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## **SI files for "A new NiCe complex derived from ortho-vanillin: Structural characterization and luminescence properties"**

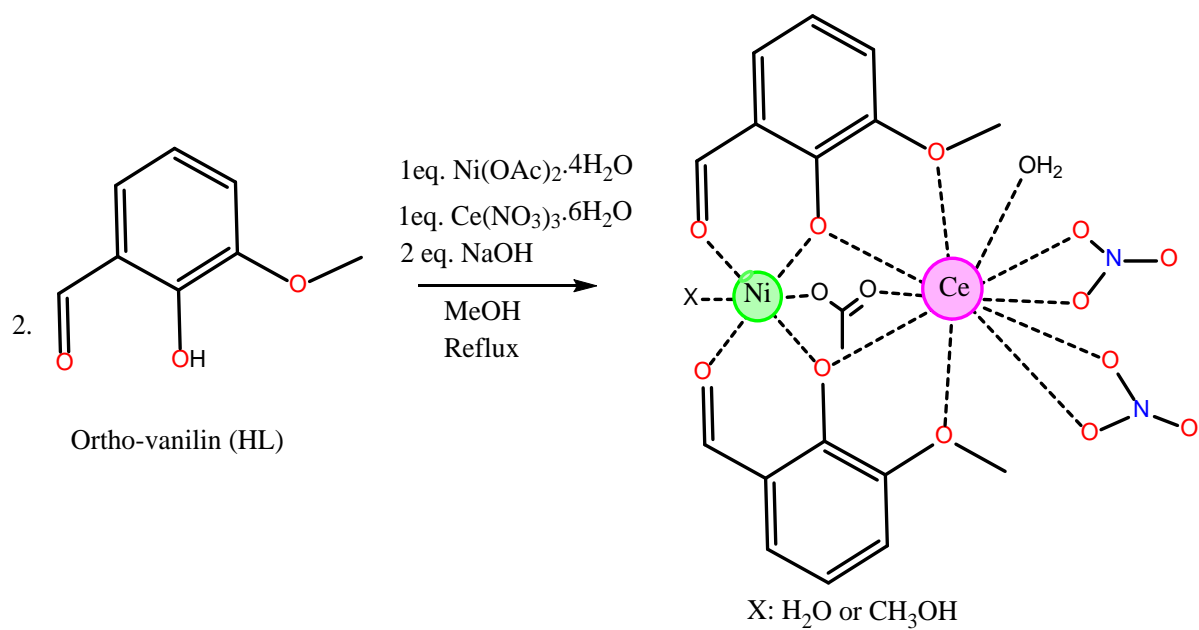
