

Table S1 Selected geometric bond lengths, bond angles and dihedral angles of the optimized ligand and its complexes using B3LYP/GEN

Ligand/ complexes	Bond lengths (Å)		Bond angles		Dihedral angles	
Scna	S23-O24	1.451	<O2-4S2-3N26	109.7	<C21-C20-S23-O24	23.552
	S23-O25	1.458	<O24-S23-C20	109.0	<O24-S23-N26-C27	-34.307
	S23-N26	1.719	<O25-S23-N26	101.4	<C20-S23-N26-C27	82.3
	N26-C27	1.388	<O25-S23-C20	108.8	<S23N-26-C27-N28	-27.3
	S23-C20	1.789	<S23-N26-C27	125.9	<S23-N26-C27-C32	154.9
	C10-O14	1.324	<O12-C11-C9	122.4	<C19-C20-S23-O25	-19.166
	C10-C9	1.407	<C11-C9-C10	118.2	<C7-C8-C9-C10	0.556
	C10-C1	1.435	<O14-C10-C9	122.2	<O14-C10-C9-C11	-0.096
	C9-C11	1.476	<O14-C10-C1	117.4	<C10-C9-C11-O12	0.721
	C11-O12	1.222	<O12-C11-O13	118.2	<C10-C9-C11-O13	-179.217
	C11-O13	1.342	<C10-C9-C8	118.1		
	C9-C8	1.407	<C11-C9-C8	123.7		
Pd-(Scna)	S23-O24	1.521	<O24-Pd-N26	68.3	<C20-S23-N26-C27	-53.5
	S23-O25	1.452	<N26-Pd-Cl50	103.9	<C21-C20-S23-O24	61.3
	S23-N26	1.631	<Cl50-Pd-O49	82.9	<O24-S23-N26-C27	-165.9
	N26-C27	1.402	<O49-Pd-O24	104.8	<S23-O24-Pd-N26	-6.5
	S23-C20	1.792	<N26-Pd-O49	172.8	<O24-S23-N26-Pd	-8.2
	Pd-O24	2.168	<O24-Pd-Cl50	171.8	<S23-N26-Pd-Cl50	-176.3
	Pd-N26	2.029				
	Pd-O49	2.156				
Ni-(Scna)	Pd-Cl50	2.332				
	S23-O24	1.52958	<O49-Ni-O24	92.826	<C20-S23-N26-C27	-100.172
	S23-O25	1.46121	<O47-Ni-Cl50	86.090	<C21-C20-S23-O24	12.513
	S23-N26	1.59696	<O24-Ni-O47	92.145	<O24-S23-N26-C27	152.277
	N26-C27	1.38821	<O49-Ni-Cl50	88.801	<S23-O24-Ni-N26	-170.602
	S23-C20	1.80089	<O48-Ni-Cl50	87.518	<O24-S23-N26-Ni	6.441

Cu ₂ -(Scna)	Ni-O24	1.92224	<O47-Ni-N26	92.647	<S23-O24-Ni-O49	97.039
	Ni-N26	2.25801	<O49-Ni-O48	84.328	<S23-O24-Ni-O48	-178.639
	Ni-O49	2.24613	<O24-Ni-N26	68.196	<S23-N26-Ni-C150	172.694
	Ni-C150	2.21938	<N26-Ni-O48	169.806	<S23-N26-Ni-O47	85.789
	Ni-O47	2.24946				
	Ni-O48	2.26200				
	S23-O24	1.47544	<O24-Cu57-N26	64.598	<C20-S23-N26-C27	76.626
	S23-O25	1.45949	<N26-Cu57-O48	123.978	<C21-C20-S23-O24	-31.708
	S23-N26	1.65849	<O48-Cu57-O47	106.214	<O24-S23-N26-C27	-172.158
	N26-C27	1.37822	<O47-Cu57-O24	105.816	<S23-O24-Cu57-N26	-10.598
	S23-C20	1.78568	<O13-Cu56-O14	94.183	<O24-S23-N26-Cu57	-14.689
	Cu57-O24	2.43470	<O14-Cu56-O46	113.310	<S23-N26-Cu57-O48	-117.158
	Cu57-N26	1.99746	<O46-Cu56-O45	101.673	<O14-C10-C9-C11	11.602
	Cu57-O47	2.20768	<O45-Cu56-O13	103.200	<C10-C9-C11-O12	177.183
	Cu57-O48	1.84819			<C10-C9-C11-O13	-4.611
	O13-C11	1.28499			<O14-Cu56-O13-C11	-5.617
	C11-O12	1.22524			<C11-O13-Cu56-O45	-126.494
	O14-C10	1.25905			<C10-O14-Cu56-O46	-121.926
	Cu56-O13	1.95006				
	Cu56-O14	2.02948				
	Cu56-O45	2.18674				
	Cu56-O46	2.12506				
Zn-(Scna) ₂	S23-O24	1.45806	<O13-Zn-O14	86.815	<O14-C10-C9-C11	2.333
	S23-O25	1.45510	<O59-Zn-O60	85.269	<C10-C9-C11-O12	175.171
	S23-N26	1.73345	<O13-Zn-O60	89.690	<C10-C9-C11-O13	-9.224
	N26-C27	1.40166	<O14-Zn-O59	98.816	<O60-C56-C55-C56	-0.288
	S23-C20	1.79382	<O13-Zn-O93	82.974	<C56-C55-C57-O58	-167.839
	S69-O70	1.46184	<O39-Zn-O60	94.923	<C56-C55-C57-O59	12.472
	S69-O71	1.44953	<O14-Zn-O96	85.801	<C11-O13-Zn-O60	4.116
	S69-N72	1.72405	<O96-Zn-O59	87.625	<C10-O14-Zn-O59	171.854

N72-C73	1.38714	<O13-Zn-O59	172.413	<O60-Zn-O59-C57	-1.985
S69-C66	1.79483	<O14-Zn-O60	172.674	<C11-O13-Zn-O60	-166.564
O13-C11	1.30188			<C10-O14-Zn-O59	171.854
O12-C11	1.21506			<O14-Zn-O13-C11	6.994
O14-C10	1.38861				
O13-Zn	1.95054				
O14-Zn	2.15163				
O59-C57	1.29810				
O58-C57	1.21575				
O60-C56	1.38163				
O59-Zn	1.94275				
O60-Zn	2.16987				
O93-Zn	2.24332				
O96-Zn	2.27951				