

Supplementary materials for the paper

Melt synthesis of molecular complexes *trans*-[MBr₄(OPPh₃)₂] (*M* = Zr, Hf) and their luminescence properties

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Table S1. Comparison of unit cell parameters of the *trans*-[ZrBr₄(OPPh₃)₂] (**1**) structure at 100 K, 200 K and 295 K from one single crystal

Parameter	100 K	200 K	295 K
<i>a</i> , Å	9.5133(8)	9.5891(7)	9.621(5)
<i>b</i> , Å	9.5519(8)	9.6154(7)	9.683(5)
<i>c</i> , Å	10.8232(9)	10.8507(8)	10.857(4)
α , °	107.511(4)	107.986(4)	108.23(2)
β , °	101.781(4)	102.118(5)	102.43(3)
γ , °	93.940(4)	93.426(5)	92.79(2)
<i>V</i> , Å ³	909.2(1)	922.0(1)	930.8(7)
Zr–Br, Å	2.6204(5)–2.6233(5); 2.6219	2.6182(5) – 2.6250(6); 2.6216	2.611(1) — 2.619(1); 2.6148
Zr–O, Å	2.045(2)	2.045(2)	2.0460(34)
P–O, Å	1.5341(25)	1.525(3)	1.521(3)
Angle Br–M–Br (<i>cis</i>), °	90.02(1)	89.92(2)	89.95(3)
Angle Br–M–Br (<i>trans</i>), °	180	180	180
Angle Br–M–O, °	90.00(8)–90.19(8); 90.10	89.817(9) — 90.21(9); 90.01	89.8(1) — 90.5(1); 90.2
Angle O–M–O, °	180	180	180

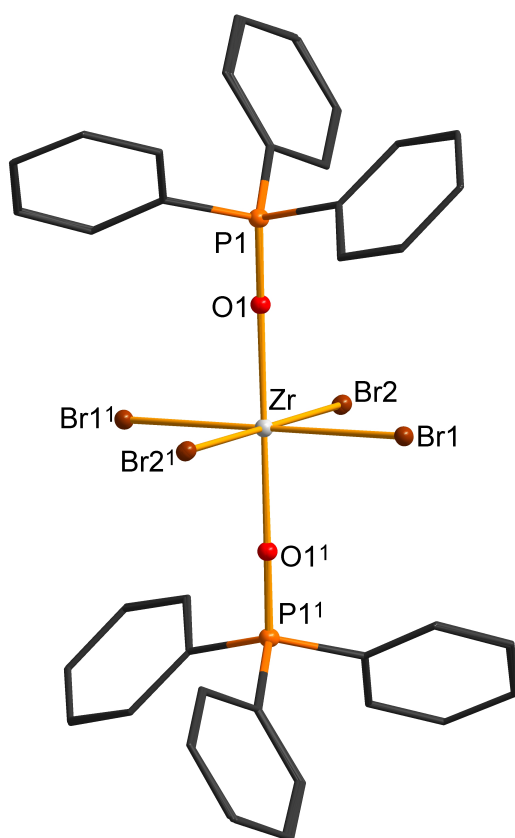


Figure S1. Comparison of the structures of *trans*-[ZrBr₄(OPPh₃)₂] (**1**) from one single crystal at 100, 200 and 295 K. Atomic coordinates are normalized to the Zr atom