

Supplementary Material

**Synthesis, crystal structure and electroluminescent properties of *fac*-
bromotricarbonyl ([1,2,5]oxadiazolo[3',4':5,6]pyrazino-
[2,3-*f*][1,10]phenanthroline) rhenium (I)**

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Table S1. Crystal data and structure refinement parameters for **5a** and **9a**

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Table S1. Crystal data and structure refinement parameters for **5a** and **9a**

	5a	9a
Formula	C ₁₄ H ₆ N ₆ O	C ₁₇ H ₆ BrN ₆ O ₄ Re
M	274.25	624.39
T, K	120	120
System	Monoclinic	Orthorhombic
Space group	P2 ₁ /c	Pnma
Z (Z')	4(1)	4(0.5)
a, Å	10.506(3)	12.2376(8)
b, Å	11.619(4)	12.6448(8)
c, Å	9.378(3)	11.0808(7)
α, °	90	90
β, °	107.655(7)	90
γ, °	90	90
V, Å ³	1090.9(6)	1714.67(19)
d _{calc} , gcm ⁻³	1.670	2.419
μ, cm ⁻¹ , F(000)	1.15, 560	94.59, 1168
2θ _{max} , °	53	58
Collected refl.	9421	31683
Independent refl	2263	2380
Observed refl.	841	2181
R1	0.0746	0.0406
wR2	0.2037	0.1026
GOF	0.958	1.057
ρ _{min} /ρ _{max} , e·Å ⁻³	0.477/-0.260	1.733/-1.794