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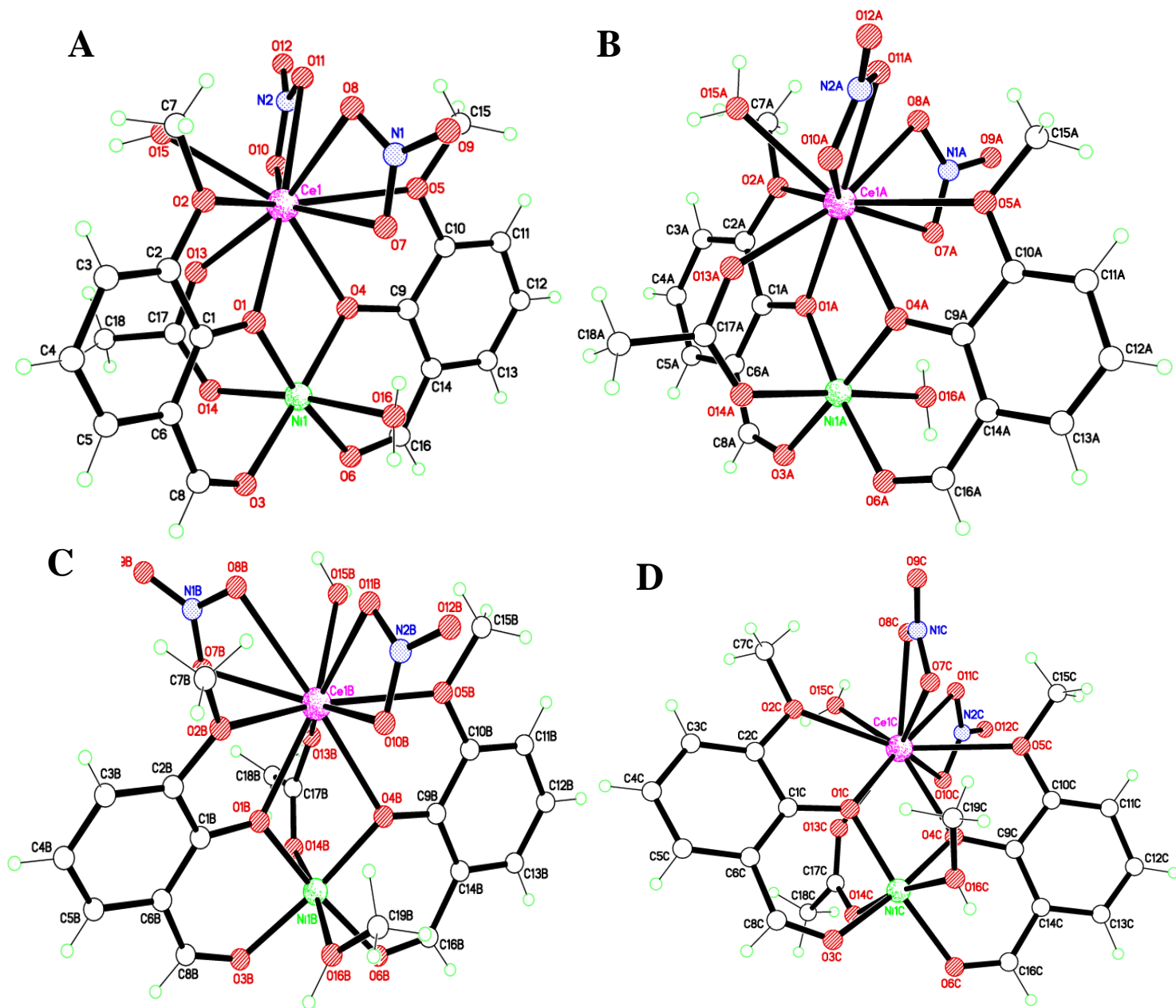
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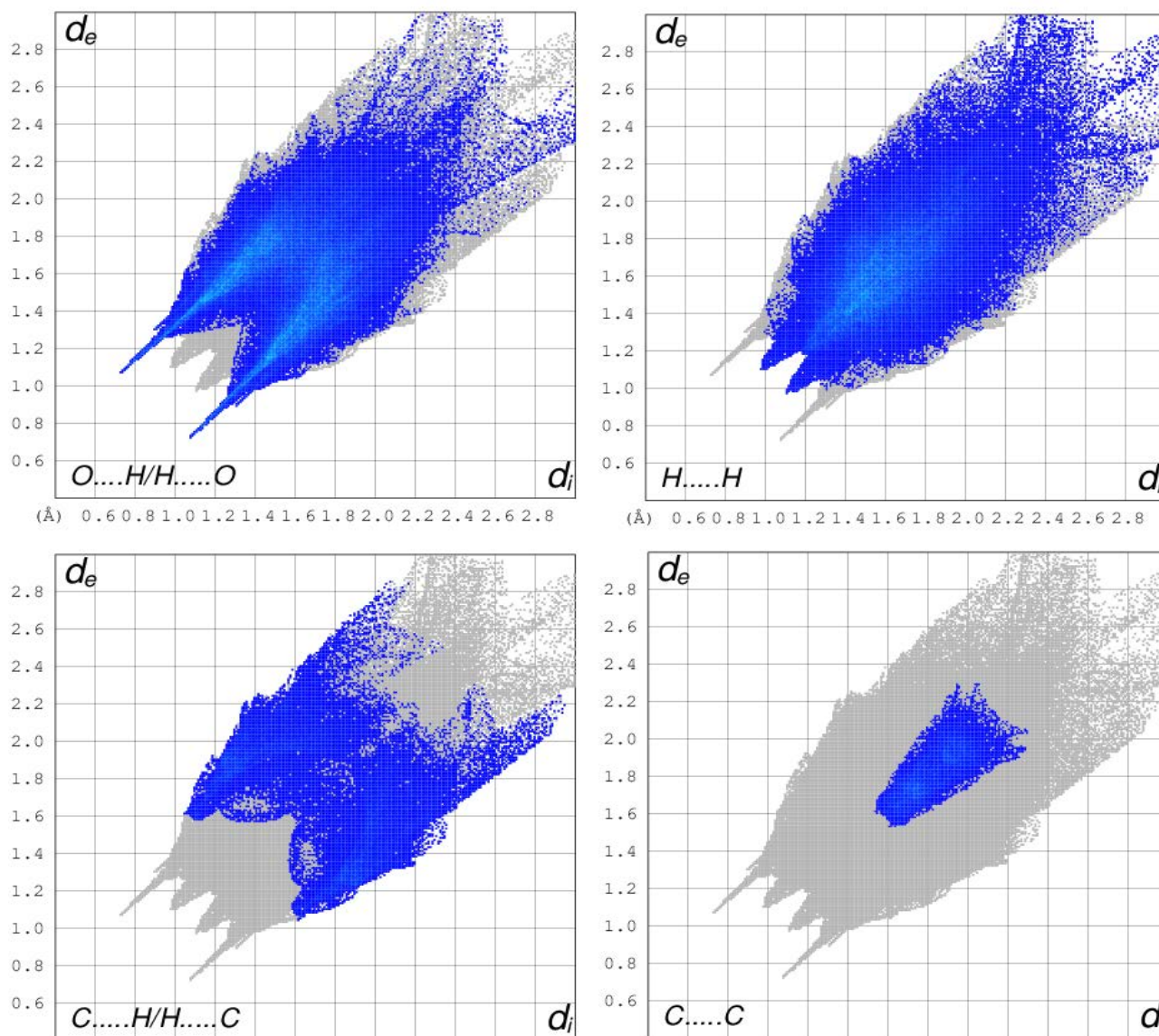
Kirpik, Hilal, Muhammet Kose, Mark Elsegood, and Cameron Carpenter-Warren. 