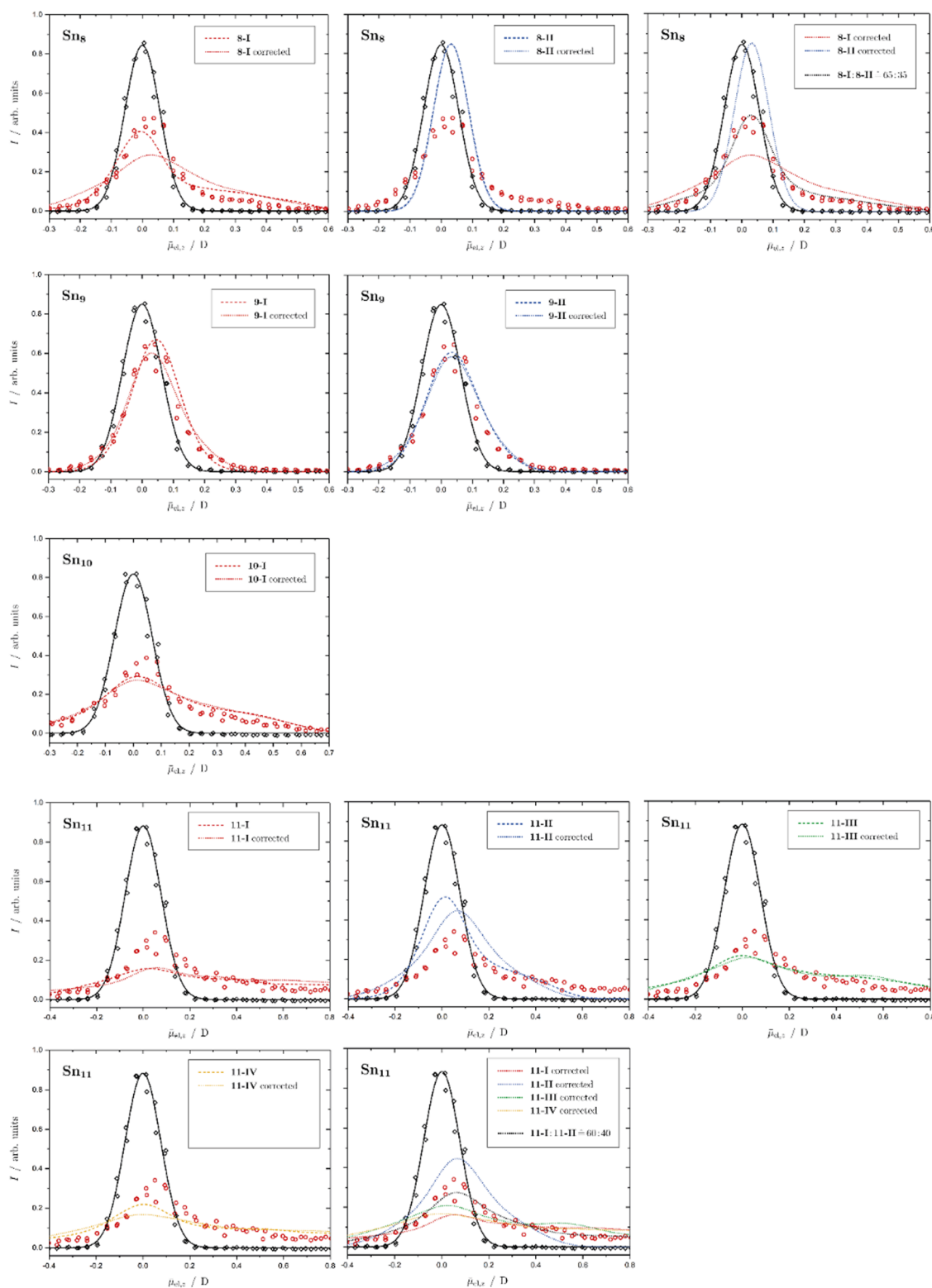
The authors would like to point out that while reevaluating the data published in the original paper, a systematic error was observed, which has a minor impact on several figures, but does not change the conclusions drawn and thus the text in the published paper.

The errors were made in the molecular dynamics simulations of the electric deflection beam profiles. By mistake, the computed electric dipole moment components  $\mu_x$ ,  $\mu_y$  and  $\mu_z$ , which serve as input for the molecular dynamics simulations, did not coincide with the centre-of-mass-based depiction of the cluster's coordination frame.

