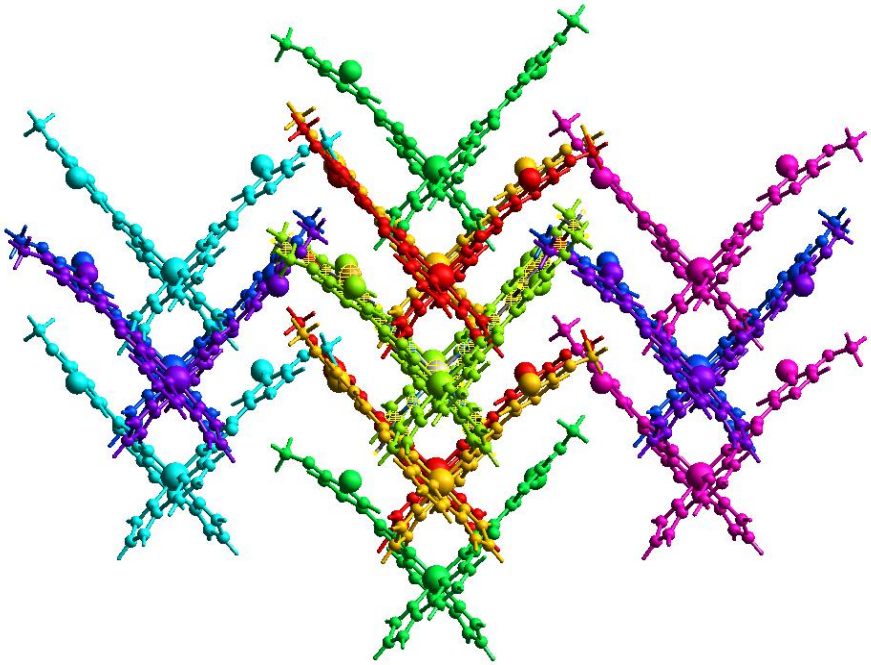
Supporting file S1

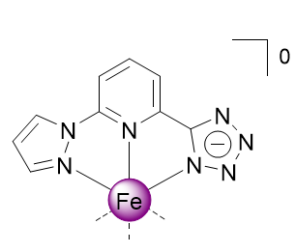
Energy framework analysis

The full colour-coded interaction mappings of a central reference molecule for the title compound. Full details of the various contributions to the total energy (E_{tot}) are also given.

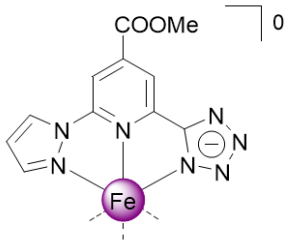


	N	Symop	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	2	-x+1/2, y+1/2, z+1/2	8.27	-33.8	-27.9	-100.6	68.7	-87.6
	2	-x+1/2, y+1/2, z+1/2	8.27	-32.7	-28.9	-91.6	61.9	-84.6
	2	x, y, z	12.67	15.4	-3.0	-7.3	0.8	7.9
	2	x, y, z	10.64	-38.2	-10.2	-38.7	18.9	-65.2
	2	-x, -y, z+1/2	14.70	-10.9	-4.8	-18.0	8.6	-23.4
	2	x+1/2, -y+1/2, z	15.32	3.5	-1.2	-7.9	2.5	-2.3
	2	x+1/2, -y+1/2, z	14.91	2.3	-2.8	-13.3	4.5	-7.7
	2	-x, -y, z+1/2	14.74	-9.3	-3.9	-20.3	15.8	-17.5

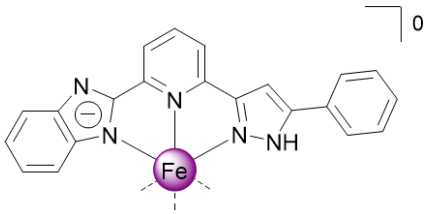
Figure S1. Schematic structure of neutral Fe^{II} complexes with deprotonable azol-based ligands.



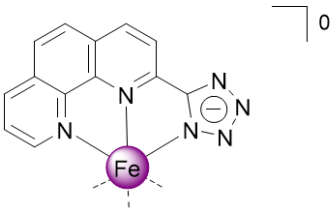
IGERIX



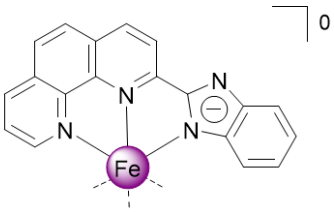
LUTGEO



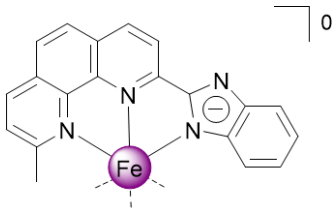
XODCEB



QIDJET



DOMQIH



DOMQUT