

Fig. 1 The synthesis of the heteronuclear NiCe complex.

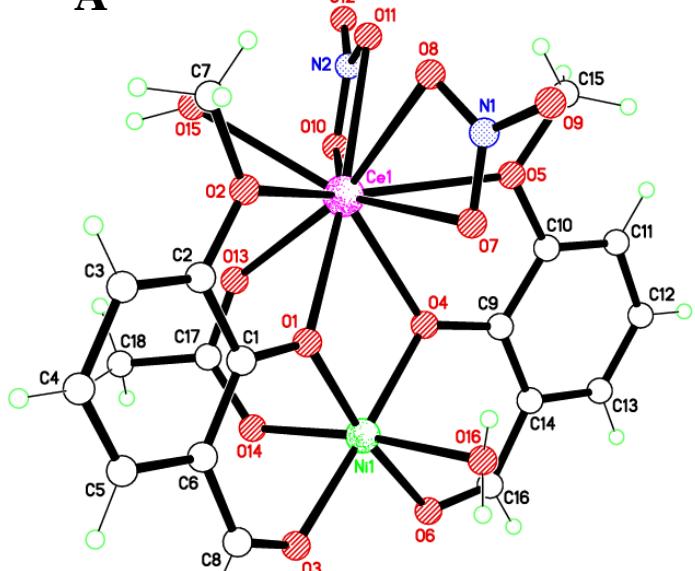
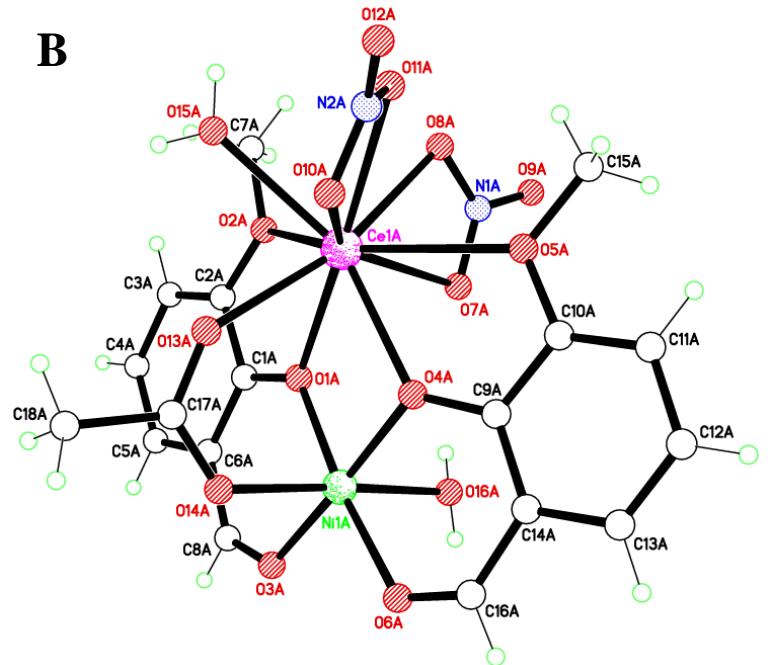
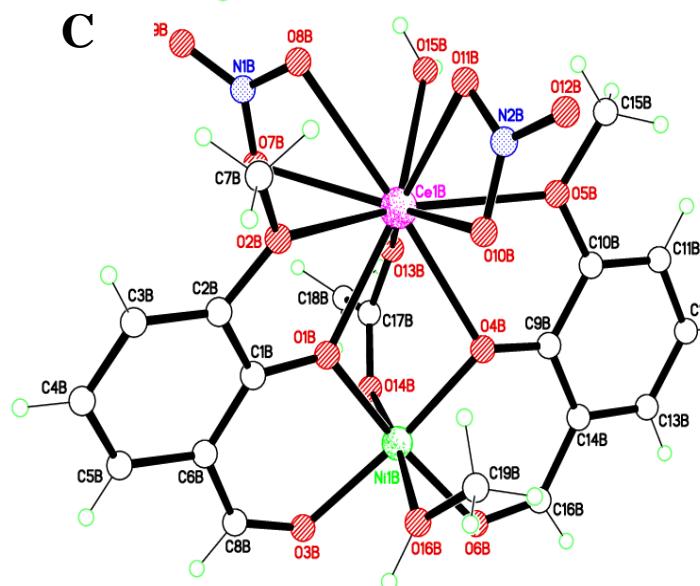
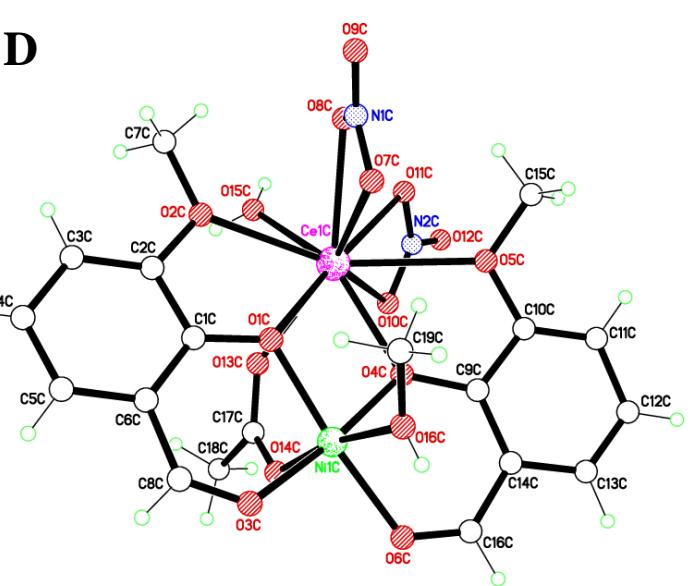
A**B****C****D**