This affects partly the simulated electric deflection profiles (dashed lines in Fig. 5–9 of the original manuscript) of the tin clusters  $\text{Sn}_N$  with  $N \leq 25$ . The corrected simulations are presented in Fig. C1–C4 (dotted lines) herein. While for many clusters, the corrected simulated beam profiles differ insignificantly from the original simulated beam profiles, less symmetric clusters can show clearly visible changes that either slightly improve on the agreement with experimental results or slightly deteriorate this agreement. In none of these cases the conclusions drawn from these results are altered and thus the text in the original paper is not affected. Only regarding the  $\text{Sn}_{19}$  cluster, when assuming two isomers to be present in the molecular beam experiment, the isomer ratio changes slightly in favour of isomer 19-I. This is now in slightly better agreement with the thermodynamic considerations in Section S3 of the electronic supplementary information (ESI) associated with the published paper.

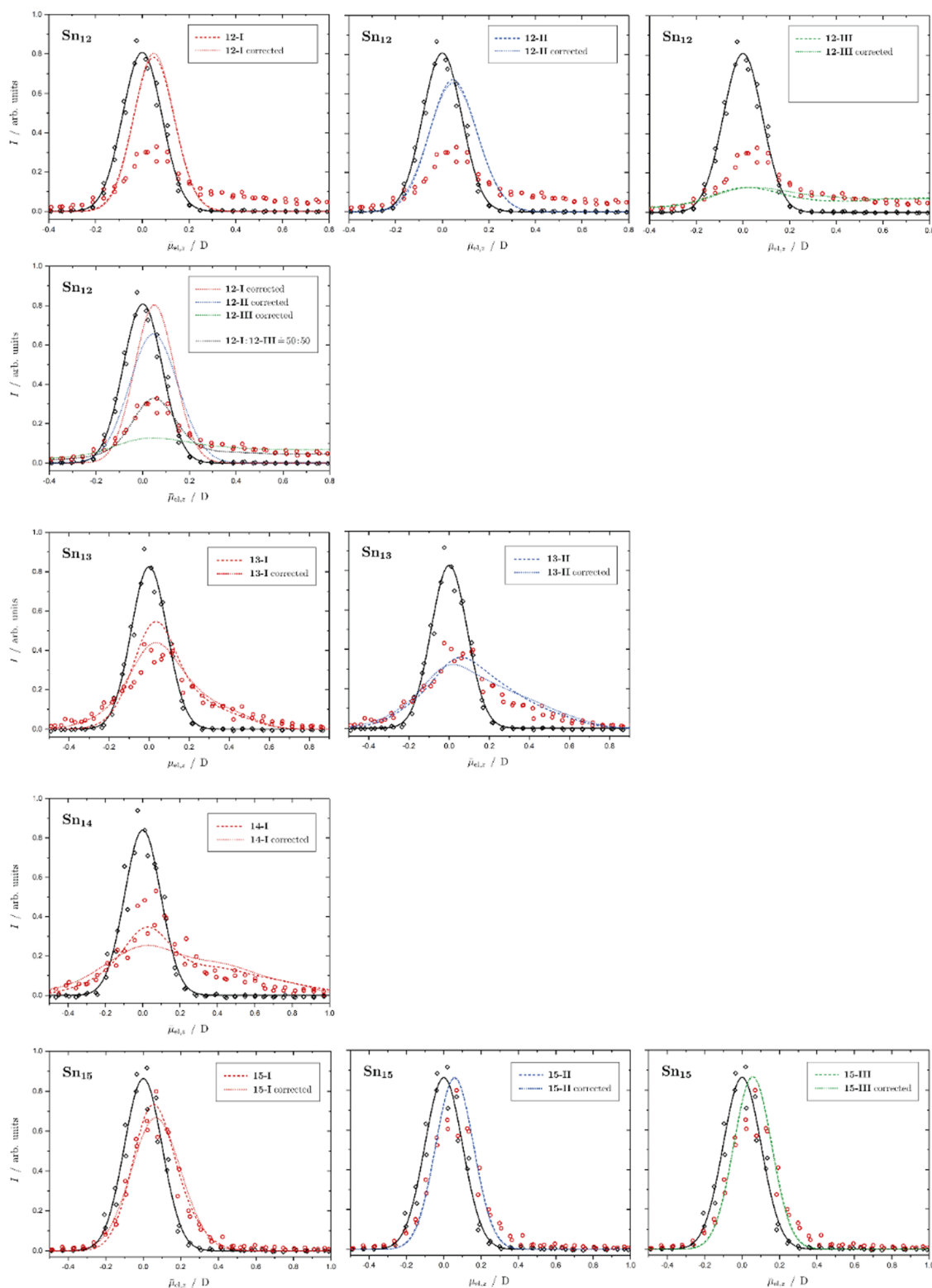
The electric dipole moment components  $\mu_x$ ,  $\mu_y$  and  $\mu_z$  as well as the total electric dipole moment  $\mu_{\text{iso}}$  were given in Table S3 of the ESI. Here, three transmission errors regarding the isomers 8-I, 30-III and 40-II occurred when setting up the table. The correct values have been updated in the ESI associated with the original paper.





