Supporting Information

Theoretical evaluation of trends in the bond distances and dissociation energies of actinide oxides AnO and AnO_2

By:
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STable1. Computed molecular properties of AnO species

An	m	ΔE (kJ/mol)	Bond (Å)	1-electron orbitals
Bk	8	0.0	1.835	$5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+2}$, $5f_{+3}$, 7s
		5.9	1.827	$5f_{-3}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+2}$, $5f_{+3}$, 7s
		73.4	1.849	$5f_{-3}$, $5f_{-2}$, $5f_{-1}$, $5f_{+1}$, $5f_{+2}$, $5f_{+3}$, 7s
	6	20.4	1.835	$5f_{-3}$, $5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+2}$, $7s^{\beta}$
		27.4	1.828	$5f_{-3}$, $5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+3}$, $7s^{\beta}$
		80.0	1.844	$5f_{-3}$, $5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+2}$, $5f_{+3}$, $7s^{\beta}$
		108.7	1.859	$5f_{-3}$, $5f_{-2}$, $5f_{-1}$, $5f_{+1}$, $5f_{+2}$, $5f_{+3}$, $7s^{\beta}$
	4	225.6	1.826	$5f_{-3}$, $5f_{-2}$, $5f_{+1}$, $5f_{+2}$, $7s^{\beta}$
	10	256.7	1.803	$6d_{+2}$, $5f_{-3}$, $5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+2}$, $5f_{+3}$, 7s
Cf	7	0.0	1.822	$5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+3}$, 7s
		31.5	1.836	$5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+2}$, $5f_{+3}$, 7s
		32.2	1.836	$5f_{-3}$, $5f_{-2}$, $5f_{-1}$, 5f0, $5f_{+2}$, 7s
		42.7	1.836	$5f_{-1}$, $5f_{-2}$, $5f_0$, $5f_{+1}$, $5f_{+2}$, 7s
		45.2	1.814	$5f_{-3}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+3}$, 7s
		71.3	1.834	$5f_{-3}$, $5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+3}$, 7s
		130.0	1.846	$5f_{-3}$, $5f_{-2}$, $5f_0$, $5f_{+2}$, $5f_{+3}$, 7s
	5	14.0	1.827	$5f_{-3}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+2}$, $7s^{\beta}$
		42.8	1.840	$5f_{-3}$, $5f_{-2}$, $5f_0$, $5f_{+1}$, $5f_{+2}$, $7s^{\beta}$
		58.6	1.819	$5f_{-3}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+3}$, $7s^{\beta}$
		92.8	1.840	$5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+2}$, $7s^{\beta}$
		100.7	1.886	$5f_{-3}$, $5f_0$, $5f_{+2}$, $5f_{+3}$
		104.7	1.849	$5f_{-3}$, $5f_{-1}$, $5f_{+1}$, $5f_{+2}$, $5f_{+3}$, $7s^{\beta}$
	3	237.5	1.848	$5f_{-3}$, $5f_{-1}$, $5f_{+1}$, $7s^{\beta}$
	9	336.7	1.804	$6d_{+2}$, $5f_{-3}$, $5f_{-2}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, $5f_{+2}$, 7s
Es	6	0.0	1.822	$5f_{-3}$, $5f_{-2}$, $5f_0$, $5f_{+3}$, 7s
		27.0	1.845	$5f_{-3}$, $5f_{-2}$, $5f_{-1}$, $5f_{+1}$, 7s
		28.2	1.810	$5f_{-3}$, $5f_{-1}$, $5f_0$, $5f_{+1}$, 7s
		51.7	1.837	$5f_{-2}$, $5f_0$, $5f_{+2}$, $5f_{+3}$, 7s
		69.5	1.828	$5f_{-1}$, $5f_{-2}$, $5f_0$, $5f_{+1}$, 7s

