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Supporting information for article:

Fluxional seven-coordinated fluorido- and oxofluoridotantalates

Anatoly A. Udovenko, Arseny B. Slobodyuk, Tatiana B. Emelina and Natalia M. Laptash

Table S1. The temperature change of parameters U (Å^2) for F3 in structures I and II

			I		
	F3 (0.25, *Y, Z*), unsplit position, *P*4/*nmm*				
	297 K	**180 K**	**165 K**	**143 K**	**120 K**
U11	0.28(1)	0.27(2)	0.29(2)	0.33(2)	0.32(2)
U_{eq}	0.123(4)	0.111(5)	0.115(5)	0.127(7)	0.124(6)
	F3 (*X, Y, Z*), split position, *P*4/*nmm*				
U11	0.14(2)	0.092(4)	0.086(4)	0.069(4)	0.061(2)
U_{eq}	0.078(8)	0.050(2)	0.047(1)	0.039(1)	0.036(1)

		II	
	F3, unsplit position		
	297 K	**193 K**	**123 K**
	*P*4/*nmm*	*P*4/*nmm*	*Cmma*
U11	0.22(1)	0.132(8)	0.053(4)
U_{eq}	0.096(4)	0.060(2)	0.040(2)
	F3, split position		
U11	0.126(8)	0.099(6)	
U_{eq}	0.067(3)	0.050(2)	

Table S2. Escape of F atoms from the BP TaF_7 equatorial plane (Å) for I and II at different temperatures

			I		
	297 K	180 K	165 K	143 K	120 K
F1	0	0	0	0	0
F2	0.25	0.22	0.21	0.20	0.20
F2A	-0.25	-0.22	-0.21	-0.20	-0.20
F3	0.42	0.38	0.37	0.34	0.34
F3A	-0.42	-0.38	-0.37	-0.34	-0.34

		II	
	297 K	193 K *P*4/*nmm*	123 K
	*P*4/*nmm*		*Cmma*
F1	0	0	0
F2 (F4)	0.28	0.30	0.35
F2A (F4A)	-0.28	-0.30	-0.35
F3	0.47	0.53	0.68
F3A	-0.47	-0.53	-0.68

Table S3. Hydrogen-bond parameters (Å, °) in (I) at 120 K

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
N1–H1···F2 × 8	0.70	2.46	2.966(1)	131
N1–H1···F1 × 4	0.70	2.54	2.980(1)	123
N2–H2···F3 × 2	0.74	2.21	2.864(3)	148