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Supporting information for article:

New $Tl_{4.86}Fe_{0.82}Hf_{1.18}(MoO_4)_6$ ternary molybdate: crystal structure and properties

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Table S1 Atomic coordinates, site occupancies (q) and equivalent ADPs (U_{eq}) for $Tl_{4.86}Fe_{0.82}Hf_{1.18}(MoO_4)_6$.

Atom	*x*/*a*	*y*/*b*	*z*/*c*	*q*	U_{eq} (Å^2)
Tl1_1	0.0545 (18)	0.3412 (16)	0.0839 (3)	0.33 (1)	0.036 (3)
Tl1_1′	0.0480 (8)	0.3240 (9)	0.0835 (2)	0.60 (1)	0.040 (2)
Tl1_1″	0.0817 (19)	0.3755 (13)	0.0807 (4)	0.07 (1)	0.022 (2)
Tl1_3	0.3320 (2)	0.0511 (1)	0.4167 (1)	0.96 (1)	0.0402 (5)
Tl1_3′	0.3867 (20)	0.0943 (16)	0.4172 (5)	0.04 (1)	0.036 (7)
Tl1_5	0.9416 (8)	0.2883 (8)	0.4163 (2)	0.49 (1)	0.043 (2)
Tl1_5′	0.9521 (7)	0.2737 (7)	0.4172 (2)	0.51 (1)	0.035 (1)
Tl1_9	0.6583 (4)	0.9454 (4)	0.5836 (1)	0.75 (1)	0.037 (1)
Tl1_9′	0.6942 (11)	0.9553 (9)	0.5828 (3)	0.25 (1)	0.032 (2)
Tl1_10	0.2750 (13)	0.3205 (15)	0.5830 (2)	0.32 (1)	0.038 (3)
Tl1_10′	0.2840 (7)	0.3396 (8)	0.5835 (1)	0.66 (1)	0.041 (1)
Tl1_11	0.0523 (1)	0.7178 (1)	0.5833 (1)	0.97 (1)	0.0410 (4)
Tl1_11′	0.0389 (21)	0.7651 (19)	0.5872 (5)	0.03 (1)	0.025 (4)
Tl2_1	0.3326 (3)	0.6673 (2)	0.0196 (4)	0.67 (1)	0.0189 (4)
Tl2_1′	0.3383 (10)	0.6659 (9)	0.0255 (2)	0.20 (1)	0.051 (3)
Tl2_5	0.6674 (1)	0.3336 (1)	0.4773 (1)	1	0.0379 (4)
Tl2_6	0.6673 (1)	0.3338 (1)	0.9772 (1)	1	0.0375 (4)
Tl2_11	0.3323 (3)	0.6670 (3)	0.5197 (1)	0.65 (1)	0.0190 (5)
Tl2_11′	0.339711)	0.6668 (9)	0.5251 (2)	0.22 (1)	0.044 (2)
Hf1_1/Fe1_1	0	0	0	0.77 / 0.23 (1)	0.0116 (1)
Hf1_4/Fe1_4	0	0	0.5	0.77 / 0.23	0.0116
Hf2_1/Fe2_1	0.6667 (1)	0.3333 (1)	0.0833 (1)	0.50 / 0.50 (1)	0.0040 (2)
Hf2_10/Fe2_10	0.6667 (2)	0.3333 (1)	0.5832 (1)	0.32 / 0.68 (1)	0.0260 (5)
Mo1_1	0.7075 (1)	0.0602 (1)	0.0337 (1)	1	0.0158 (1)
Mo1_2	–0.0602	0.6473	0.0337	1	0.0158
Mo1_3	–0.6473	–0.7075	0.0337	1	0.0158
Mo1_4	0.0602	0.7075	0.4663	1	0.0158
Mo1_5	0.6473	–0.0602	0.4663	1	0.0158
Mo1_6	–0.7075	–0.6473	0.4663	1	0.0158
Mo1_7	–0.7075	–0.0602	–0.0337	1	0.0158
Mo1_8	0.0602	–0.6473	–0.0337	1	0.0158
Mo1_9	0.6473	0.7075	–0.0337	1	0.0158
Mo1_10	–0.0602	–0.7075	0.5337	1	0.0158
Mo1_11	–0.6473	0.0602	0.5337	1	0.0158
Mo1_12	0.7075	0.6473	0.5337	1	0.0158
O1_1	0.7521 (15)	0.2349 (14)	0.0522 (3)	1	0.019 (4)
O1_2	0.7652 (14)	0.5206 (13)	0.0519 (3)	1	0.019 (4)
O1_3	0.4880 (16)	0.2533 (15)	0.0517 (3)	1	0.026 (6)
O1_4	0.2379 (15)	0.7514 (13)	0.4479 (3)	1	0.021 (5)
O1_5	0.5156 (13)	0.7641 (11)	0.4464 (3)	1	0.013 (3)
O1_6	0.2518 (16)	0.4881 (14)	0.4473 (4)	1	0.023 (5)
O1_7	0.2514 (15)	0.7647 (13)	0.9475 (3)	1	0.019 (4)
O1_8	0.2365 (15)	0.4903 (13)	0.9470 (4)	1	0.021 (4)
O1_9	0.5168 (13)	0.7514 (12)	0.9470 (3)	1	0.015 (4)

