Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 85 (5) S212–S213 (2020)
Supplementary material

SUPPLEMENTARY MATERIAL TO

Decomposition mechanism of dihydroxylammonium 5,5'-bis(tetrazole)-1,1'-diolate on Al(111) surface by periodic DFT calculation

YING ZHAO[1], XIAOLING XING[2], SHENGXIANG ZHAO[2] and XUEHAI JU[1]*

[1]*School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China and* [2]*Xi'an Modern Chemistry Research Institute, Xi'an 710065, P. R. China*

J. Serb. Chem. Soc. 85 (5) (2020) 651–660

TABLE S-I. Equilibrium structure based on different methods and experimental parameters of TKX-50 molecule; $r_{GGA\text{-}PBE}$, $r_{GGA\text{-}pw91}$, $r_{GGA\text{-}RPBE}$, $r_{GGA\text{-}WC}$ and $r_{experiment}$ are the bond lengths in Å obtained from GGA-PBE, GGA-PW91, GGA-RPBE, GGA-WC and experiment, respectively

Species	$r_{GGA\text{-}PBE}$	$r_{GGA\text{-}pw91}$	$r_{GGA\text{-}RPBE}$	$r_{GGA\text{-}WC}$	$r_{experiment}$
O_1-N_1, O'_1-N'_1	1.316	1.332	1.335	1.323	1.317
C_1-N_1, C'_1-N'_1	1.366	1.366	1.368	1.364	1.336
N_1-N_2, N'_1-N'_2	1.371	1.366	1.367	1.333	1.343
N_2-N_3, N'_2-N'_3	1.337	1.335	1.335	1.358	1.306
N_3-N_4, N'_3-N'_4	1.357	1.360	1.361	1.351	1.351
N_4-C_1, N'_4-C'_1	1.349	1.351	1.353	1.351	1.332
C_1-C'_1	1.437	1.428	1.432	1.428	1.444
N_5-O_2	1.415	1.427	1.431	1.416	1.408
N_5-H_{1A}	1.120	1.285	1.325	1.242	0.970
N_5-H_{1B}	1.030	1.035	1.033	1.038	0.880
N_5-H_{1C}	1.030	1.034	1.034	1.038	0.87
O_2-H_2	1.083	1.041	1.034	1.051	0.90

TABLE S-II. Al cell parameters (*a*, b, *c* in Å) optimized by different methods

Method	*a*	*b*	*c*
GGA-PBE	4.058	4.058	4.058
GGA-PW91	4.062	4.062	4.062
GGA-RPBE	4.145	4.145	4.145
GGA-WC	4.152	4.152	4.152
Experiment	4.050	4.050	4.050

* Corresponding author. E-mail: xhju@njust.edu.cn

TABLE S-III. Hirshfeld atomic charge (charge in e) of TKX-50 anion in adsorption of Al(111)

Configuration	O_1	O'_1	N_1	N'_1	N_2	N'_2	N_3	N'_3	N_4	N'_4	C_1	C'_1
Initial	−0.24	−0.14	0.09	0.11	−0.10	−0.04	−0.10	−0.16	−0.28	−0.08	0.03	0.08
T1	−0.21	−0.21	−0.11	0.08	−0.08	−0.05	−0.24	−0.05	−0.27	−0.03	0.01	0.07
T2	−0.31	−0.14	−0.28	0.10	−0.25	−0.04	−0.04	−0.08	−0.10	−0.07	0.05	0.07
V1	−0.23	−0.14	0.07	0.11	−0.25	−0.03	−0.04	−0.06	−0.12	−0.02	0.03	0.09
V2	−0.20	−0.15	0.01	0.10	−0.25	−0.04	−0.22	−0.08	−0.09	−0.08	0.05	0.07
P	−0.32	−0.32	−0.15	−0.27	−0.1	−0.25	−0.09	−0.10	−0.10	−0.01	0.05	0.06

TABLE S-IV. Hirshfeld atomic charge (e) of hydroxylammonium anion in adsorption of Al(111)

Configuration	O_2	O'_2	N_5	N'_5	H_{1A}	H'_{1A}	H_{1B}	H'_{1B}	H_{1C}	H'_{1C}	H_2	H'_2
Initial	−0.19	−0.17	−0.02	−0.04	0.09	0.09	0.17	0.15	0.17	0.15	0.08	0.10
T1	−0.21	−0.14	−0.08	0.04	0.09	0.10	0.12	0.17	0.12	0.17	0.08	0.01
T2	−0.13	−0.18	0.01	−0.05	0.09	0.08	0.16	0.14	0.09	0.14	0.09	0.10
V1	−0.20	−0.17	−0.06	−0.04	0.09	0.09	0.13	0.13	0.13	0.15	0.08	0.01
V2	−0.17	−0.18	0.03	−0.05	0.09	0.09	0.17	0.14	0.17	0.14	0.09	0.10
P	−0.17	−0.36	−0.09	−0.15	0.09	0.15	0.15	0.15	0.12	0.14	0.13	0.14