THE “LEGO BRICK” APPROACH AT WORK: A COST-EFFECTIVE STRATEGY FOR PREDICTING ACCURATE ROTATIONAL CONSTANTS

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The “Lego brick” model [a] is based on the idea that a molecular system can be seen as formed by different fragments (“Lego bricks”). If accurate semi-experimental equilibrium geometries are available for these fragments, then the template molecule approach [b] can be used to account for the modifications occurring when going from the isolated fragment to the molecular system under investigation. The linear regression model [c] can be employed to correct the linkage between the different fragments. The application of the “Lego brick” approach to substituted (mainly CN and CCH) benzenes and small PAHs will be presented. Rotational constants will be used to test the accuracy of these structures.

[a] A. Melli, F. Tonolo, V. Barone, C. Puzzarini, J. Phys. Chem. A **125**, 9904 (2021)

[b] M. Piccardo, E. Penocchio, C. Puzzarini, M. Biczysko, V. Barone, J. Phys. Chem. A **119**, 2058 (2015)

[c] G. Ceselin, V. Barone, N. Tasinato, J. Chem. Theory Comput. **17**, 7290 (2021)