O1_10	0.7680 (13)	0.2496 (13)	0.5529 (3)	1	0.016 (4)
O1_11	0.4860 (16)	0.2341 (14)	0.5511 (4)	1	0.027 (5)
O1_12	0.7524 (14)	0.5191 (12)	0.5523 (3)	1	0.015 (4)
O2_1	0.8695 (14)	0.0391 (14)	0.0328 (3)	1	0.022 (5)
O2_2	0.9663 (15)	0.8305 (11)	0.0328 (3)	1	0.024 (5)
O2_3	0.1697 (14)	0.1334 (13)	0.0334 (3)	1	0.020 (3)
O2_4	0.0339 (15)	0.8607 (13)	0.4668 (3)	1	0.023 (4)
O2_5	0.8325 (14)	0.9639 (14)	0.4665 (3)	1	0.024 (5)
O2_6	0.1335 (15)	0.1688 (13)	0.4665 (3)	1	0.021 (4)
O2_7	0.1388 (13)	0.9664 (14)	0.9667 (3)	1	0.022 (4)
O2_8	0.0362 (14)	0.1711 (13)	0.9672 (3)	1	0.021 (4)
O2_9	0.8286 (15)	0.8622 (14)	0.9675 (3)	1	0.027 (3)
O2_10	0.9624 (15)	0.1317 (13)	0.5326 (3)	1	0.024 (5)
O2_11	0.1720 (12)	0.0341 (14)	0.5328 (3)	1	0.018 (4)
O2_12	0.8626 (13)	0.8285 (11)	0.5327 (3)	1	0.018 (4)
O3_1	0.5610 (13)	0.9194 (15)	0.0554 (3)	1	0.027 (5)
O3_2	0.0805 (16)	0.64042 (14)	0.0543 (3)	1	0.028 (5)
O3_3	0.3521 (15)	0.4370 (13)	0.0547 (3)	1	0.027 (5)
O3_4	0.9151 (14)	0.5620 (13)	0.4456 (3)	1	0.024 (4)
O3_5	0.6474 (14)	0.0860 (13)	0.4446 (3)	1	0.022 (5)
O3_6	0.4329 (15)	0.3544 (15)	0.4452 (4)	1	0.031 (6)
O3_7	0.4381 (15)	0.0822 (14)	0.9450 (4)	1	0.029 (5)
O3_8	0.9163 (14)	0.3530 (14)	0.9440 (3)	1	0.021 (5)
O3_9	0.6409 (15)	0.5606 (13)	0.9442 (3)	1	0.025 (5)
O3_10	0.0798 (15)	0.4371 (14)	0.5556 (4)	1	0.029 (5)
O3_11	0.3600 (16)	0.9217 (13)	0.5552 (3)	1	0.028 (5)
O3_12	0.5574 (13)	0.6436 (14)	0.5558 (3)	1	0.023 (4)
O4_1	0.6635 (17)	0.0661 (16)	0.9905 (3)	1	0.036 (6)
O4_2	0.9385 (17)	0.5978 (15)	0.9898 (3)	1	0.031 (6)
O4_3	0.3993 (17)	0.3351 (16)	0.9904 (4)	1	0.042 (6)
O4_4	0.0606 (17)	0.6611 (15)	0.5100 (3)	1	0.028 (6)
O4_5	0.5994 (15)	0.9380 (15)	0.5104 (3)	1	0.027 (5)
O4_6	0.3385 (16)	0.3985 (15)	0.5105 (3)	1	0.028 (6)
O4_7	0.3439 (15)	0.9457 (14)	0.0098 (2)	1	0.023 (5)
O4_8	0.0584 (16)	0.3943 (14)	0.0097 (3)	1	0.025 (5)
O4_9	0.6000 (14)	0.6569 (13)	0.0097 (3)	1	0.022 (4)
O4_10	0.9386 (18)	0.3367 (16)	0.4902 (3)	1	0.029 (6)
O4_11	0.3969 (15)	0.0577 (17)	0.4901 (3)	1	0.029 (6)
O4_12	0.6593 (15)	0.5988 (14)	0.4902 (3)	1	0.028 (5)

