UNIWERSYTET OPOLSKI

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THEORETICAL STUDIES ON CHEMICAL SHIFTS OF 3,6-DIIODO-9-ETHYL-9H-CARBAZOLE

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KAPITAŁ LUDZKI
NARODOWA STRATEGIA SPÓJNOŚCI

Klaudia Radula-Janik is a recipient of a Ph.D. fellowship from a project funded by the European Social Fund Stypendia doktoranckie-inwestycja w kadrę naukową województwa opolskiego.T. Kupka and K. Ejsmont acknowledges financial support from 8/WCh/2012-S and 7/WCh/2012-S projects.

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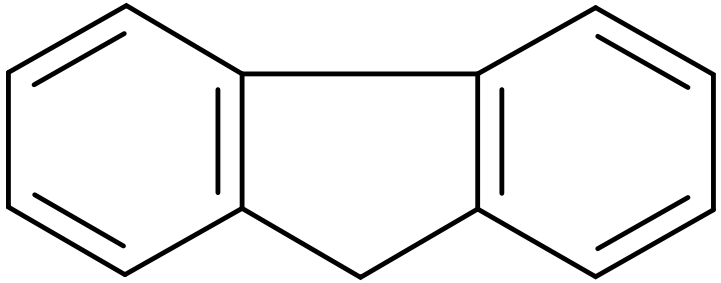
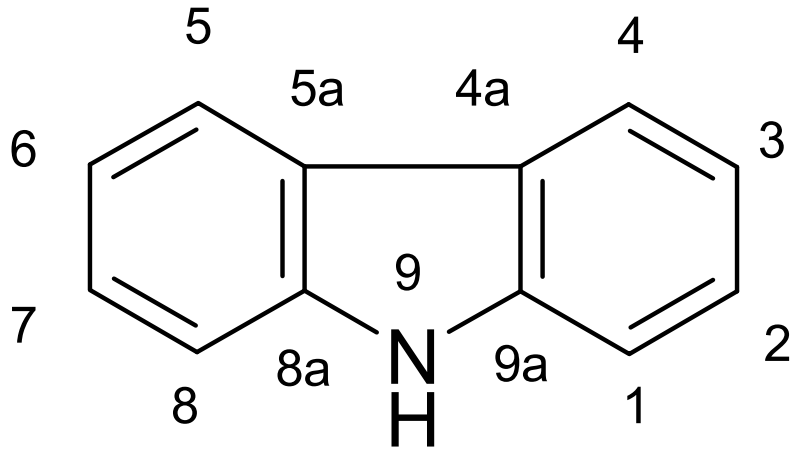
FUNDUSZ SPOŁECZNY

$C_{12}H_9N$

- Carbazole (9-azafluorene, dibenzopyrrole, diphenylenimine, diphenyleneimide)



Fluorene



Carbazole

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$C_{12}H_9N$

- 9*H*-carbazole is a very cheap starting material;
- it is a fully aromatic unit providing a better chemical and environmental stability;
- the nitrogen atom can be easily substituted with a wide variety of functional groups to help polymer solubility and to tune the optical and electrical properties;
- it possesses a bridged biphenyl unit resulting in materials with a lower band gap than traditional poly(p-phenylene)s.

Jean-Francois Morin, Mario Leclerc, Dominique Ades, Alain Siove *Macromol. Rapid Commun.* 2005, **26**, 761–778

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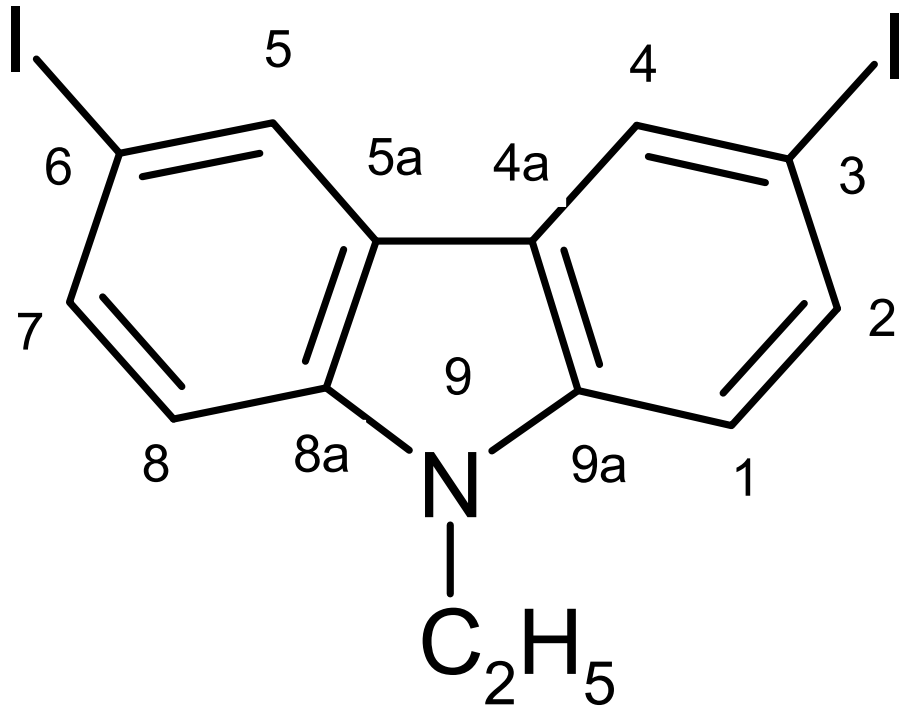