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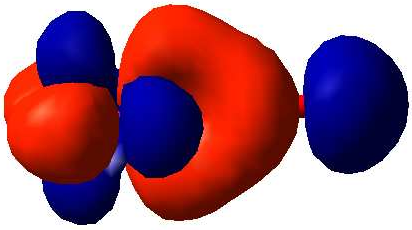
		91.2	1.822	$5f_{-2}$, $5f_{-1}$, $5f_{0}$, $5f_{+1}$, 7s
		108.6	1.852	$5f_{-2}$, $5f_{-1}$, $5f_{+1}$, $5f_{+2}$, 7s
	4	0.2	1.835	$5f_{-1}$, $5f_{0}$, $5f_{+1}$, $5f_{+2}$, $7s^{\beta}$
		20.1	1.839	$5f_{-1}$, $5f_{0}$, $5f_{+1}$, $5f_{+3}$, $7s^{\beta}$
		104.0	1.853	$5f_{-2}$, $5f_{-1}$, $5f_{0}$, $5f_{+1}$, $7s^{\beta}$
		109.8	1.826	$5f_{-3}$, $5f_{-1}$, $5f_{0}$, $5f_{+3}$, $7s^{\beta}$
	2	102.0	1.829	$5f_{-3}$, $5f_{0}^{\beta}$, $5f_{+1}$, $5f_{+2}$, $7s^{\beta}$
	8	418.5	1.967	$6d_{-2}$, $5f_{-3}$, $5f_{-2}$, $5f_{0}$, $5f_{+1}$, 7s, O2pz
Fm	3	0.0	1.850	$5f_{-3}$, $5f_{-2}$, $5f_{0}$, $7s^{\beta}$
		17.5	1.892	$5f_{-2}$, $5f_{0}$
		22.2	1.881	$5f_{-1}$, $5f_{+1}$
		28.9	1.860	$5f_{-3}$, $5f_{0}$
		43.4	1.860	$5f_{-2}$, $5f_{0}$, $5f_{+2}$, $7s^{\beta}$
		47.3	1.856	$5f_{-2}$, $5f_{0}$, $5f_{+1}$, $7s^{\beta}$
	5	17.8	1.823	$5f_{-2}$, $5f_{0}$, $5f_{+3}$, 7s
		33.5	1.848	$5f_{-2}$, $5f_{-1}$, $5f_{+1}$, 7s
		66.2	1.829	$5f_{-2}$, $5f_{0}$, $5f_{+2}$, 7s
	1	182.9	1.860	($5f_{0}$, 7s empty)
Md	2	0.0	1.898	$5f_{-1}$
		3.8	1.899	$5f_{0}$
		7.1	1.901	$5f_{+2}$
		32.2	1.890	$5f_{+3}$
	4	64.2	1.845	$5f_{-1}$, $5f_{0}$, 7s
		70.9	1.878	$5f_{-1}$, $5f_{+1}$, 7s
		91.7	2.169	$5f_{-1}$, 7s, $O2p_{y}$
	6	547.4	1.963	$5f_{-1}$, $5f_{+1}$, 7s, $7p_{x}$, $O2p_{z}$
No	1	0.0	1.923	$5f_{0}$, 7s2
	3	65.3	2.163	7s, $O2p_{x}$
	5	594.7	2.264	$6d_{+2}$, 7s, $O2p_{y}$, $O2p_{x}$
Lr	2	0.0	1.871	7s
	4	344.0	2.116	$6d_{+2}$, 7s, $O2p_{y}$
	6	916.8	2.896	$6d_{-2}$, $6d_{+2}$, 7s, $O2p_{x}$, $O2p_{y}$

