Semiempirical Molecular Dynamics Study of Empty $C_2(3)$-$C_{82}$

Fullerene in Neutral and Charged Forms: Geometrical and Spectroscopic Characterization

Roland Šolc$^1$, Vladimír Lukeš$^{1,*}$, Michal Ilčin$^1$, Peter Rapta$^{1,2}$, Michal Zalibera$^{1,2}$ and Lothar Dunsch$^{2,*}$

$^1$ Institute of Physical Chemistry and Chemical Physics, Slovak University of Technology, Radlinského 9, SK-81 237 Bratislava, Slovakia

$^2$ Department of Electrochemistry and Conducting Polymers, Leibniz-Institute of Solid State and Materials Research, IFW Dresden, Helmholtzstrasse 20, D-01069 Dresden, Germany

*e-mail of corresponding authors: vladimir.lukes@stuba.sk, l.dunsch@ifw-dresden.de
Figure 1S: The visualisation of the optimal AM1 structures and 3-dimensional mapped AM1 electrostatic potentials.