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Stability prediction in C_{40} fullerenes

MARCELA F. DINCA, SIMONA CIGHER, MONICA ŞTEFU, F. GHERMAN,
KATALIN MIKLOS, CSABA L. NAGY and OLEG URSU

ABSTRACT. The well-known "isolated pentagon rule" IPR is described in quantitative terms provided by the layer matrix of valences, constructed on the dual of the associate molecular graph of fullerenes. The derived pentagon valence pv parameter correlates well (it describes more than 90% of variance) with the $PM3$ heat of formation of small fullerenes C_{40}. The equivalence classes of their vertices, edges and faces are also deducible from some layer matrix invariants. They are important in simulating the $^{13}C\ NMR$ spectrum and/or in predicting the products of addition reactions of fullerenes.

"BABEŞ-BOLYAI" UNIVERSITY
FACULTY OF CHEMISTRY AND CHEMICAL ENGINEERING
ARANY JÁNOS 11, 40028 CLUJ-NAPOCA
ROMANIA
E-mail address: diudea@chem.ubbcluj.ro