Fig. 2 Four independent complex molecules (prefixed with A-D) in the asymmetric unit.

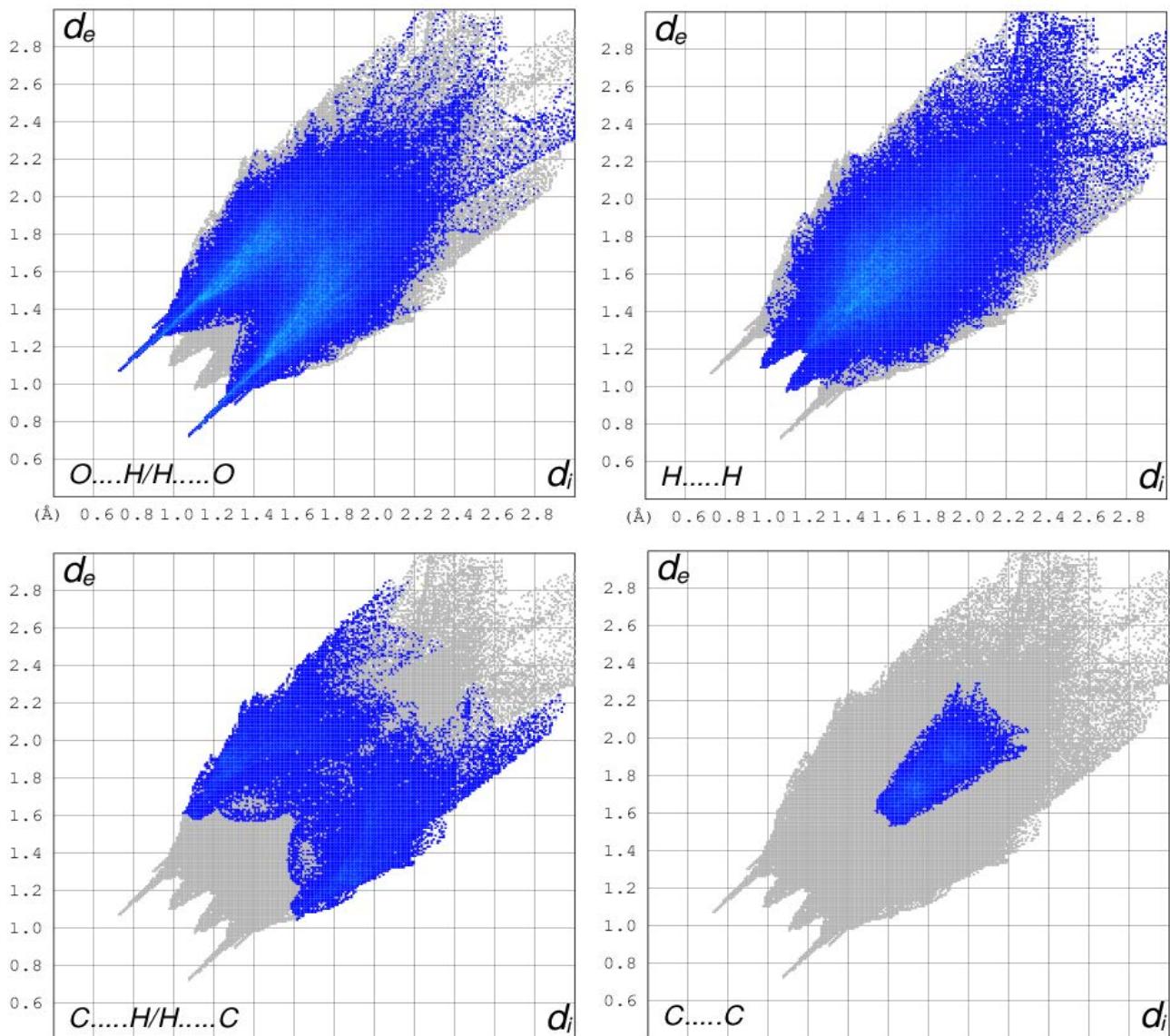


Fig. 3 Finger print plots of the complex showing