Table S2 Local symmetry operators for transition from space group $R\bar{3}c$ to space group $R1$.

Number	Operator
1	x, y, z
2	$\bar{y}, x-y, z$
3	$\bar{x}+y, \bar{x}, z$
4	$y, x, \bar{z}+1/2$
5	$x-y, \bar{y}, \bar{z}+1/2$
6	$\bar{x}, \bar{x}+y, \bar{z}+1/2$
7	$\bar{x}, \bar{y}, \bar{z}$

8	$y, \overline{x} + y, \overline{z}$
9	$x - y, x, \overline{z}$
10	$\overline{y}, \overline{x}, z + 1/2$
11	$\overline{x} + y, y, z + 1/2$
12	$x, x - y, z + 1/2$

Table S3 Selected interatomic distances (Å) for $Tl_{4.86}Fe_{0.82}Hf_{1.18}(MoO_4)_6$.

Hf/Fe-octahedra					
Hf1_1–O2_1*	2.046 (15)	Hf2_1–O1_1	2.051 (17)	Hf2_10–O1_7	2.022 (17)
Hf1_1–O2_2	2.055 (12)	Hf2_1–O1_2	2.084 (12)	Hf2_10–O1_8	1.983 (12)
Hf1_1–O2_3	2.065 (11)	Hf2_1–O1_3	2.025 (14)	Hf2_10–O1_9	2.035 (12)
Hf1_1–O2_7	2.091 (15)	Hf2_1–O1_4	2.028 (17)	Hf2_10–O1_10	2.044 (16)
Hf1_1–O2_8	2.063 (13)	Hf2_1–O1_5	2.012 (12)	Hf2_10–O1_11	2.050 (14)
Hf1_1–O2_9	2.065 (11)	Hf2_1–O1_6	2.005 (13)	Hf2_10–O1_12	2.062 (11)
Average, $\Delta_{max-min}$	2.064, 0.045	Average, $\Delta_{max-min}$	2.034, 0.079	Average, $\Delta_{max-min}$	2.033, 0.079
Hf1_4–O2_4	2.096 (15)				
Hf1_4–O2_5	2.050 (14)				
Hf1_4–O2_6	2.061 (10)				
Hf1_4–O2_10	2.039 (15)				
Hf1_4–O2_11	2.075 (13)				
Hf1_4–O2_12	2.069 (10)				
Average, $\Delta_{max-min}$	2.065, 0.057				
Mo-tetrahedra					
Mo1_1–O1_1	1.801 (14)	Mo1_5–O1_5	1.833 (10)	Mo1_9–O1_9	1.813 (15)
Mo1_1–O2_1	1.832 (17)	Mo1_5–O2_5	1.841 (16)	Mo1_9–O2_9	1.791 (11)
Mo1_1–O3_1	1.725 (11)	Mo1_5–O3_5	1.748 (15)	Mo1_9–O3_9	1.733 (15)
Mo1_1–O4_1	1.704 (14)	Mo1_5–O4_5	1.737 (12)	Mo1_9–O4_9	1.718 (10)
Average, $\Delta_{max-min}$	1.767, 0.130	Average, $\Delta_{max-min}$	1.790, 0.104	Average, $\Delta_{max-min}$	1.764, 0.095
Mo1_2–O1_2	1.787 (11)	Mo1_6–O1_6	1.832 (17)	Mo1_10–O1_10	1.789 (13)
Mo1_2–O2_2	1.811 (13)	Mo1_6–O2_6	1.824 (10)	Mo1_10–O2_10	1.829 (17)
Mo1_2–O3_2	1.712 (17)	Mo1_6–O3_6	1.676 (17)	Mo1_10–O3_10	1.716 (12)
Mo1_2–O4_2	1.736 (13)	Mo1_6–O4_6	1.735 (11)	Mo1_10–O4_10	1.710 (12)
Average, $\Delta_{max-min}$	1.762, 0.099	Average, $\Delta_{max-min}$	1.767, 0.156	Average, $\Delta_{max-min}$	1.761, 0.119
Mo1_3–O1_3	1.807 (19)	Mo1_7–O1_7	1.819 (14)	Mo1_11–O1_11	1.789 (12)
Mo1_3–O2_3	1.818 (10)	Mo1_7–O2_7	1.780 (16)	Mo1_11–O2_11	1.786 (14)
Mo1_3–O3_3	1.723 (15)	Mo1_7–O3_7	1.721 (11)	Mo1_11–O3_11	1.709 (16)
Mo1_3–O4_3	1.702 (15)	Mo1_7–O4_7	1.720 (10)	Mo1_11–O4_11	1.714 (12)
Average, $\Delta_{max-min}$	1.763, 0.116	Average, $\Delta_{max-min}$	1.760, 0.099	Average, $\Delta_{max-min}$	1.750, 0.080
Mo1_4–O1_4	1.830 (16)	Mo1_8–O1_8	1.846 (12)	Mo1_12–O1_12	1.787 (15)
Mo1_4–O2_4	1.772 (16)	Mo1_8–O2_8	1.804 (14)	Mo1_12–O2_12	1.791 (9)
Mo1_4–O3_4	1.723 (11)	Mo1_8–O3_8	1.740 (15)	Mo1_12–O3_12	1.774 (15)
Mo1_4–O4_4	1.721 (11)	Mo1_8–O4_8	1.698 (11)	Mo1_12–O4_12	1.718 (12)
Average, $\Delta_{max-min}$	1.762, 0.109	Average, $\Delta_{max-min}$	1.772, 0.148	Average, $\Delta_{max-min}$	1.768, 0.073
Tl-polyhedra					