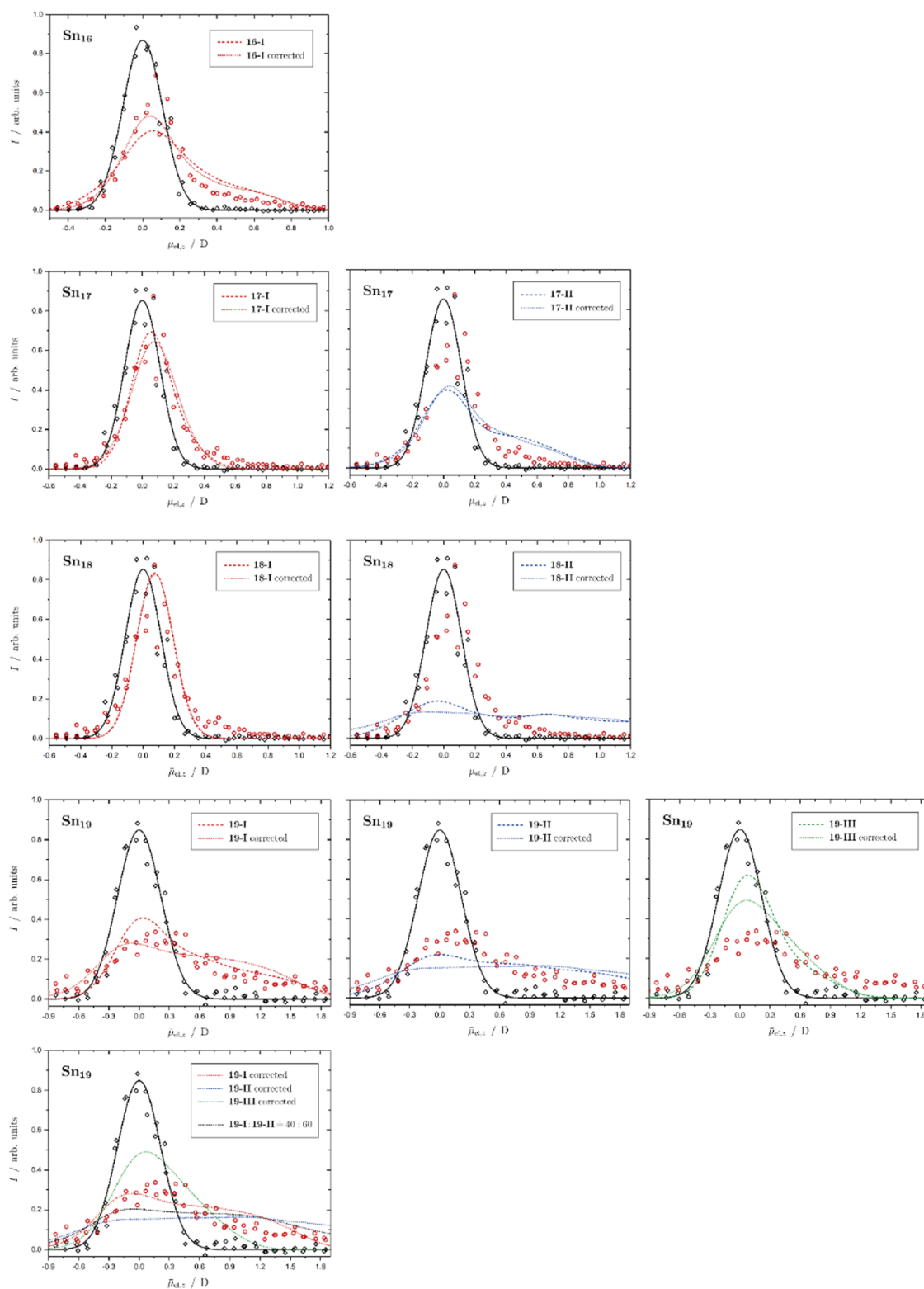
**Fig. C1** Corrected simulated electric deflection profiles (dotted lines) in direct comparison with the erroneous electric deflection profiles of the original manuscript (dashed lines) for the  $\text{Sn}_N$  clusters with  $N = 8$ –11. Details of this figure are given in the caption of Fig. 4 of the original paper.





