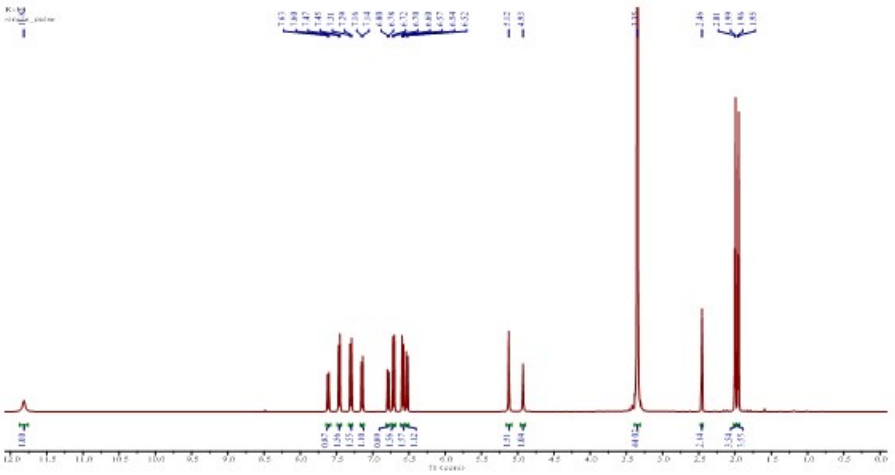


Figure. 1SI ^{1}H-NMR of (3Z, 2'E, 3'Z)-N2, N2'-biylbis (N3-hydroxybutane-2, 3-diimine)

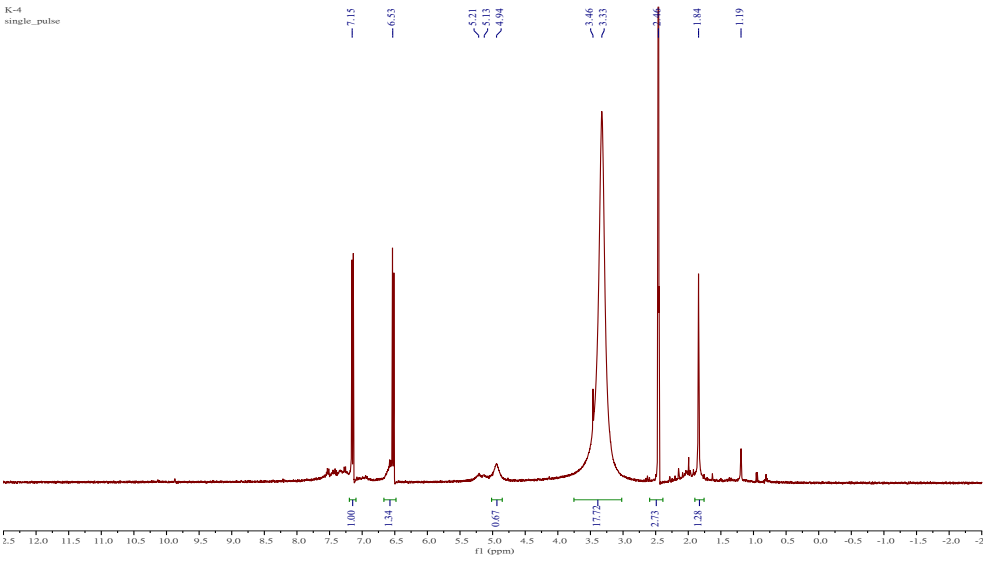


Figure. 2SI ^{1}H-NMR of bis-benzidinedioxime palladium II.