different intermolecular contacts.

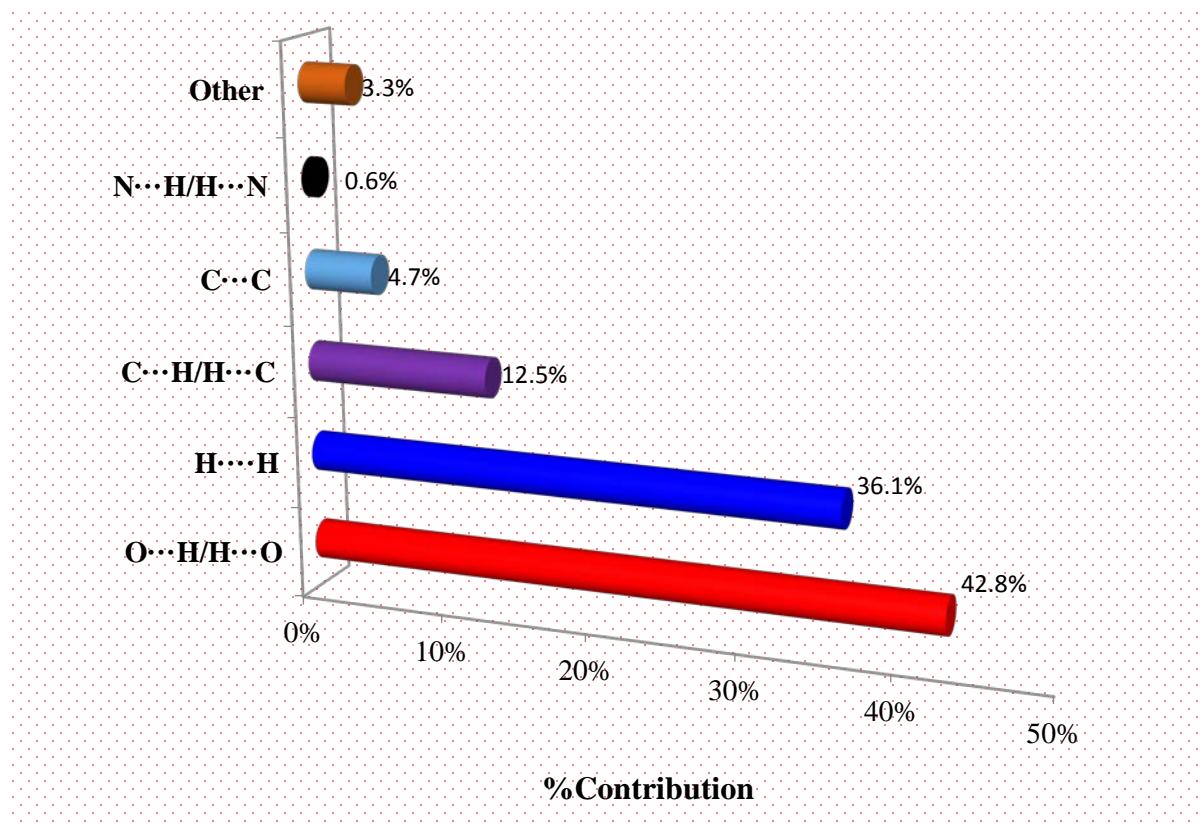


Fig. 4 Percentage contribution of different intermolecular contacts in the structure of the complex.