STabl2. Computed molecular properties of AnO_2 species

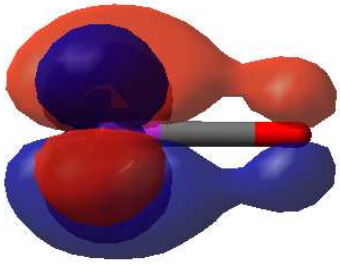
An	m	ΔE (kJ/mol)	Bond (Å)	Angle (°)	1-electron orbitals
Bk	6	0.0	1.820	180.0	$5f_{-3}$ $5f_{-1}$ $5f_{+1}$ $5f_{+2}$ $5f_{+3}$
		0.0	1.820	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{-1}$ $5f_{+1}$ $5f_{+3}$
		0.8	1.834	180.0	$5f_{-2}$ $5f_{-1}$ $5f_{+1}$ $5f_{+2}$ $5f_{+3}$
		0.8	1.834	180.0	$5f_{-2}$ $5f_{-1}$ $5f_{+1}$ $5f_{+2}$ $5f_{-3}$
	4	134.4	1.808	180.2	$5f_{-3}^{0}$ $5f_{-2}$ $5f_{-1}$ $5f_{0}$ $5f_{+2}$ $5f_{+3}^{\beta}$
	8	76.9	1.783	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{-1}$ $5f_{+1}$ $5f_{+2}$ $5f_{+3}$ 7s
Cf	5	0.0	1.817	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{-1}$ $5f_{+1}$
		0.1	1.816	180.0	$5f_{-3}$ $5f_{-1}$ $5f_{+1}$ $5f_{+2}$
		33.7	1.803	180.0	$5f_{-3}$ $5f_{-1}$ $5f_{+1}$ $5f_{+3}$
		63.0	1.840	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{+1}$ $5f_{+2}$
		63.1	1.840	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{-1}$ $5f_{+2}$
		112.3	1.826	180.0	$5f_{-3}$ $5f_{-1}$ $5f_{+2}$ $5f_{+3}$
		112.9	1.831	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{-1}$ $5f_{+3}$
		120.6	1.829	180.0	$5f_{-2}$ $5f_{-1}$ $5f_{+1}$ $5f_{+2}$
	3	185.0	1.784	180.0	$5f_{-3}$ $5f_{-1}^{0}$ $5f_{+1}$
	7	124.9	1.780	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{-1}$ $5f_{+1}$ $5f_{+2}$ 7s
		128.3	1.769	180.0	$5f_{-3}$ $5f_{-1}$ $5f_{+1}$ $5f_{+2}$ $5f_{+3}$ 7s
		128.3	1.769	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{-1}$ $5f_{+1}$ $5f_{+3}$ 7s
	9	269.9	1.844	106.7	$6d_{-1}$ $5f_{-2}$ $5f_{-1}$ $5f_{0}$ $5f_{+1}$ $5f_{+2}$ $5f_{+3}$ 7s $7p_{y}^{\beta}$ O 2s
Es	4	0.0	1.795	180.0	$5f_{-1}$ $5f_{+1}$ $5f_{+3}$
		6.9	1.817	180.0	$5f_{-1}$ $5f_{+1}$ $5f_{+2}$
		6.9	1.817	180.0	$5f_{-2}$ $5f_{-1}$ $5f_{+1}$
		42.0	1.818	180.0	$5f_{+1}$ $5f_{+2}$ $5f_{+3}$
		42.3	1.824	180.0	$5f_{-2}$ $5f_{+1}$ $5f_{+3}$
		81.9	1.817	180.0	$5f_{-2}$ $5f_{-1}$ $5f_{+1}$
		98.3	1.841	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{+2}$
		98.8	1.806	180.0	$5f_{-2}$ $5f_{-1}$ $5f_{+1}$
		99.2	1.842	180.0	$5f_{-2}$ $5f_{+2}$ $5f_{+3}$
		122.3	1.810	180.0	$5f_{-3}$ $5f_{+1}$ $5f_{+3}$
	2	83.3	1.788	180.0	$5f_{-3}^{\beta}$ $5f_{-1}$ $5f_{+1}$
		83.5	1.803	180.0	$5f_{-1}^{\beta}$ $5f_{+1}$ $5f_{+3}$
		99.5	1.811	180.0	$5f_{-2}$ $5f_{-1}^{\beta}$ $5f_{+3}$
		135.0	1.812	180.0	$5f_{-3}^{\beta}$ $5f_{-1}$ $5f_{+2}$
		135.1	1.813	180.0	$5f_{-2}$ $5f_{+1}$ $5f_{+3}^{\beta}$
		175.4	1.798	180.0	$5f_{-1}$ $5f_{+1}$ $5f_{+2}^{\beta}$
		184.5	1.803	180.0	$5f_{-3}$ $5f_{+1}$ $5f_{+3}^{\beta}$
	6	97.5	1.891	113.3	$6d_{-1}$ $5f_{-2}$ $5f_{-1}$ $5f_{+2}$ $5f_{+3}$
	8	357.1	1.945	180.0	$5f_{-3}$ $5f_{-2}$ $5f_{+3}$ 7s + O: $2p_{x}$ $2p_{y}$ $2p_{z}$
Fm	3	0.0	1.791	180.0	$5f_{-1}$ $5f_{+3}$
		0.1	1.794	180.0	$5f_{-3}$ $5f_{+1}$
		3.3	1.797	180.0	$5f_{+1}$ $5f_{+3}$
		18.1	1.813	180.0	$5f_{+2}$ O: $2p_{x}$
		20.7	1.815	180.0	$5f_{-2}$ O: $2p_{x}$
		32.5	1.780	180.0	$5f_{-1}$ $5f_{+1}$

