

Three new trifluoromethyl derivatives of [60]fullerene, $C_{60}(CF_3)_{12}$

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The negative ion MALDI mass spectra of isolated fractions were acquired with the use of a Bruker AutoFlex II reflector time-of-flight mass spectrometer (N_2 laser, 337 nm, 2.5 ns pulse). Trans-2- [3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]malonodinitrile (DCTB) in a molar ratio of >1000:1 relatively to the analyte was employed as a MALDI matrix.

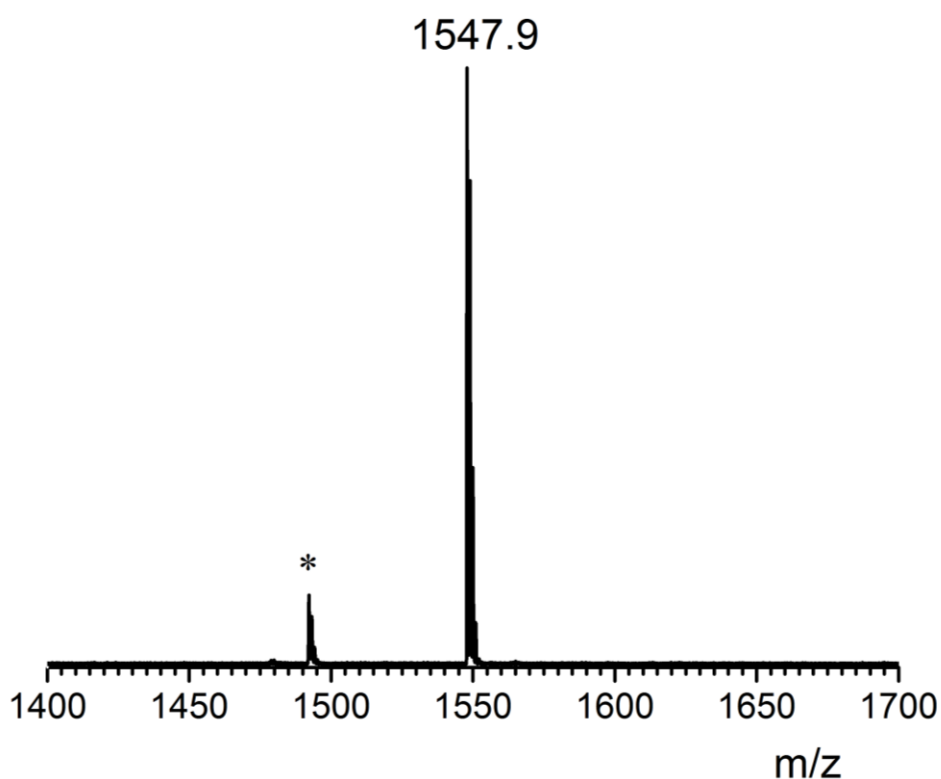


Figure S1 MALDI-TOF spectrum of the fraction containing $C_{60}(CF_3)_{12}$ -VIII. 1547.9 ($C_{60}(CF_3)_{12}^-$, M_1^- , 100%), 1492.2 ($[M_1-CF_3]^-$, 11.6%).

UV/Vis spectra of $C_{60}(CF_3)_{12}$ -I in *o*-DHB and *n*-hexane^{S1} and the rest compounds in toluene solution were obtained using the HPLC DAD detector in the 290–900 nm range with 2 nm resolution.

UV/Vis spectra of $C_{60}(CF_3)_{12}$ -II and $C_{60}(CF_3)_{12}$ -IV have not been reported in the original works.^{S2,3}

