

Theoretical study on phosphorus substitutionally doped fullerenes

LILIANA PĂCUREANU, MIRCEA V. DIUDEA and MIRCEA MRACEC

ABSTRACT. Since Karfunkel predicted the stability of azafullerenes by semiempirical calculation, a sustaining effort was paid to quantum-chemical calculation of substitutionally doped fullerenes. While the N and B hetero-fullerenes are the most known, in the last years Si, Co, Ni, Fe, Rh, Ir doped C_{60} have been modeled⁴⁻⁶. This paper reports semiempirical *PM3* calculations of phosphorus substituted fullerenes $C_{60-n}P_n$, $n = 1 - 6$. The *C* by *P* replacement appears to not dramatically influence the thermal stability of substituted C_{60} but electronic structure is changed. The degeneracy of HOMO and LUMO levels is reduced or destroyed while the HOMO-LUMO gap is, in some cases, as high as in the parent C_{60} and consistent with a good kinetic stability. The difference between *C* and *P* electronegativity determines the partial positive charge at phosphorus and a negative charge at the neighboring *C* atoms. The displacement of a number of phosphorus atoms on the same polygon diminishes the positive charge at phosphorus. Angles at phosphorus are larger when phosphorus is on a hexagon. The reverse situation is found for bond length that increases for *P* - *C* [5, 6] with respect to [6, 6] bonds. The bonding energy of P-doped fullerenes decrease with increasing the number of phosphorus atoms, as the strength of *P* - *C* bonds decreases with respect to *C* - *C* bonds. From energetic considerations, we can draw the conclusion that phosphorus doped fullerenes may be stable molecules.

ROMANIAN ACADEMY
INSTITUTE OF CHEMISTRY
MIHAI VITEAZUL 24, 300233 TIMIȘOARA
ROMANIA

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