Tl1_1–O1_1	3.05 (2)	Tl1_9–O1_8	3.039 (17)	Tl2_1′–O1_7	3.402 (17)
Tl1_1–O1_5	2.980 (30)	Tl1_9–O1_10	3.045 (14)	Tl2_1′–O1_8	3.378 (16)
Tl1_1–O2_1	3.385 (18)	Tl1_9–O2_7	3.434 (12)	Tl2_1′–O1_9	3.387 (14)
Tl1_1–O2_4	3.431 (19)	Tl1_9–O2_8	3.275 (14)	Tl2_1′–O3_1	2.768 (13)
Tl1_1–O2_5	3.250 (20)	Tl1_9–O2_10	3.401 (13)	Tl2_1′–O3_2	2.820 (20)
Tl1_1–O3_2	3.230 (20)	Tl1_9–O3_7	3.055 (18)	Tl2_1′–O3_3	2.725 (19)
Tl1_1–O3_3	2.990 (20)	Tl1_9–O3_9	3.334 (11)	Tl2_1′–O4_7	2.980 (20)
Tl1_1–O3_4	3.030 (30)	Tl1_9–O3_11	3.215 (18)	Tl2_1′–O4_8	2.973 (13)
Tl1_1–O3_6	3.392 (17)	Tl1_9–O3_12	2.998 (15)	Tl2_1′–O4_9	2.870 (20)
Tl1_1–O4_8	2.857 (16)	Tl1_9–O4_3	2.865 (15)	Average, $\Delta_{max-min}$	3.034, 0.677
Tl1_1–O4_12	2.854 (17)	Tl1_9–O4_5	2.826 (12)		
Average, $\Delta_{max-min}$	3.132, 0.577	Average, $\Delta_{max-min}$	3.135, 0.608	Tl2_5–O1_10	3.316 (13)
				Tl2_5–O1_11	3.245 (14)
Tl1_1′–O1_1	3.015 (17)	Tl1_9′–O1_8	3.230 (20)	Tl2_5–O1_12	3.301 (11)
Tl1_1′–O1_5	3.050 (19)	Tl1_9′–O1_10	3.019 (17)	Tl2_5–O3_4	2.790 (11)
Tl1_1′–O2_1	3.251 (14)	Tl1_9′–O2_10	3.131 (16)	Tl2_5–O3_5	2.802 (14)
Tl1_1′–O2_4	3.443 (19)	Tl1_9′–O2_12	3.302 (19)	Tl2_5–O3_6	2.863 (18)
Tl1_1′–O2_5	3.393 (16)	Tl1_9′–O3_7	2.890 (20)	Tl2_5–O4_10	2.890 (20)
Tl1_1′–O3_2	3.367 (19)	Tl1_9′–O3_9	3.102 (14)	Tl2_5–O4_11	2.924 (12)
Tl1_1′–O3_3	3.013 (17)	Tl1_9′–O3_12	3.032 (16)	Tl2_5–O4_12	2.883 (17)
Tl1_1′–O3_4	2.970 (20)	Tl1_9′–O4_3	2.843 (19)	Average, $\Delta_{max-min}$	3.002, 0.526
Tl1_1′–O3_6	3.273 (14)	Tl1_9′–O4_5	2.886 (17)		
Tl1_1′–O4_8	2.872 (13)	Average, $\Delta_{max-min}$	3.048, 0.459	Tl2_6–O1_1	3.297 (14)
Tl1_1′–O4_12	2.840 (14)			Tl2_6–O1_2	3.299 (12)
Average, $\Delta_{max-min}$	3.135, 0.603	Tl1_10–O1_7	3.102 (19)	Tl2_6–O1_3	3.259 (13)
		Tl1_10–O1_11	3.050 (20)	Tl2_6–O3_7	2.821 (11)
