Supporting Information for

Synthesis, X-Ray crystal structures, optical properties and modelling data of neutral bis(1,2-dithiolene) nickel complexes

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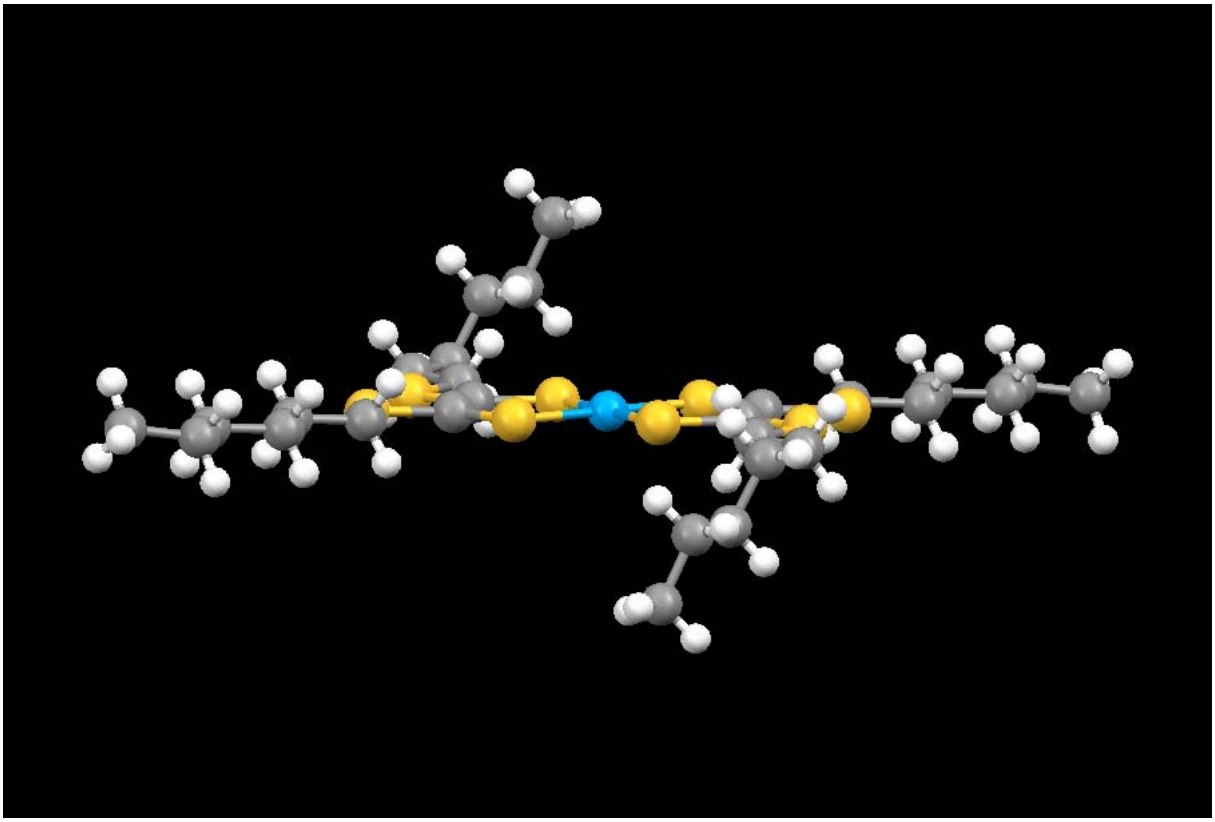


Figure SI-1 : X-Ray Structure of **complex 1**: side view.

