Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2016

Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Impact of the Si/Al ratio on the selective capture of iodine compounds in silver-mordenite: a periodic DFT study—Supporting Information

Siwar Chibani,*[a] Mouheb Chebbi,[a] Sébastien Lebègue,[b] Laurent Cantrel,[c] Michael Badawi*[a]

Table S1 The Al−Ag distances (Å) in the Ag-MOR with a Al/Si ratio of 47 (1 Ag^+ per cell) calculated for bare external cations alone and after adsorption of ICH_3, I_2, CO and water.

Sites	Ag^+	ICH_3	I_2	CO	H_2O
T1-E	3.02	3.08	3.07	3.06	3.00
T2-D	3.14	3.01	3.01	3.00	3.09
T4-D	3.09	3.11	3.07	3.07	3.12
T2-E	3.13	3.03	3.05	3.03	3.06
T4-E	3.00	2.93	2.90	2.89	3.04

Table S2 The Al−Ag distances (Å) in the Ag-MOR with a Al/Si ratio of 23 (2 Ag^+ per cell) calculated for bare external cations alone and after adsorption of ICH_3, I_2, CO and water with the adsorption modes.

Sites	Cations		ICH_3			I_2			CO			H_2O		
	$Ag^+(1)$	$Ag^+(2)$	Ads. Modes	$Ag^+(1)$	$Ag^+(2)$	Ads. Modes	$Ag^+(1)$	$Ag^+(2)$	Ads. Modes	$Ag^+(1)$	$Ag^+(2)$	Ads. Modes	$Ag^+(1)$	$Ag^+(2)$
T1(5-II)-E/T1(7-I)-E	3.02	2.98	A	3.16	3.12	A	3.16	3.08	A	3.03	3.00	I	3.08	3.00
T1(5-II)-E/T1(8-II)-E	3.02	3.01	I	3.10	2.99	M	3.09	3.08	I	3.04	3.00	I	2.99	3.08
T1(5-II)-E/T1(8-I)-E	2.99	3.00	I	2.98	3.00	I	3.07	3.01	I	3.03	3.00	I	3.07	3.00
T1(5-II)-E/T1(5-I)-E	3.02	3.23	A	3.09	3.33	A	3.09	3.34	A	3.09	3.21	I	3.20	3.12
T1(5-II)-E/T1(6-I)-E	2.99	3.00	M	3.14	3.11	M	3.10	3.04	I	3.04	3.00	I	2.99	3.08
T4(1-III)-D/T4(11-II)-D	3.10	3.08	M	3.13	3.04	M	2.97	3.13	I	3.11	3.02	I	3.12	3.12
T4(1-III)-D/T4(12-II)-D	3.07	3.08	M	3.04	3.03	M	3.00	3.03	I	2.99	3.07	I	3.15	3.10
T4(1-III)-E/T1(5-II)-E	3.09	3.04	A	2.97	3.17	A	3.17	2.95	A	2.91	3.04	M	3.09	3.06
T4(1-III)-D/T4(2-I)-D	3.07	3.05	A	3.09	3.09	A	3.09	3.10	A	3.09	3.08	A	3.08	3.11
T4(1-III)-D/T4(12-II)-E	3.03	3.08	I	2.92	3.09	I	2.87	3.09	I	2.90	3.10	I	3.04	3.11
T4(1-III)-D/T4(1-I)-D	3.04	3.05	A	3.10	3.10	A	3.08	3.09	A	3.07	3.06	A	3.08	3.08
T4(1-III)-D/T1(5-II)-E	3.12	3.01	A	3.04	3.05	A	3.00	3.05	A	2.98	3.01	M	3.15	3.06
T4(1-III)-D/T4(1-I)-E	2.99	3.07	A	2.84	3.17	A	3.16	2.83	I	3.09	2.99	I	3.07	3.12
T4(1-III)-D/T4(11-II)-E	3.01	3.10	M	2.91	3.04	M	2.91	3.04	I	3.02	3.01	I	3.06	3.03
T4(1-III)-D/T4(2-I)-E	3.01	3.07	I	3.00	3.10	I	3.00	3.09	I	3.02	3.09	I	3.12	3.20
T4(1-III)-E/T4(12-II)-E	3.03	3.02	M	3.00	3.03	M	3.02	3.00	I	3.02	3.08	I	3.02	3.01
T4(1-III)-E/T4(2-I)-E	3.01	2.98	I	3.00	3.01	I	3.00	3.02	I	3.00	2.94	I	3.05	3.00
T4(1-III)-E/T4(1-I)-E	2.70	2.99	I	3.01	3.02	I	2.88	3.01	I	2.99	3.01	I	2.99	3.08
T4(1-III)-E/T4(11-II)-E	2.70	3.03	M	2.97	2.90	M	2.78	3.01	I	3.02	3.01	I	2.96	3.01