2018. "SI Files for "A New Nice Complex Derived from Ortho-vanillin: Structural Characterization and Luminescence Properties"". figshare. <https://doi.org/10.17028/rd.lboro.7172516.v1>.



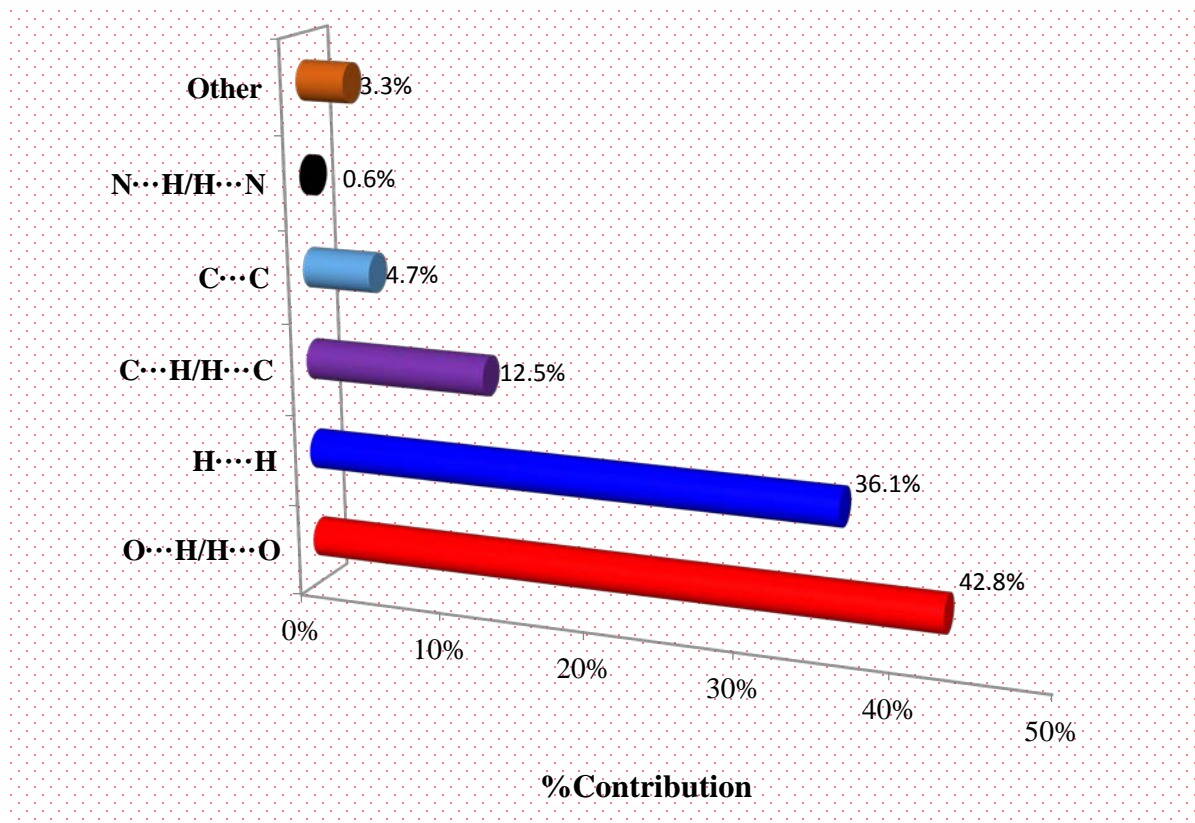
**Fig. 1** The synthesis of the heteronuclear NiCe complex.