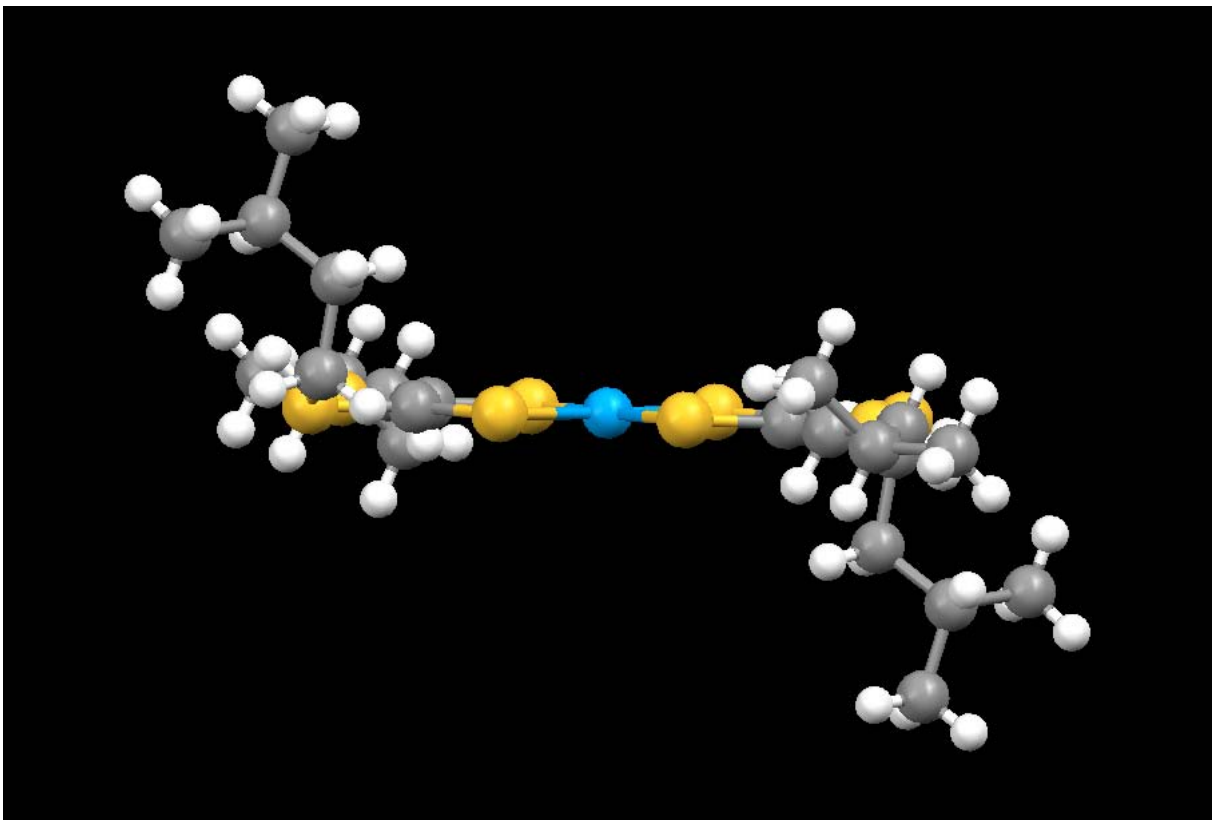


Figure SI-1 : X-Ray Structure of **complex 3**: side view.

