

A theoretical study of the ground state and lowest excited states of $\text{PuO}^{0/+/+2}$ and $\text{PuO}_2^{0/+/+2}$

Giovanni La Macchia^a, Ivan Infante^a, Juraj Raab^a, John K. Gibson^{*b} and Laura Gagliardi^{*a}

^aDepartment of Physical Chemistry University of Geneva, 30 Quai Ernest Ansermet, CH-1211 Geneva,
Switzerland

^bChemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA.

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^{*}Corresponding author: laura.gagliardi@unige.ch

Table S1 Total energy (a.u.) for the species reported in Table 1 of the paper.

Species	State	Method	R(Pu-O)	Energy [a.u.]
PuO	$^7\Pi$	B3LYP	1.834	-29623.3731681406
	“	CASPT2(12,16)	1.818	-29615.0452765335
	$\Omega = 0$	CASPT2-SO	1.820	-29615.0753157635
PuO ⁺	$^6\Pi$	B3LYP	1.788	-29623.1411380087
	“	CASPT2(11,16)	1.784	-29614.8188161611
	$\Omega = 0.5$	CASPT2-SO	1.789	-29614.8483975936
PuO ²⁺	$^6\Gamma$	B3LYP	1.720	-29622.6076291824
	“	CASPT2(10,16)	1.724	-29614.2837297927
	$\Omega = 2$	CASPT2-SO	1.731	-29614.3208327027
	“	B3LYP	1.818	-29698.7600087617
	“	CASPT2(12,14)	1.792	-29690.2939796187
	$\Omega = 1g$	CASPT2-SO	1.744	-29690.3023934874
PuO ₂ ⁺	$^4\Phi_u$	B3LYP	1.718	-29698.5136950023
	“	CASPT2(11,14)	1.703	-29690.0466487729
	$\Omega = 1.5u$	CASPT2-SO	1.704	-29690.0743863829
PuO ₂ ²⁺	3H_g	B3LYP	1.678	-29697.9145351395
	3H_g	CASPT2(10,14)	1.675	-29689.4777059243
	$\Omega = 4g$	CASPT2-SO	1.675	-29689.5093927543