Synthesis and Crystal Structure of δ-TaON, a Metastable Polymorph of Tantalum Oxide Nitride

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Table S1: Gaussian-type basis sets for Ta, O, N

Element	Shell type	Exponent	Coefficient
Ta (SD60MWB)	5*s*	13.92894522	-0.65530133
		11.99334000	0.99999851
		5.13783577	-0.75340391
	6*s*	0.81369698	1.00000000
	7*s*	0.20617834	1.00000000
	5*p*	7.39668050	0.58299598
		5.71622490	-0.99750066
	6*p*	1.11480608	0.53922059
		0.48684871	0.43278257
	7*p*	0.20000020	1.00000000
	5*d*	3.89501783	-0.07125693
		1.54623255	0.18750222
		0.78972687	0.33933435
		0.39161871	0.46423064
	6*d*	0.20001481	1.00000000
	4*f*	0.69700000	1.00000000
O	1*s*	17236.81829238	0.00074182
		2751.75465497	0.00535982
		644.13976274	0.02693106
		186.54606980	0.10368114
		62.05370174	0.30631113
		22.40522705	0.63919506
		8.63211071	0.69861249
		3.43665812	0.23444923
	2*s*	31.23086387	-0.03031382
		8.75022651	-0.16427606
		0.99708039	0.97908082
	3*s*	0.29679220	1.00000000
	2*p*	37.97017643	0.01498951

		8.81023497	0.09235816
		2.57513767	0.29875716
		0.80224337	0.49916591
	3*p*	0.23077580	1.00000000
	3*d*	0.28447631	1.00000000
N	1*s*	19610.14142999	0.00067103
		2918.28119664	0.00524937
		662.82669961	0.02721870
		188.48972830	0.10851369
		61.86476194	0.33759047
		22.40189484	0.75710716
		8.70806179	1.04888702
		3.43054032	0.59027045
	2*s*	19.83643370	0.75107092
		5.74154083	3.14684949
		0.85051883	-14.22933913
	3*s*	0.26704755	1.00000000
	2*p*	40.95912588	0.01123324
		9.12783302	0.08265355
		2.53467765	0.31399797
		0.78249957	0.62944112
	3*p*	0.20016341	1.00000000
	3*d*	0.51431751	1.00000000