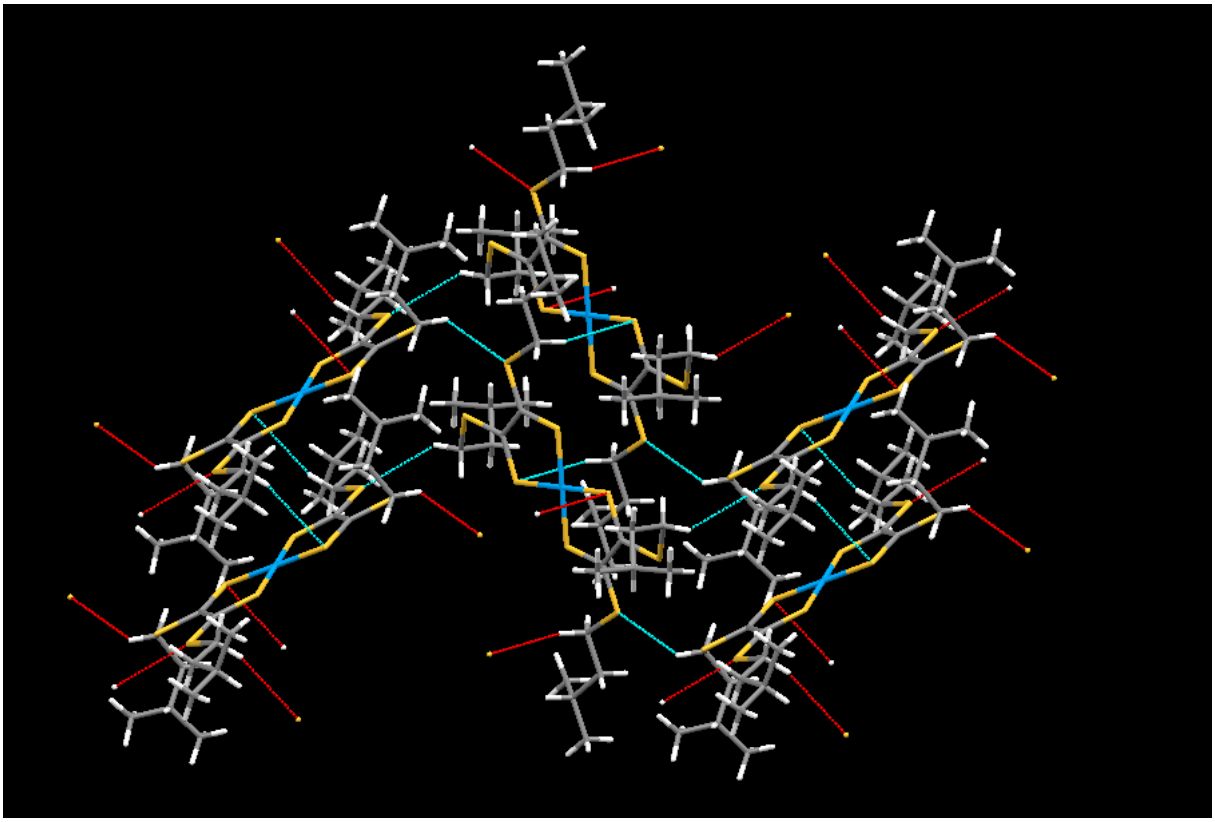
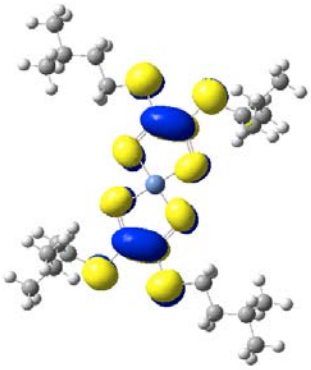
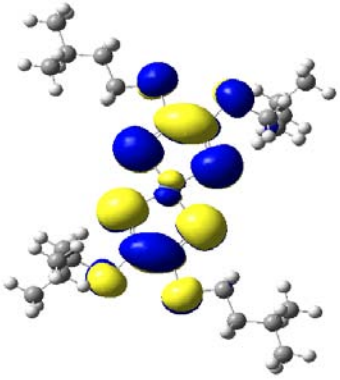


Figure SI-3 : packing of **complex 3** in the crystal with expanded (blue) and hanging (red) short contacts.



HOMO



LUMO

Figure SI-4: HOMO and LUMO Orbitals of complex 3.

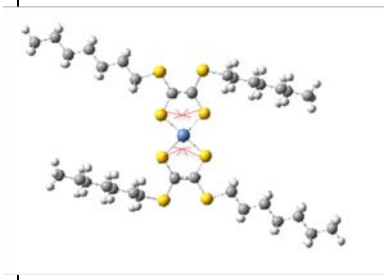
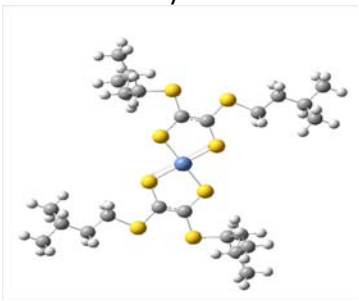
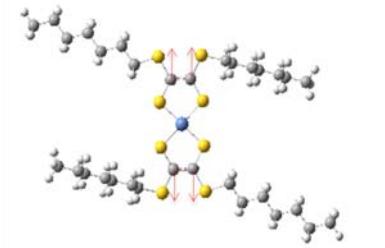
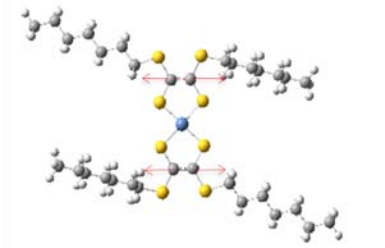
Assignment	***Complex 1***	***Complex 2***	***Complex 3***
$\bar{\nu}$ Ni–S	377	375	376/382
			
$\bar{\nu}$ C–S	983	930	984
			
$\bar{\nu}$ C–C	1393	1416	1393
			

Figure SI-5: Calculated Raman frequencies of the three complexes and schematic representation of the normal modes. For **complex 3**, the representation of the second band (if any) has been added in the last column.