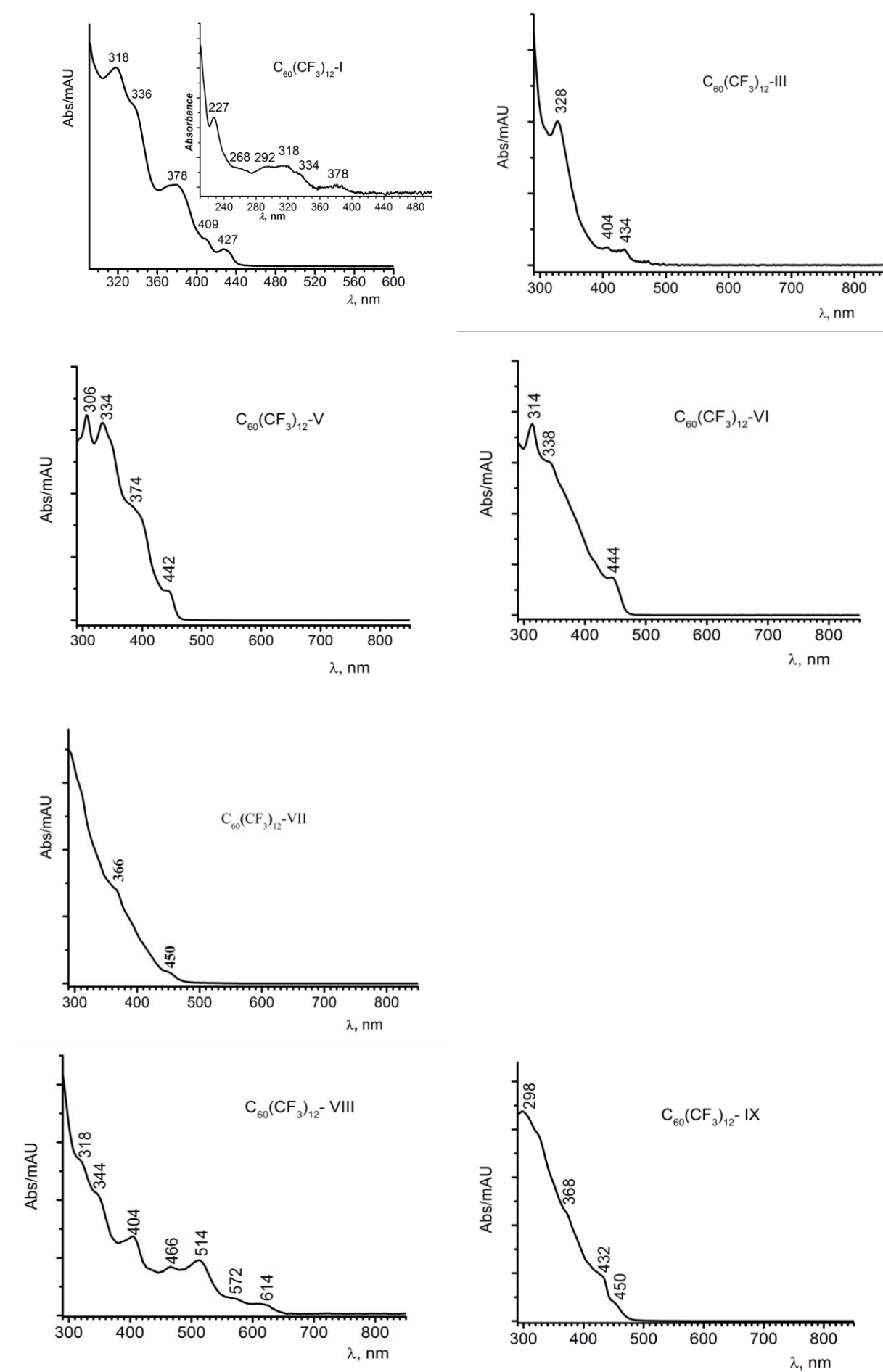


Figure S2 UV/Vis spectra of $C_{60}(CF_3)_{12}$ isomers I, III, V, VI, VII, VIII, IX

References

- S1. N. A. Romanova, V. Yu. Markov and A. A. Goryunkov, *Russ. J. Phys. Chem. A*, 2023, **97**, 1964.
- S2. I. E. Kareev, N. B. Shustova, D. V. Peryshkov, S. F. Lebedkin, S. M. Miller, O. P. Anderson, A. A. Popov, O. V. Boltalina and S. H. Strauss, *Chem. Commun.*, 2007, 1650.
- S3. N. B. Shustova, O. P. Anderson, O. V. Boltalina, S. H. Strauss and I. E. Kareev, *Acta Crystallogr.*, 2008, **E64**, o159.