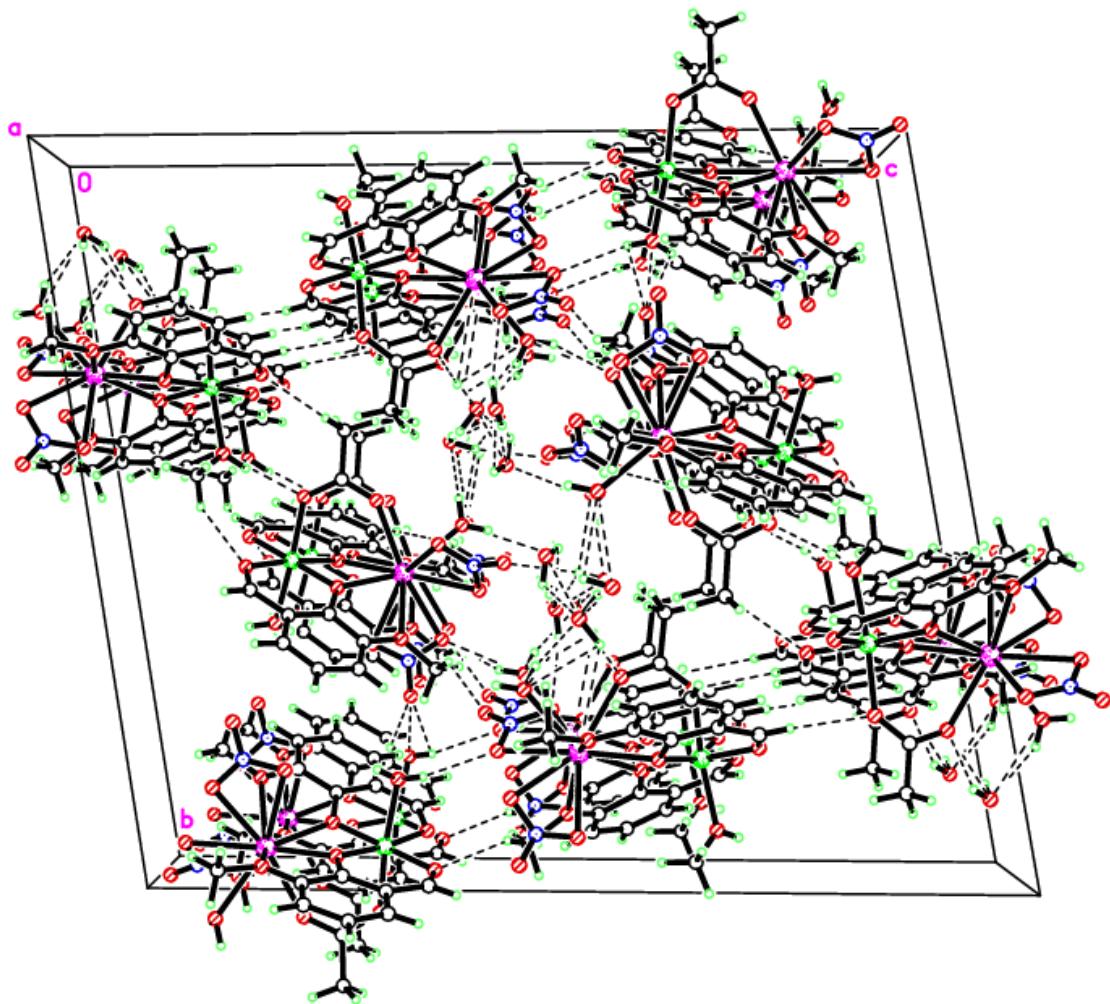


Fig. 5 Packing plot of the complex, showing all four molecules from the asymmetric unit stacking linearly parallel to the *a* axis.