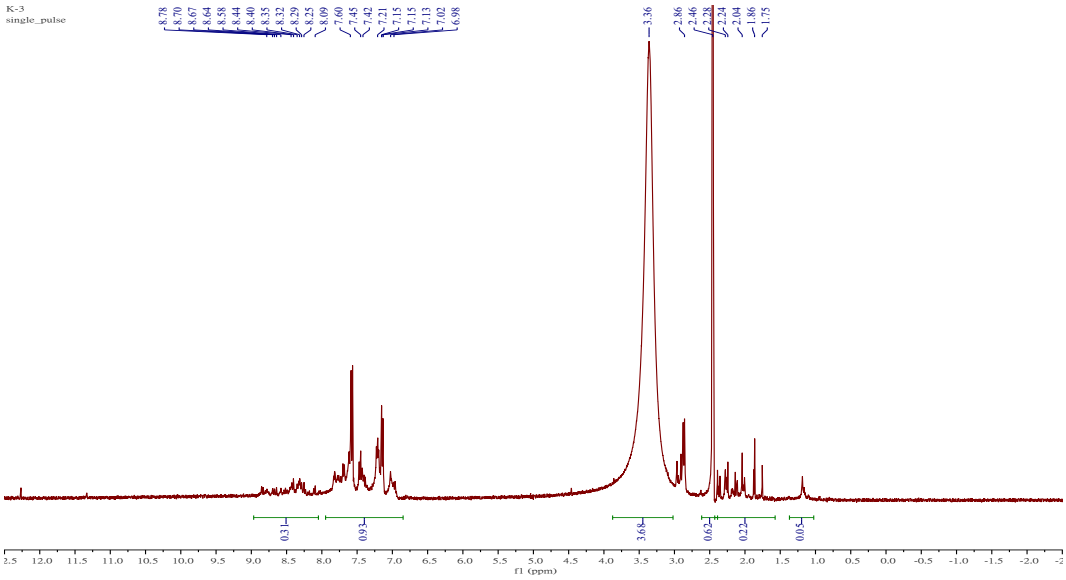


Figure. 3SI[1]H-NMR of bis-benzidinedioxime Platinum(IV) .

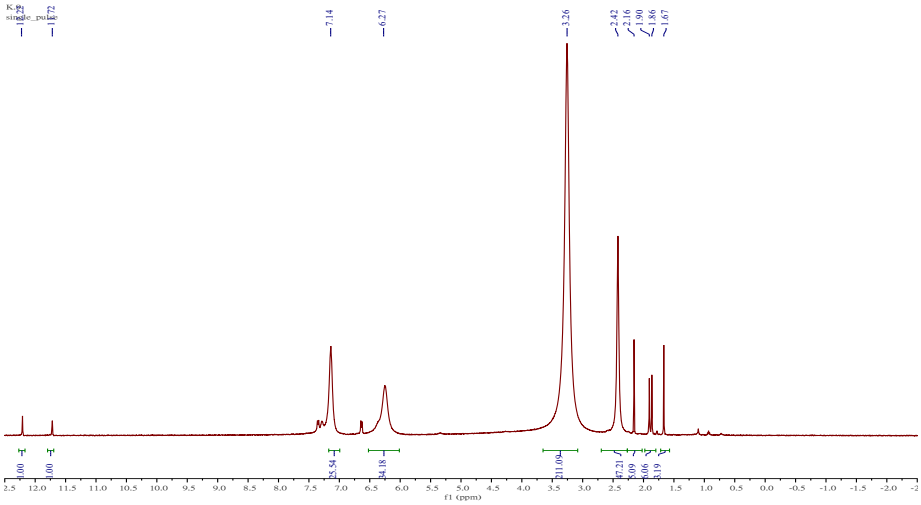


Figure. 4SI [1]H-NMR of bis-benzidinedioxime nickel II.

