Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS
*J. Serb. Chem. Soc. 79* (11) S158–S159 (2014) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

# The formation of hydride bonds in cationic complexes of $nBeH_2\cdots mX$ with $n$ = 1 or 2, $m$ = 1 or 2 and X = $Li^+$ or $Na^+$

BOAZ G. OLIVEIRA*

*Institute of Environmental Sciences and Sustainable Development (ICADS), Federal University of Bahia, 47801-100, Barreiras – BA, Brazil*

*J. Serb. Chem. Soc.* 79 (11) (2014) 1413–1420

ADDITIONAL PARAMETERS AN D THE COORDINATES OF THE OPTIMIZED GEOMETRIES OF THE $BEH_2\cdots NA^+$, $2BEH_2\cdots NA^+$, $BEH_2\cdots 2NA^+$, $BEH_2\cdots LI^+$, $2BEH_2\cdots LI^+$ AND $BEH_2\cdots 2LI^+$ DIHYDRIDE COMPLEXES OBTAINED BY CALCULATIONS AT THE BHANDHLYP/6-31G(D,P) LEVEL OF THEORY

| I | | | II | | | III | | |
|---|---|---|---|---|---|---|---|---|
| Be | 0.000000 | 0.000000 | Be | 0.000000 | 0.000000 | Be | 0.000000 | 0.023301 |
| | | –2.228812 | | | 3.446979 | | | 0.000000 |
| H | 0.000000 | 0.000000 | H | 0.000000 | 0.000000 | H | 1.312989 | –0.253010 |
| | | –3.535955 | | | 4.754689 | | | 0.000000 |
| H | 0.000000 | 0.000000 | H | 0.000000 | 0.000000 | H | –1.316371 | 0.282492 |
| | | –0.876694 | | | 2.098770 | | | 0.000000 |
| Na | 0.000000 | 0.000000 | Na | 0.000000 | 0.000000 | Na | –3.809335 | 0.800534 |
| | | 1.21162 | | | 0.001256 | | | 0.000000 |
| | | | Be | 0.000000 | 0.000000 | Na | 3.809642 | –0.811688 |
| | | | | | –3.449485 | | | 0.000000 |
| | | | H | 0.000000 | 0.000000 | | | |
| | | | | | –4.757655 | | | |
| | | | H | 0.000000 | 0.000000 | | | |
| | | | | | –2.099599 | | | |
| Energy = –177.9874194 Hartree | | | Energy = –193.9091853 Hartree | | | Energy = –339.98752 Hartree | | |
| ZPE = 38849.9 J $mol^{-1}$ | | | ZPE = 78231.9 J $mol^{-1}$ | | | ZPE = 38931.2 J $mol^{-1}$ | | |
| Dipole = 4.2231 Debye** | | | Dipole = 0.0022 Debye | | | Dipole = 0.0197 Debye | | |
| Imaginary frequency = 0 | | | Imaginary frequency = 0 | | | Imaginary frequency = 1 | | |

* E-mail: boazgaldino@gmail.com
** 1 C m = $3\times10^{29}$ Debye

| IV | | | V | | | VI | | |
|---|---|---|---|---|---|---|---|---|
| Be | 0.000000 | 0.000000 | Be | 0.000000 | 0.000000 | Be | 0.000000 | 0.002194 |
| | 1.045934 | | | 3.113729 | | | 0.000000 | |
| H | 0.000000 | 0.000000 | H | 0.000000 | 0.000000 | H | 1.021994 | –0.873035 |
| | 2.351700 | | | 4.420169 | | | 0.000000 | |
| H | 0.000000 | 0.000000 | H | 0.000000 | 0.000000 | H | –1.022169 | 0.877178 |
| | –0.312529 | | | 1.762821 | | | 0.000000 | |
| Li | 0.000000 | 0.000000 | Be | 0.000000 | 0.000000 | Li | –2.602736 | 2.221883 |
| | –2.074303 | | | –3.113728 | | | 0.000000 | |
| | | | H | 0.000000 | 0.000000 | Li | 2.602794 | –2.226190 |
| | | | | –4.420169 | | | 0.000000 | |
| | | | H | 0.000000 | 0.000000 | | | |
| | | | | –1.762820 | | | | |
| | | | Li | 0.000000 | 0.000000 | | | |
| | | | | –0.000001 | | | | |
| Energy = –23.2126542 Hartree | | | Energy = –39.1426661 Hartree | | | Energy = –30.4242061 Hartree | | |
| ZPE = 39836.4 J mol-1 | | | ZPE = 80967.2 J mol-1 | | | ZPE = 41292.0 J mol-1 | | |
| Dipole = 8.0368 Debye | | | Dipole = 0.0000 Debye | | | Dipole = 0.0211 Debye | | |
| Imaginary frequency = 0 | | | Imaginary frequency = 0 | | | Imaginary frequency = 0 | | |