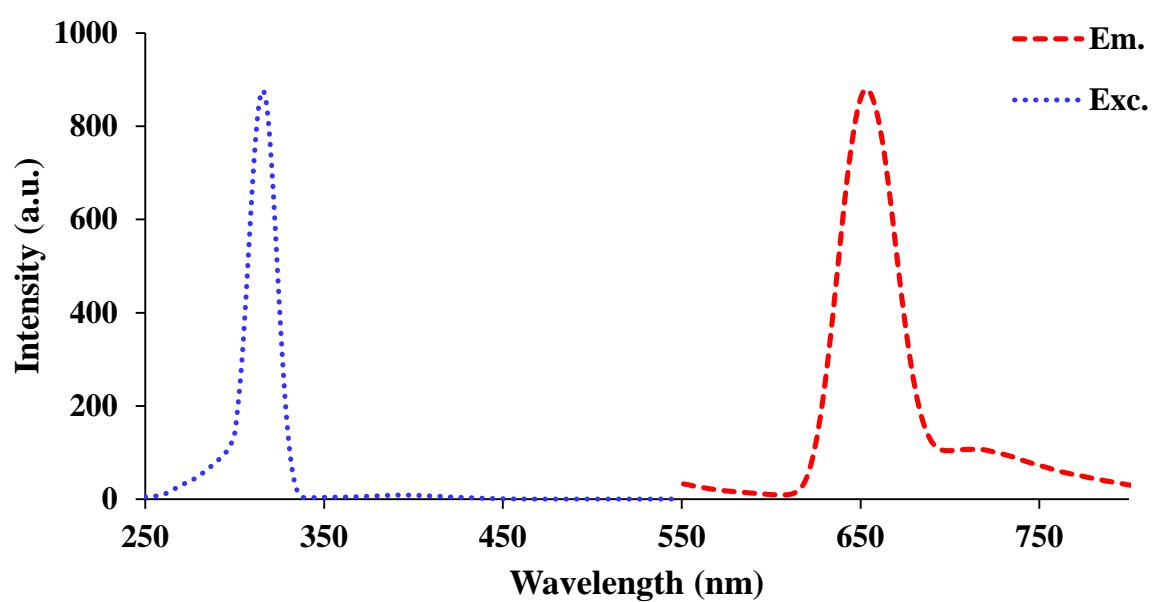
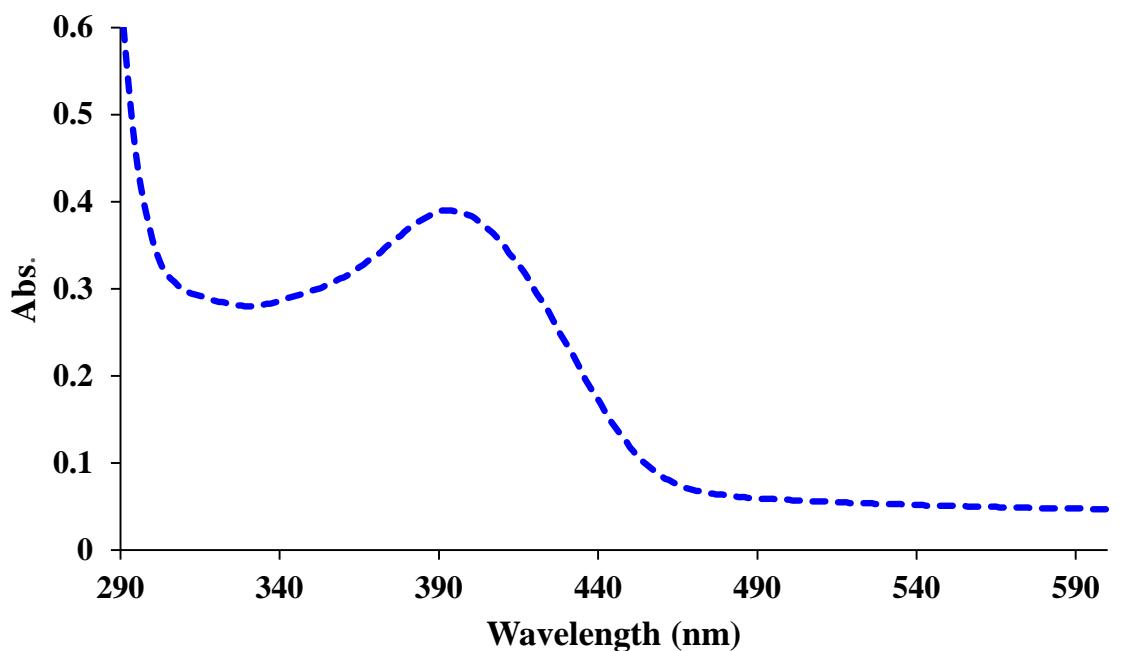


Fig. 6 Absorption and excitation-emission spectra of the complex in DMF (10^{-5} M).