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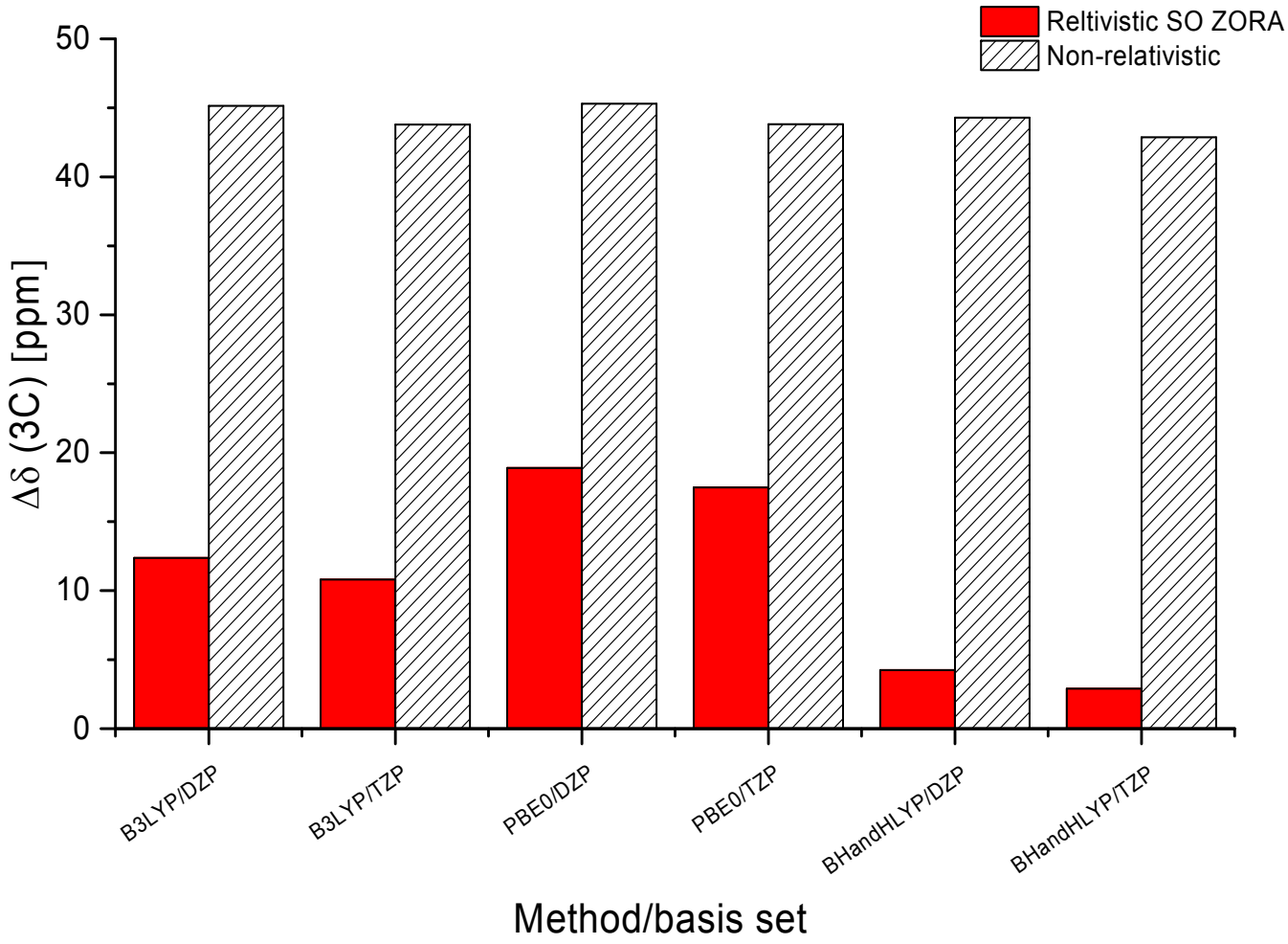