Tl1_1″–O1_1	3.210 (20)	Tl1_10–O2_7	3.460 (16)	Tl2_6–O3_8	2.826 (15)
Tl1_1″–O1_5	3.050 (30)	Tl1_10–O2_10	3.452 (16)	Tl2_6–O3_9	2.833 (16)
Tl1_1″–O2_4	3.280 (20)	Tl1_10–O2_11	3.262 (18)	Tl2_6–O4_1	2.851 (19)
Tl1_1″–O2_5	3.090 (20)	Tl1_10–O3_8	3.220 (20)	Tl2_6–O4_2	2.864 (12)
Tl1_1″–O3_2	2.970 (20)	Tl1_10–O3_9	3.010 (20)	Tl2_6–O4_3	2.880 (20)
Tl1_1″–O3_3	2.770 (30)	Tl1_10–O3_10	3.060 (20)	Average, $\Delta_{max-min}$	2.992, 0.478
Tl1_1″–O3_4	3.110 (30)	Tl1_10–O3_12	3.378 (15)		
Tl1_1″–O4_8	2.711 (19)	Tl1_10–O4_2	2.833 (16)	Tl2_11–O1_4	3.167 (15)
Tl1_1″–O4_12	3.070 (20)	Tl1_10–O4_6	2.845 (13)	Tl2_11–O1_5	3.235 (12)
Average, $\Delta_{max-min}$	3.029, 0.569	Average, $\Delta_{max-min}$	3.152, 0.627	Tl2_11–O1_6	3.186 (14)
				Tl2_11–O3_10	2.893 (12)
Tl1_3–O1_2	3.008 (17)	Tl1_10′–O1_7	3.047 (16)	Tl2_11–O3_11	2.883 (15)
Tl1_3–O1_4	3.039 (14)	Tl1_10′–O1_11	3.110 (20)	Tl2_11–O3_12	2.856 (16)
Tl1_3–O2_2	3.373 (14)	Tl1_10′–O2_7	3.307 (13)	Tl2_11–O4_4	2.860 (19)
Tl1_3–O2_4	3.346 (12)	Tl1_10′–O2_9	3.446 (18)	Tl2_11–O4_5	2.862 (11)
Tl1_3–O2_6	3.476 (16)	Tl1_10′–O2_11	3.415 (15)	Tl2_11–O4_6	2.888 (18)
Tl1_3–O3_1	3.035 (18)	Tl1_10′–O3_8	3.369 (17)	Average, $\Delta_{max-min}$	2.981, 0.379
Tl1_3–O3_3	3.330 (11)	Tl1_10′–O3_9	3.047 (16)		
Tl1_3–O3_5	3.332 (16)	Tl1_10′–O3_10	3.010 (20)	Tl2_11′–O1_4	3.382 (17)
Tl1_3–O3_6	3.022 (16)	Tl1_10′–O3_12	3.236 (12)	Tl2_11′–O1_5	3.382 (14)
Tl1_3–O4_9	2.862 (10)	Tl1_10′–O4_2	2.851 (14)	Tl2_11′–O1_6	3.363 (16)
Tl1_3–O4_11	2.849 (12)	Tl1_10′–O4_6	2.826 (11)	Tl2_11′–O3_10	2.842 (14)
Average, $\Delta_{max-min}$	3.152, 0.627	Average, $\Delta_{max-min}$	3.151, 0.620	Tl2_11′–O3_11	2.825 (19)
				Tl2_11′–O3_12	2.690 (20)
Tl1_3′–O1_2	3.050 (30)	Tl1_11–O1_9	3.021 (10)	Tl2_11′–O4_4	2.970 (20)
Tl1_3′–O1_4	3.350 (20)	Tl1_11–O1_12	3.026 (12)	Tl2_11′–O4_5	2.859 (14)