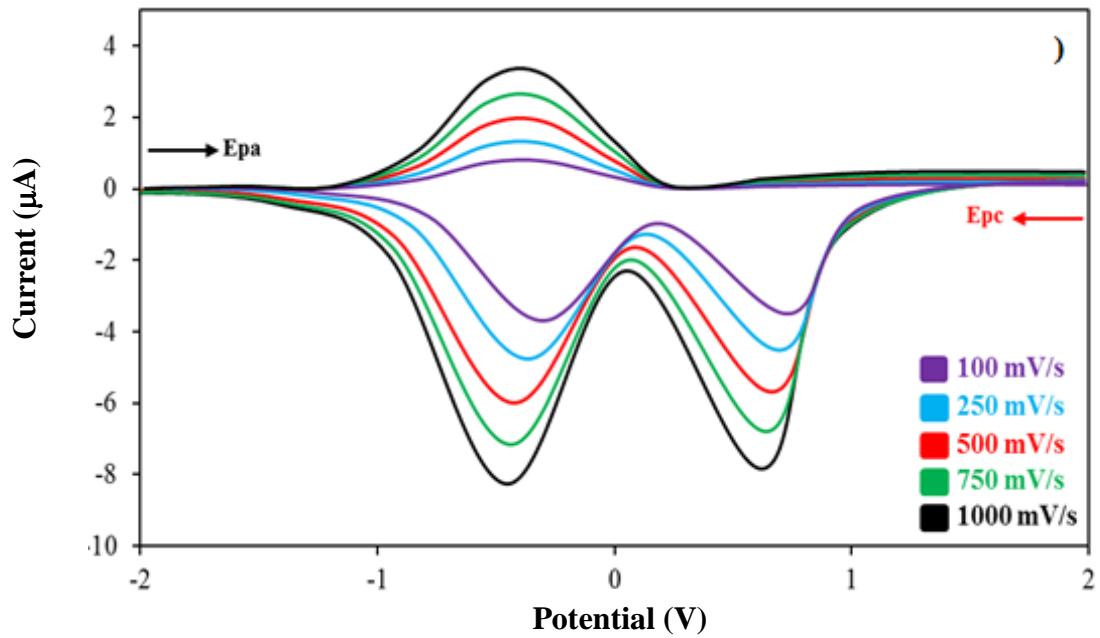


Fig. 7 CV curves of the complex.

Table 1 X-ray data for the complex

Empirical formula	C _{73.28} H _{96.56} Ce ₄ N ₈ Ni ₄ O ₆₉
Formula weight	2988.75
Crystal size (mm ³)	0.20 × 0.08 × 0.04
Crystal color	Green
Crystal system	Triclinic
Space group	P $\bar{1}$
Unit cell	
a (Å)	9.2061(9)
b (Å)	22.683(2)
c (Å)	26.087(3)
α (°)	80.3211(13)
β (°)	85.7890(13)
γ (°)	86.6485(14)
Volume (Å ³)	5349.6(9)
Z	2
Abs. coeff. μ (mm ⁻¹)	2.47
Refl. collected	59816
Ind. Refl. [R_{int}]	21898 [0.071]
$R[F^2 > 2\sigma(F^2)]$	0.055
$wR(F^2)$	0.131
GOOF, S	1.01
Largest diff peak/hole (e Å ⁻³)	1.97/-1.11
CCDC	1842328

Table 2 Electrochemical data for the complex.

Scan rate(mV/s)	E_{pa} (V)	E_{pc} (V)	E_{pa}/E_{pc}	$E_{1/2}$ (V)	ΔE_p (V)
100	-0.36	0.80, -0.29	1.24	-	-0.07
250	-0.37	0.76, -0.37	1.00	0.37	0.00
500	-0.38	0.71, -0.43	0.93	-	0.05
750	-0.39	0.69, -0.47	0.82	-	0.08
1000	-0.40	0.67, -0.50	0.80	-	0.10