**Table 1.** Theoretical vertical ionization energies (eV) of the eight highest occupied MOs (denoted as H, …, H-7) and electron affinities of the lowest unoccupied MO (denotes as L) in I computed using the Koopmans' theorem (HF, DFT/B3LYP, DFT/CAMB3LYP) and OVGF methods (cc-pVTZ basis set). The Mulliken populations in the molecular orbitals (percent) are also shown. The calculation results are compared with experimental data [].

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| MO | Type | Ionization energies a | | | | | Atomic populations in MOs b | | | | |
| HF | B3LYP | CAMB3LYP | OVGF | Expt. [] | O | 2Cβ | CγH | 2Me | X |
| L |  |  |  |  |  |  |  |  |  |  |  |
| H |  |  |  |  |  |  |  |  |  |  |  |
| H-1 |  |  |  |  |  |  |  |  |  |  |  |
| H-2 |  |  |  |  |  |  |  |  |  |  |  |
| H-3 |  |  |  |  |  |  |  |  |  |  |  |
| H-4 |  |  |  |  |  |  |  |  |  |  |  |
| H-5 |  |  |  |  |  |  |  |  |  |  |  |
| H-6 |  |  |  |  |  |  |  |  |  |  |  |
| H-7 |  |  |  |  |  |  |  |  |  |  |  |

a OVGF - без сдвига

CAMB3LYP – сдвиг 0.5 эВ надо определить средний сдвиг

B3LYP – сдвиг 2.0 эВ надо определить средний сдвиг

b Вклады CAMB3LYP

X=OH (I), NH2 (II), NH-Me (III), 2 NH-CH2 (IV)

Для соединения IV в шапке указываем 2O 4Cβ 2CγH 4Me X

Таблица 1 – соединение I

Таблица 2 – соединения II и III

Таблица 3 – соединение IV

Орбиталей сколько видим на спектрах + 1