Tl1_3′–O2_1	3.190 (20)	Tl1_11–O2_8	3.495 (13)	Tl2_11′–O4_6	2.880 (20)
Tl1_3′–O2_2	3.020 (20)	Tl1_11–O2_9	3.363 (16)	Average, $\Delta_{max-min}$	3.021, 0.692
Tl1_3′–O3_1	3.090 (30)	Tl1_11–O2_11	3.490 (13)		
Tl1_3′–O3_5	2.980 (30)	Tl1_11–O2_12	3.373 (14)		
Tl1_3′–O3_6	2.750 (20)	Tl1_11–O3_7	3.319 (18)		
Tl1_3′–O4_9	3.040 (20)	Tl1_11–O3_8	2.986 (11)		
Tl1_3′–O4_11	2.790 (20)	Tl1_11–O3_10	3.290 (17)		
Average, $\Delta_{max-min}$	3.029, 0.600	Tl1_11–O3_11	3.054 (13)		
Tl1_5–O1_3	3.048 (14)	Tl1_11–O4_1	2.871 (14)		
Tl1_5–O1_6	3.104 (15)	Tl1_11–O4_4	2.846 (12)		
Tl1_5–O2_2	3.414 (16)	Average, $\Delta_{max-min}$	3.178, 0.649		
Tl1_5–O2_3	3.221 (17)				
Tl1_5–O2_6	3.443 (19)	Tl1_11′–O1_9	3.330 (20)		
Tl1_5–O3_1	3.388 (19)	Tl1_11′–O1_12	3.127 (19)		
Tl1_5–O3_2	3.097 (14)	Tl1_11′–O2_11	3.210 (20)		
Tl1_5–O3_4	3.232 (18)	Tl1_11′–O2_12	3.070 (30)		
Tl1_5–O3_5	2.951 (14)	Tl1_11′–O3_7	2.890 (30)		
Tl1_5–O4_7	2.873 (13)	Tl1_11′–O3_8	2.641 (18)		
Tl1_5–O4_10	2.840 (14)	Tl1_11′–O3_11	3.180 (20)		
Average, $\Delta_{max-min}$	3.146, 0.603	Tl1_11′–O4_1	2.670 (20)		
		Tl1_11′–O4_4	3.170 (20)		
Tl1_5′–O1_3	3.146 (14)	Average, $\Delta_{max-min}$	3.032, 0.689		
Tl1_5′–O1_6	3.045 (14)				
Tl1_5′–O2_3	3.429 (17)	Tl2_1–O1_7	3.178 (14)		
Tl1_5′–O2_5	3.411 (15)	Tl2_1–O1_8	3.188 (13)		
Tl1_5′–O2_6	3.239 (18)	Tl2_1–O1_9	3.221 (13)		
Tl1_5′–O3_1	3.210 (18)	Tl2_1–O3_1	2.881 (11)		
Tl1_5′–O3_2	3.015 (13)	Tl2_1–O3_2	2.851 (17)		
Tl1_5′–O3_4	3.428 (18)	Tl2_1–O3_3	2.864 (16)		
Tl1_5′–O3_5	2.995 (14)	Tl2_1–O4_7	2.905 (17)		
Tl1_5′–O4_7	2.859 (12)	Tl2_1–O4_8	2.912 (11)		
Tl1_5′–O4_10	2.857 (14)	Tl2_1–O4_9	2.902 (17)		
Average, $\Delta_{max-min}$	3.149, 0.572	Average, $\Delta_{max-min}$	2.989, 0.370		

