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Chemical bond in FmO_2

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Table S1 MO compositions (shares) and energies E_0 [a](eV) for the FmO_8 (D_{4h}) cluster at R_{Fm-O} = 0.2279 nm and photoemission cross-sections σ_i[b].

MO		- E_0, eV	MO composition												
			Fm										O		
			6s	$6p_{1/2}$	$6p_{3/2}$	$6d_{3/2}$	$6d_{5/2}$	7s	$5f_{5/2}$	$5f_{7/2}$	$7p_{1/2}$	$7p_{3/2}$	2s	$2p_{1/2}$	$2p_{3/2}$
			σ_i [b] 1.28	0.88	1.48	0.64	0.56	0.10	7.17	6.66	0.04	0.06	0.96	0.07	0.07
OVMO	25 γ_6^+	-10.53				0.51	0.35						0.05		0.09
	22 γ_7^+	-10.50				0.40	0.47						0.05	0.03	0.05
	21 γ_7^+	-10.42				0.12	0.75						0.05	0.05	0.03
	24 γ_6^+	-8.62						0.88					0.06	0.02	0.04
	23 γ_6^+	-7.59				0.35	0.52							0.04	0.09
	20 γ_7^+	-7.58				0.35	0.52							0.04	0.09
	28 γ_6^-	-7.04									0.91		0.04	0.04	0.01
	27 γ_6^-	-4.92										0.90	0.02		0.08
	24 γ_7^-	-4.82										0.90	0.02		0.08
	23 γ_7^-	-0.71							0.03	0.53			0.01	0.19	0.24
	26 γ_6^-	-0.07								0.72				0.25	0.03
	22 γ_7^- [c]	0.00			0.01				0.01	0.70		0.01		0.06	0.21
	25 γ_6^-	0.00			0.01				0.01	0.70		0.01		0.03	0.24
	24 γ_6^-	0.78												0.32	0.68
	21 γ_7^-	0.79												0.32	0.68
	20 γ_7^-	0.99			0.02				0.13	0.19		0.01		0.07	0.58
	23 γ_6^-	0.99			0.02				0.12	0.19		0.01	0.01	0.06	0.59
	22 γ_6^+	1.02												0.16	0.84
	19 γ_7^+	1.02												0.14	0.86
	21 γ_6^+	1.04												0.66	0.34
	19 γ_7^-	1.22							0.24	0.30				0.03	0.43
	18 γ_7^+	1.28												0.03	0.97
	17 γ_7^+	1.32												0.50	0.50
	20 γ_6^+	1.32												0.51	0.49
	22 γ_6^-	1.89								0.27	0.02			0.69	0.02
	21 γ_6^-	1.99			0.01				0.05			0.03		0.21	0.70
	18 γ_7^-	1.99			0.01				0.05			0.03		0.40	0.51
	20 γ_6^-	2.50							0.01		0.03		0.01	0.21	0.74
	17 γ_7^-	2.56							0.35	0.09		0.01		0.09	0.46
	19 γ_6^-	2.56							0.35	0.09		0.01		0.10	0.45
	16 γ_7^-	2.67							0.17	0.16				0.59	0.08
	16 γ_7^+	2.69				0.01	0.07						0.01	0.56	0.35
	19 γ_6^+	2.71				0.05	0.03						0.01	0.01	0.90
	15 γ_7^+	2.73				0.03	0.05						0.01	0.35	0.56
	18 γ_6^+	3.11						0.05					0.01	0.32	0.62
	15 γ_7^-	3.22							0.46	0.02				0.10	0.42
	18 γ_6^-	3.22							0.45	0.03				0.08	0.44
	14 γ_7^-	3.36							0.56					0.13	0.31
	14 γ_7^+	3.59				0.06	0.08							0.28	0.58
	17 γ_6^+	3.61				0.06	0.08							0.29	0.57

IVMO	17 γ_6^-	14.47			0.47							0.03	0.48	0.01	0.01
	13 γ_7^-	14.48			0.47							0.03	0.48	0.01	0.01
	12 γ_7^-	15.78							0.01	0.01			0.98		
	13 γ_7^+	16.23					0.04						0.95		0.01
	16 γ_6^+	16.23				0.03	0.02						0.95		
	12 γ_7^+	16.23				0.03	0.02						0.95		
	16 γ_6^-	16.39		0.01							0.04		0.95		
	15 γ_6^+	16.95						0.07					0.93		
	15 γ_6^-	18.14			0.49							0.01	0.48	0.01	0.01
	11 γ_7^-	18.15			0.49							0.01	0.48	0.01	0.01
	14 γ_6^-	31.67		0.99									0.01		
	14 γ_6^+	55.51	1.00												

[a)]energies are reduced by the absolute values (shifted upward) by 15.44 eV;
[b)]photoemission cross-section σ_i (kiloBarn per electron) for O [S1] and for Fm [S2].
[c)]filling number for all the filled orbitals is 2.

References

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