[a] *Laboratoire de Chimie et Physique—Approche Multi échelle des Milieux Complexe (LCP-A2MC, EA 4632), Institut Jean-Barriol FR2843 CNRS, Université de Lorraine, Rue Victor Demange, 57500 Saint-Avold, France. E-mail: siwar.chibani@univ-lorraine.fr; E-mail: michael.badawi@univ-lorraine.fr*

[b] *Laboratoire de Cristallographie, Résonance Magnétique et Modélisations (CRM2, UMR CNRS 7036) Institut Jean Barriol, Université de Lorraine, BP 239, Boulevard des Aiguillettes 54506 Vandoeuvre-lès-Nancy,France.*

[c] *Institut de Radioprotection et de Sûreté Nucléaire, CE Cadarache, F-13115 Saint Paul lez Durance, France.*

Table S3 The Al−Ag distances (Å) in the Ag-MOR with a Al/Si ratio of 11 (4 Ag^+ per cell) calculated for bare external cations alone and after adsorption of ICH_3, I_2, CO and water

Sites	Al−Ag	Ag^+	ICH_3	I_2	CO	H_2O
T1(6−I, 7−I, 5−II, 8−II)-E	Al−Ag1	3.02	3.09	3.14	3.01	3.01
	Al−Ag2	2.96	3.15	2.75	2.97	2.98
	Al−Ag3	2.97	3.02	3.11	2.98	2.98
	Al−Ag4	3.02	2.95	3.07	3.08	
T1(5−I, 6−I, 5−II, 8−II)-E	Al−Ag1	3.15	3.00	3.06	2.98	3.12
	Al−Ag2	2.97	3.05	3.18	3.10	2.98
	Al−Ag3	2.98	3.14	3.10	3.16	3.08
	Al−Ag4	2.99	3.08	3.20	3.05	3.22
T4(1−I, 11−II, 1−III, 11−IV)-D	Al−Ag1	3.10	3.13	3.30	2.98	3.08
	Al−Ag2	3.06	3.10	3.03	3.07	3.00
	Al−Ag3	3.07	3.12	3.06	3.08	3.10
	Al−Ag4	3.05	3.08	3.06	3.06	3.09
T4(1−I, 12−II, 1−III, 12−IV)-D	Al−Ag1	3.06	3.06	3.03	3.07	3.06
	Al−Ag2	3.06	3.03	3.04	3.05	3.05
	Al−Ag3	3.06	3.08	3.07	3.08	3.04
	Al−Ag4	3.05	3.12	3.06	3.07	3.08
T4(1−I, 12−II, 1−III, 12−IV)-E	Al−Ag1	3.05	3.10	3.03	3.07	3.08
	Al−Ag2	2.71	3.03	3.05	3.03	3.07
	Al−Ag3	3.05	3.08	3.05	3.04	3.03
	Al−Ag4	3.02	3.05	3.03	3.05	3.00
T4(1−I, 11−II, 1−III, 11−IV)-E	Al−Ag1	3.02	3.04	2.99	2.95	3.04
	Al−Ag2	3.02	2.70	2.70	2.71	3.04
	Al−Ag3	2.69	3.03	2.98	2.69	3.14
	Al−Ag4	2.70	3.05	2.74	2.96	2.75