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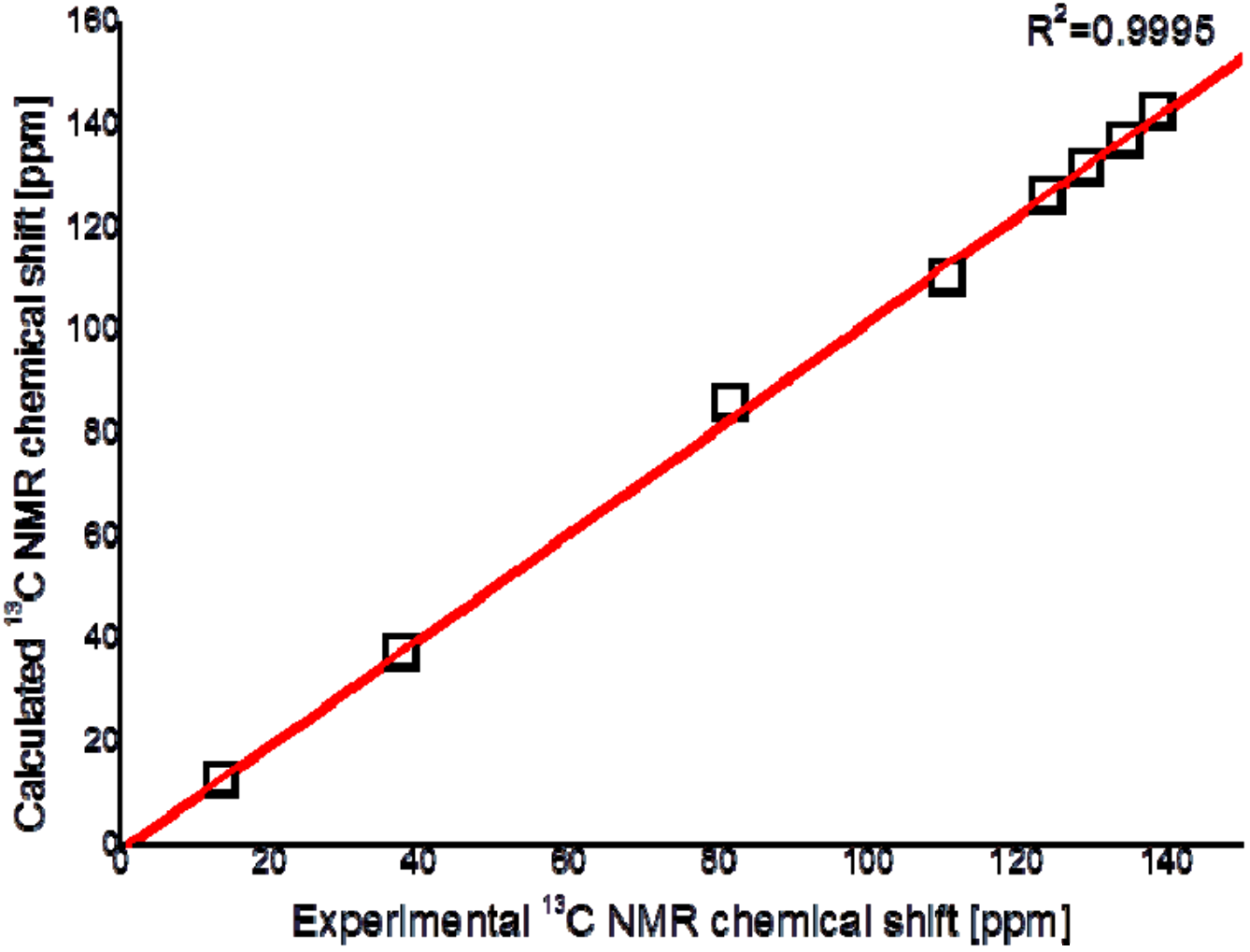

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CONCLUSIONS

- In the case of halogenated carbazoles containing “heavy atoms” (chlorine, bromine and iodine), it is important to employ the SO ZORA approach to accurately assign the observed ^{13}C NMR spectra;
- deviation from the theoretical (non-relativistic) value and observed experimentally is about 45 ppm;
- dramatic changes for ZORA results (a method accounting for relativistic effect) – deviation from the theoretical value and observed experimentally is about 5 ppm;
- a good linear correlation between theoretically predicted and experimental NMR parameters

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ACKNOWLEDGMENT

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Thank's for your attention ☺