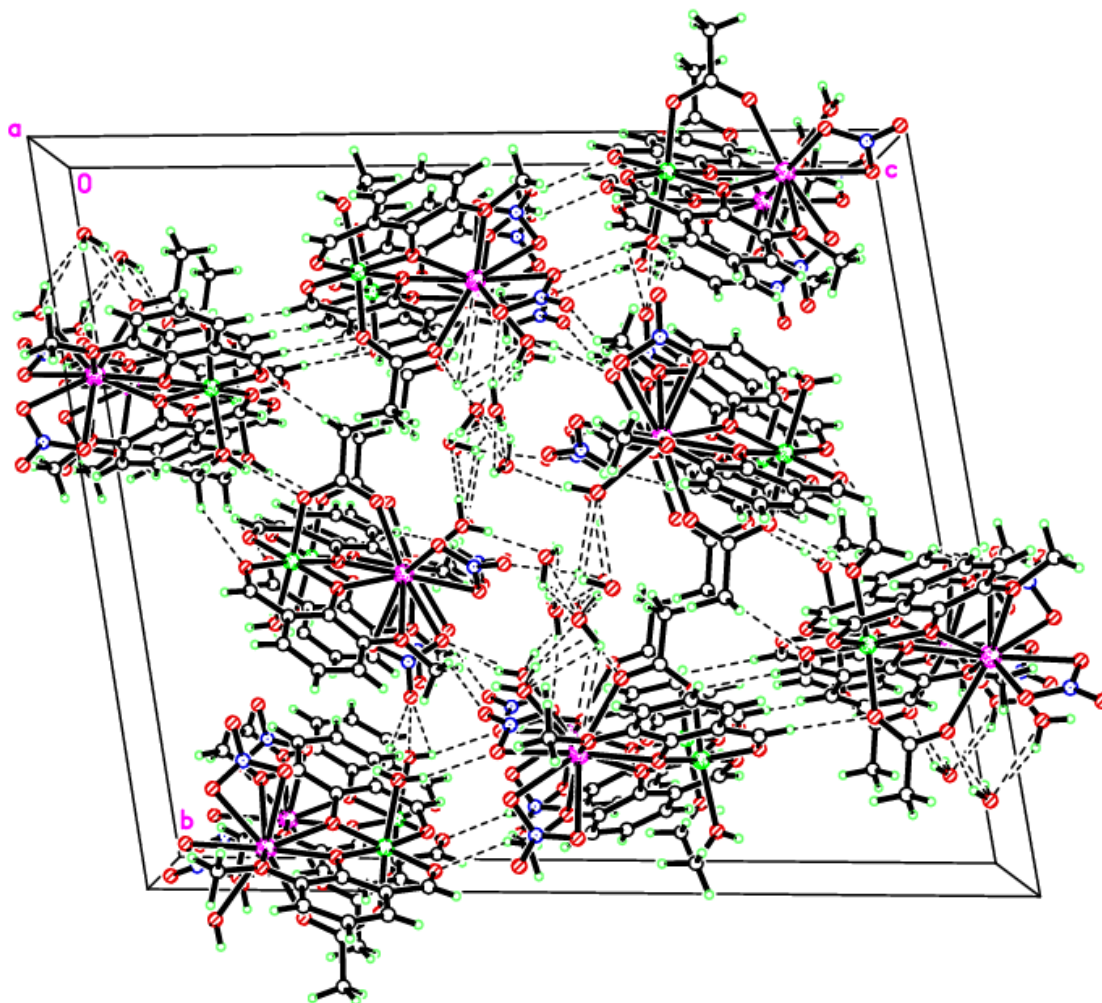
**Fig. 2** Four independent complex molecules (prefixed with A-D) in the asymmetric unit.



