Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Plutonium and transplutonium element trioxides: molecular structures, chemical bonding, isomers. Supplementary data

Table 1: Calculated equilibrium energies ΔE and enthalpies ΔH_0° at 0 K (kJ/mol) of An·3O isomers with respect to those of (AnO_2 + 1/2 O_2).

Species	ΔE	ΔH_0^0	Species	ΔE	ΔH_0^0	Species	ΔE	ΔH_0^0
PuO_3	−126	−124	$PuO(O_2)^p$	59	59			
AmO_3	−47	−45	$AmO(O_2)^p$	40	41	$AmO(O_2)^s$	55	57
CmO_3	25	26	$CmO(O_2)^p$	17	19	$CmO(O_2)^s$	−8	−5
BkO_3	−49	−47	$BkO(O_2)^p$	30	-32	$BkO(O_2)^s$	0	3
CfO_3	38	39	$CfO(O_2)^p$	53	55	$CfO(O_2)^s$	12	15

Table 2: Full list of vibrational frequencies of An·3O molecules (in cm^{-1}).

PuO_3	239	257	278	803	911	957
AmO_3	214	250	283	479	850	954
CmO_3	196	228	238	507	770	884
BkO_3	188	204	247	533	819	905
CfO_3	180	234	274	528	816	911
$PuO(O_2)^p$	109	136	477	542	842	927
$AmO(O_2)^p$	116	167	474	523	824	940
$CmO(O_2)^p$	128	159	474	518	777	936
$BkO(O_2)^p$	130	163	488	498	780	923
$CfO(O_2)^p$	160	161	401	511	791	952
$AmO(O_2)^s$	142	167	324	393	836	1201
$CmO(O_2)^s$	158	173	373	396	831	1236
$BkO(O_2)^s$	146	154	319	407	845	1210
$CfO(O_2)^s$	135	144	372	383	852	1236

Table 3: Geometrical parameters (internuclear separations r in Å, angles in degrees, see the figure below for the atom numbering) of peroxide-like structures of AnO_3 dimers. Full data on the equilibrium geometries of oxide-like structures are provided in Supplementary material for Ref. [5].

An	r(O3-O4)	r(An1-O3)	r(An1-O1)	r(An1-O2)	∠An1O3O4An2	∠O1An1O2	∠O1An1O3
Pu	1.472	2.284	1.749	1.751	143	174	94
Am	1.485	2.277	1.746	1.746	144	175	93
Bk	1.479	2.243	1.775	1.777	143	166	97