		82.9	1.834	180.0	$5f_{-2}$ $5f_{+2}$
	1	157.5	1.789	180.0	$5f_0^0$
	5	54.7	1.879	146.6	$5f_{-3}$ $5f_{-1}$ $5f_{+2}$ + O: $2p_y$
		61.8	1.878	130.0	$5f_{-3}$ $5f_{-2}$ $5f_0$ $7s^{\beta}$ + O: $2p_x$ $2p_y$
		60.8	1.879	129.1	$5f_{-1}$ $5f_{+2}$ $5f_{+3}$ + O: $2p_y$
		104.6	1.866	116.6	$5f_{-3}$ $5f_{-2}$ $5f_{-1}$ + O: $2p_y$
	7	369.1	1.918	180.0	5_{f-2} $5f_{+2}$ 7s + O: $2p_x$ $2p_y$ $2p_z$
	9	800.3	2.233	179.2	$6d_0$ 5_{f-3} $5f_{-1}$ $5f_{+1}$ 7s + O: $2p_z$ $2p_x$ $2p_x$
	11	1373.4	2.763	180.0	$6d_{-2}$ $6d_{+2}$ 5_{f0} $5f_{+2}$ $5f_{+3}$ 7s + O: $2p_x$ $2p_y$ $2p_x$ $2p_y$
Md	2	0.0	1.812	180.0	$5f_{+2}$
	4	58.2	1.917	180.0	O: $2p_x$ $2p_y$ $2p_z$
	6	312.1	1.933	180.0	$5f_{+3}$ 7s + O: $2p_x$ $2p_y$ $2p_z$
	8	930.6	2.087	180.0	$6d_{-2}$ $5f_{-1}$ $5f_{+1}$ 7s + O: $2p_x$ $2p_y$ $2p_z$
	10	1408.3	2.803	180.0	$6d_{-2}$ $6d_{+2}$ 5_{f0} $5f_{+3}$ 7s + O: $2p_x$ $2p_y$ $2p_x$ $2p_y$
No	1	0.0	1.843	180.0	-
	3	75.5	1.997	159.2	$7s^{\beta}$ + O: $2p_y$ 2pz 2pz
	5	305.3	2.148	155.9	O: $2p_y$ $2p_x$ $2p_z$ $2p_z$
	7	852.8	2.187	180.0	$6d_{+1}$ 7s O: $2p_x$ $2p_x$ $2p_y$
Lr	2	0.0	1.940	101.5	$2p_z$
	4	150.7	2.109	119.0	O: $2p_x$ $2p_z$ $2p_z$
	6	759.6	2.132	180.0	$6d_{-2}$ 7s + O: $2p_x$ $2p_y$ $2p_z$

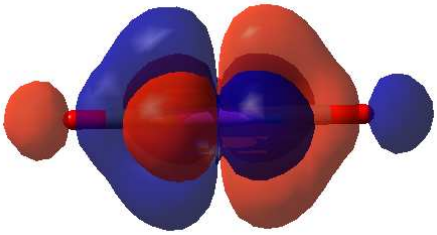
Kohn-Sham orbitals representing minor An5f – O2p overlaps in a few oxides.



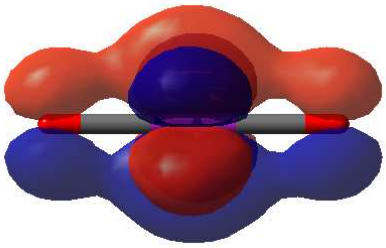
EsO



MdO



FmO_2



FmO_2