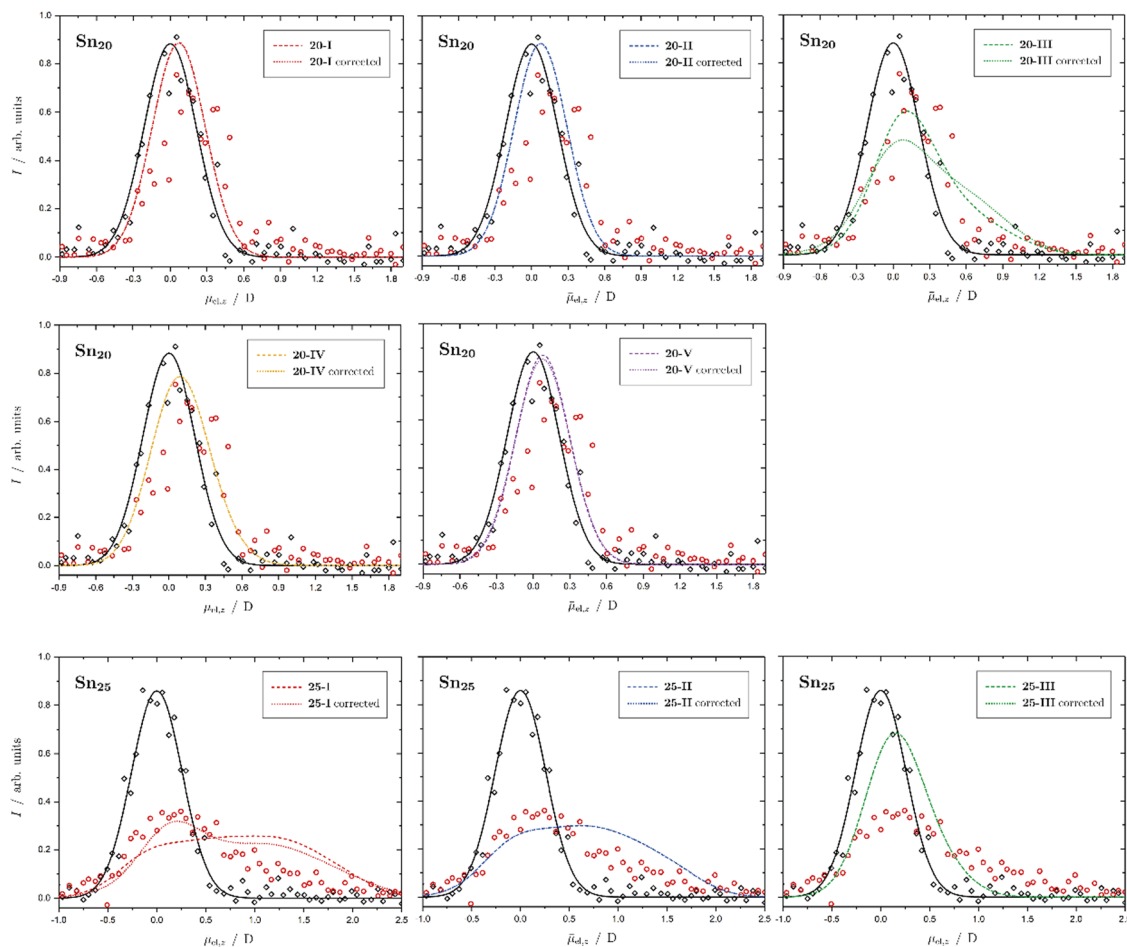
**Fig. C2** Corrected simulated electric deflection profiles (dotted lines) in direct comparison with the erroneous electric deflection profiles of the original manuscript (dashed lines) for the  $\text{Sn}_N$  clusters with  $N = 12$ –15. Details of this figure are given in the caption of Fig. 4 of the original paper.





**Fig. C3** Corrected simulated electric deflection profiles (dotted lines) in direct comparison with the erroneous electric deflection profiles of the original manuscript (dashed lines) for the  $\text{Sn}_N$  clusters with  $N = 16$ –19. Details of this figure are given in the caption of Fig. 4 of the original paper.





**Fig. C4** Corrected simulated electric deflection profiles (dotted lines) in direct comparison with the erroneous electric deflection profiles of the original manuscript (dashed lines) for the  $\text{Sn}_N$  clusters with  $N = 20$  and  $25$ . Details of this figure are given in the caption of Fig. 4 of the original paper.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