Table S4 The Al−Ag distances (Å) in the Ag-MOR with a Al/Si ratio of 5 (8 Ag^+ per cell) calculated for bare external cations alone and after adsorption of ICH_3, I_2, CO and water

Al−Ag	Ag^+	ICH_3	I_2	CO	H_2O
Al−Ag1	3.26	3.02	3.17	2.99	3.03
Al−Ag2	3.07	2.98	3.03	2.98	2.99
Al−Ag3	3.03	3.31	2.99	3.08	3.32
Al−Ag4	2.96	2.95	3.15	3.02	2.95
Al−Ag5	3.01	3.04	3.21	2.98	3.04
Al−Ag6	3.01	3.12	3.21	3.04	3.04
Al−Ag7	3.02	3.17	3.32	3.23	3.24
Al−Ag8	3.01	3.22	3.27	3.09	3.18

Table S5 I−C and I−I distances (Å) for ICH_3 and I_2 in gas phase and in Ag-MOR with a Si/Al ratio of 47.

Sites	I−C (Å)	I−I (Å)
Gas phase	2.152	2.684
T1-E(MC)	2.160	2.696
T2-D(MC)	2.165	2.704
T4-D(MC)	2.166	2.704
T2-E(MC)	2.163	2.708
T4-E(MC)	2.168	2.702

This journal is © The Royal Society of Chemistry [year]

Table S6 I−C and I−I distances (Å) for ICH_3 and I_2 in gas phase and in Ag-MOR with a Si/Al ratio of 23.

Sites	I−C (Å)	I−I (Å)
Gas phase	2.152	2.684
T1(5-II)-E/T1(7-I)-E	2.170	2.726
T1(5-II)-E/T1(8-II)-E	2.161	2.708
T1(5-II)-E/T1(8-I)-E	2.164	2.708
T1(5-II)-E/T1(5-I)-E	2.166	2.731
T1(5-II)-E/T1(6-I)-E	2.164	2.698
T4(1-III)-D/T4(11-II)-D	2.172	2.722
T4(1-III)-D/T4(12-II)-D	2.177	2.744
T4(1-III)-E/T1(5-II)-E	2.173	2.723
T4(1-III)-D/T4(2-I)-D	2.177	2.776
T4(1-III)-D/T4(12-II)-E	2.160	2.705
T4(1-III)-D/T4(1-I)-D	2.176	2.732
T4(1-III)-D/T1(5-II)-E	2.178	2.723
T4(1-III)-D/T4(1-I)-E	2.169	2.723
T4(1-III)-D/T4(11-II)-E	2.176	2.720
T4(1-III)-D/T4(2-I)-E	2.163	2.705
T4(1-III)-E/T4(12-II)-E	2.176	2.713
T4(1-III)-E/T4(2-I)-E	2.165	2.702
T4(1-III)-E/T4(1-I)-E	2.167	2.776
T4(1-III)-E/T4(11-II)-E	2.169	2.715

Table S7 I−C and I−I distances (Å) for ICH_3 and I_2 in gas phase and in Ag-MOR with Si/Al ratio of 11 and 5.

Ratio	Sites	I−C (Å)	I−I (Å)
Gas phase	2.152	2.684	
11	T1(6−I, 7−I, 5−II, 8−II)-E	2.166	2.856
	T1(5−I, 6−I, 5−II, 8−II)-E	2.168	3.059
	T4(1−I, 11−II, 1−III, 11−IV)-D	2.182	4.411
	T4(1−I, 12−II, 1−III, 12−IV)-D	2.172	4.372
	T4(1−I, 12−II, 1−III, 12−IV)-E	2.177	2.768
	T4(1−I, 11−II, 1−III, 11−IV)-E	2.179	2.816
5	T1-E	2.178	4.566