*For brevity, atoms in mixed positions Hf/Fe are labeled Hf. Distances between split sites: Tl1_1–Tl1_1′ = 0.159 (19) Å, Tl1_1–Tl1_1″ = 0.353 (17) Å, Tl1_1′–Tl1_1″ = 0.489 (14) Å, Tl1_3–Tl1_3′ = 0.527 (15) Å, Tl1_5–Tl1_5′ = 0.233 (13) Å, Tl1_9–Tl1_9′ = 0.340 (12) Å, Tl1_10–Tl1_10′ = 0.175 (16) Å, Tl1_11–Tl1_11′ = 0.600 (20) Å, Tl2_1–Tl2_1′ = 0.233 (9) Å, Tl2_11–Tl2_11′ = 0.222 (9) Å.

Table S4 The shortest distances (*x*) between positions of Tl atoms in the $Tl_{4.86}Fe_{0.82}Hf_{1.18}(MoO_4)_6$ structure and the estimated height of the potential barrier (*p*) for the possible migration of thallium ions between these positions.

Bond	*x* (Å)	*p* (meV)	Bond	*x* (Å)	*p* (meV)
Tl1_1–Tl2_1	4.035 (13)	> 2200	Tl1_5′–Tl2_5	4.063 (9)	1550
Tl1_1–Tl2_1′	3.916 (15)	2200	Tl1_9–Tl2_6	4.060 (5)	1450
Tl1_1–Tl2_5	4.046 (17)	1800	Tl1_9–Tl2_11	4.024 (4)	1850
Tl1_1′–Tl2_1	4.132 (8)	1900	Tl1_9–Tl2_11′	3.864 (9)	1650
Tl1_1′–Tl2_1′	4.017 (11)	1750	Tl1_9′–Tl2_6	3.802 (12)	1150
Tl1_1′–Tl2_5	3.932 (10)	1100	Tl1_9′–Tl2_11	4.235 (10)	2200
Tl1_1″–Tl2_1	3.698 (13)	> 2200	Tl1_9′–Tl2_11′	4.078 (12)	2000
Tl1_1″–Tl2_1′	3.575 (15)	2000	Tl1_10–Tl2_6	3.911 (10)	1400

Tl1_1″–Tl2_5	4.328 (15)	2000	Tl1_10–Tl2_11	4.155 (14)	2100
Tl1_3–Tl2_1	4.068 (3)	1950	Tl1_10–Tl2_11′	4.015 (17)	1900
Tl1_3–Tl2_1′	3.887 (11)	1450	Tl1_10′–Tl2_6	4.030 (5)	1300
Tl1_3–Tl2_5	4.015 (2)	1300	Tl1_10′–Tl2_11	4.033 (8)	2050
Tl1_3′–Tl2_1	4.430 (20)	> 2200	Tl1_10′–Tl2_11′	3.888 (12)	1900
Tl1_3′–Tl2_1′	4.250 (20)	> 2200	Tl1_11–Tl2_6	4.006 (2)	1280
Tl1_3′–Tl2_5	3.579 (16)	1150	Tl1_11–Tl2_11	4.049 (4)	1760
Tl1_5–Tl2_1	4.126 (8)	1850	Tl1_11–Tl2_11′	3.996 (12)	1350
Tl1_5–Tl2_1′	4.046 (14)	1700	Tl1_11′–Tl2_6	3.450 (20)	1125
Tl1_5–Tl2_5	3.913 (9)	1100	Tl1_11′–Tl2_11	4.520 (20)	2200
Tl1_5′–Tl2_1	4.002 (8)	1900	Tl1_11′–Tl2_11′	4.470 (30)	2200
Tl1_5′–Tl2_1′	3.911 (13)	1700			