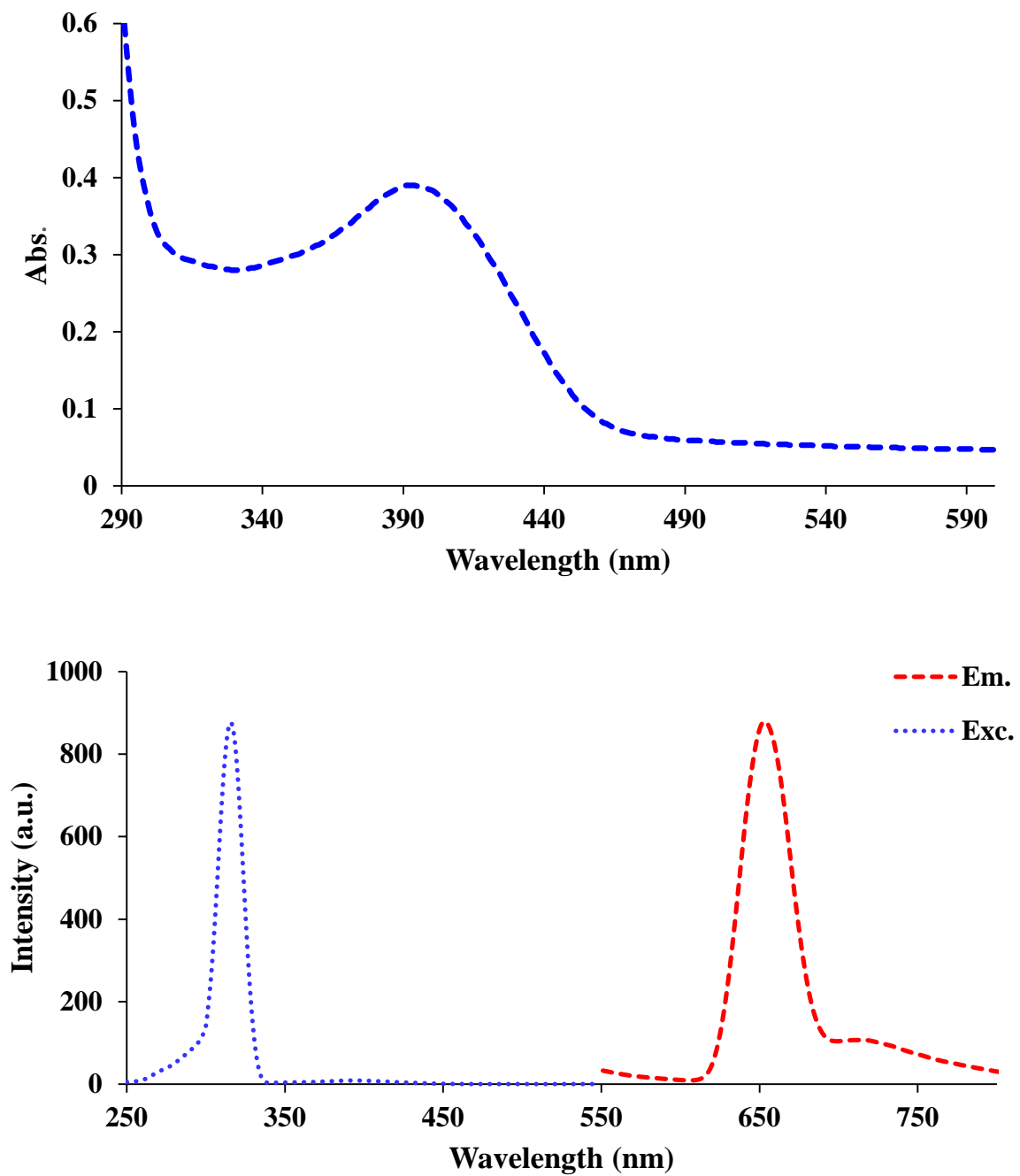
**Fig. 3** Finger print plots of the complex showing different intermolecular contacts.



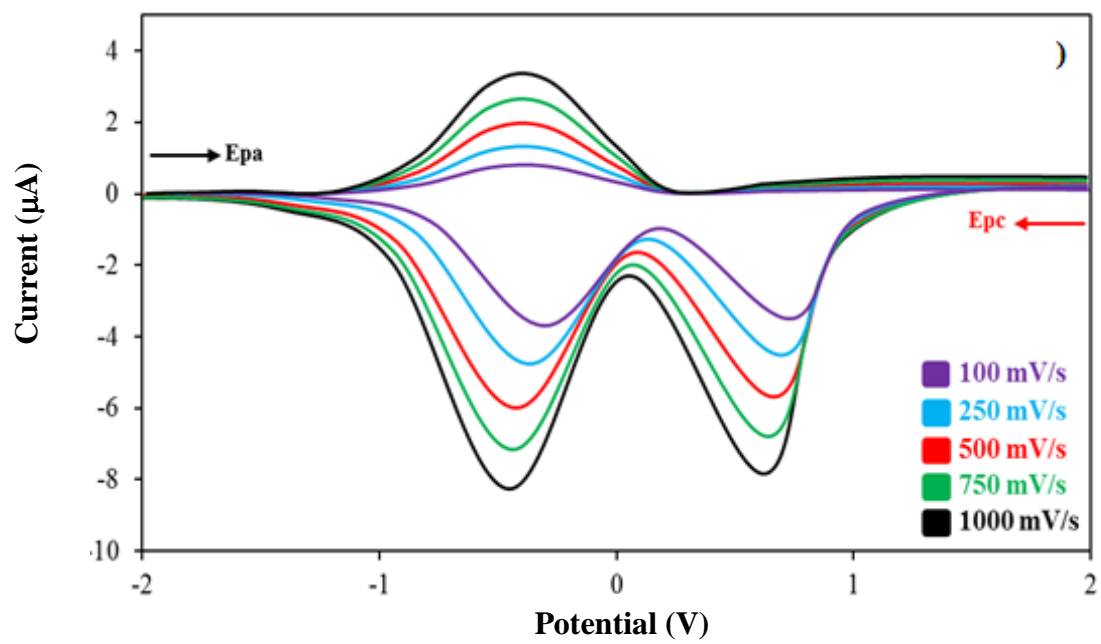
**Fig. 4** Percentage contribution of different intermolecular contacts in the structure of the complex.



**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	$C_{73.28}H_{96.56}Ce_4N_8Ni_4O_{69}$
Formula weight	2988.75
Crystal size (mm <sup>3</sup> )	0.20 × 0.08 × 0.04
Crystal color	Green
Crystal system	Triclinic
Space group	$P \bar{1}$
Unit cell	
<i>a</i> (Å)	9.2061(9)
<i>b</i> (Å)	22.683(2)
<i>c</i> (Å)	26.087(3)
<i>α</i> (°)	80.3211(13)
<i>β</i> (°)	85.7890(13)
<i>γ</i> (°)	86.6485(14)
Volume (Å <sup>3</sup> )	5349.6(9)
<i>Z</i>	2
Abs. coeff. $\mu$ (mm <sup>-1</sup> )	2.47
Refl. collected	59816
Ind. Refl. [ <i>R</i> <sub>int</sub> ]	21898 [0.071]
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )]	0.055
<i>wR</i> ( <i>F</i> <sup>2</sup> )	0.131
GOOF, <i>S</i>	1.01
Largest diff peak/hole (e Å <sup>-3</sup> )	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)	$\Delta E_p$ (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