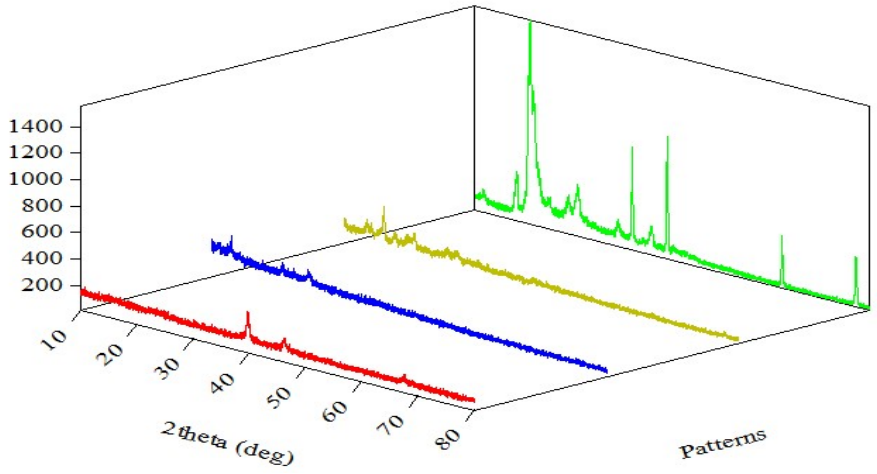
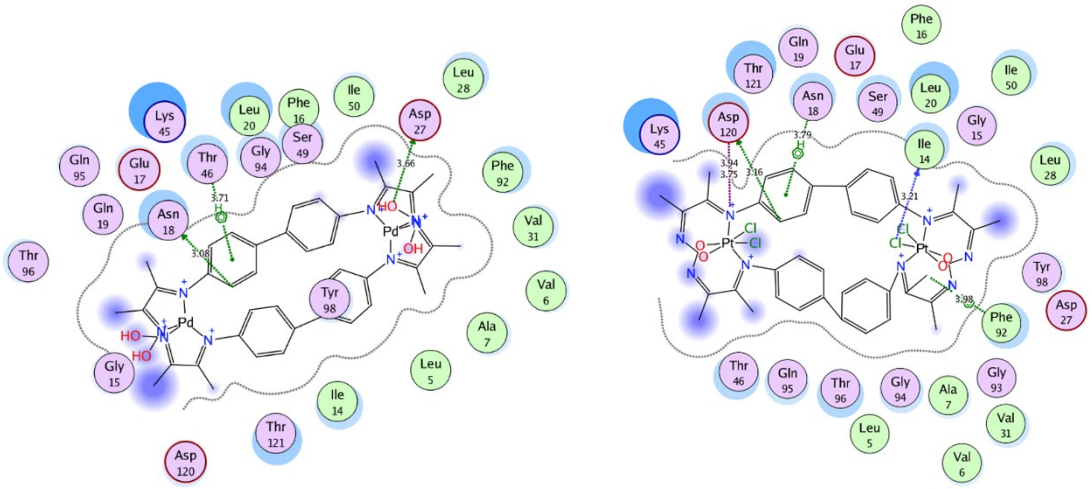
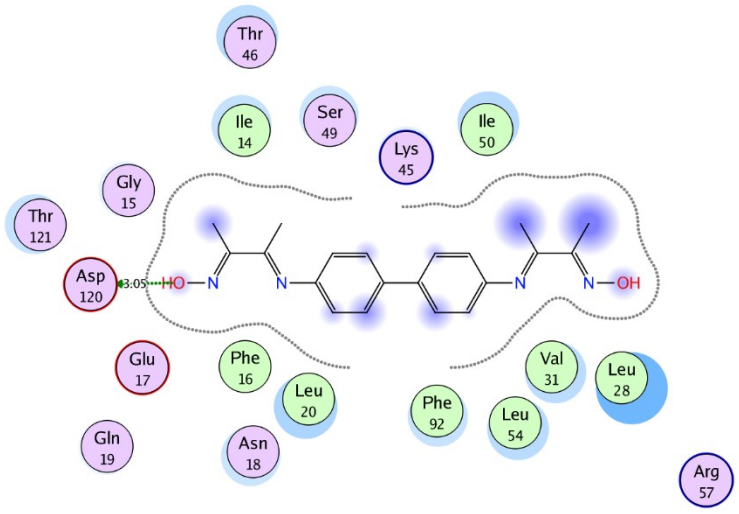


Figure. 5SI Illustrates analysis of PXRD spectrum of bis-benzidine dioxime and complexes, the green line is absorbed pattern of benzidinedioxime, the yellow line is absorbed pattern of bis-benzidinedioxime nickel II, the blue line is absorbed pattern of bis-benzidinedioxime Palladium(II) and red is absorbed pattern of bis-benzidinedioxime Platinum(IV) .

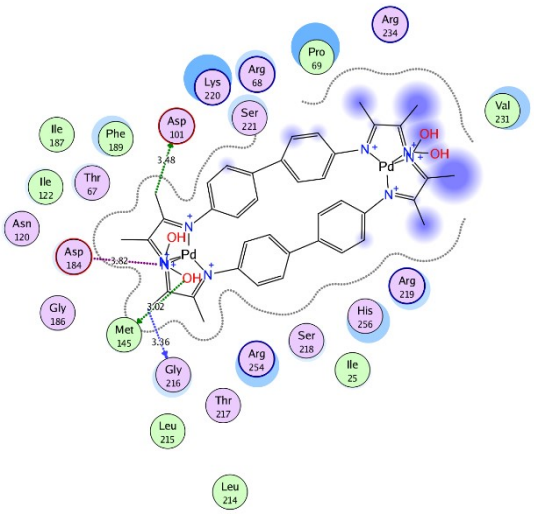


(D) (E)

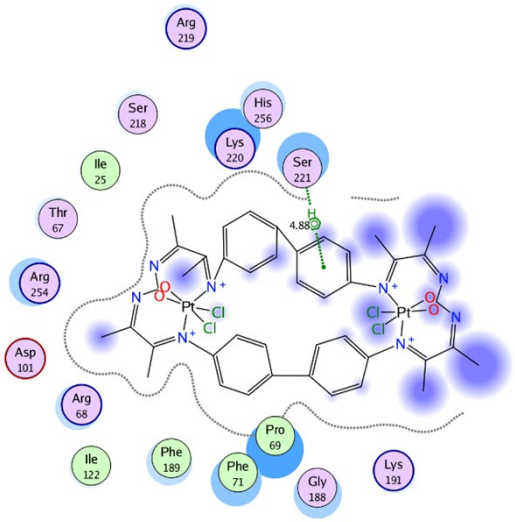


(F)

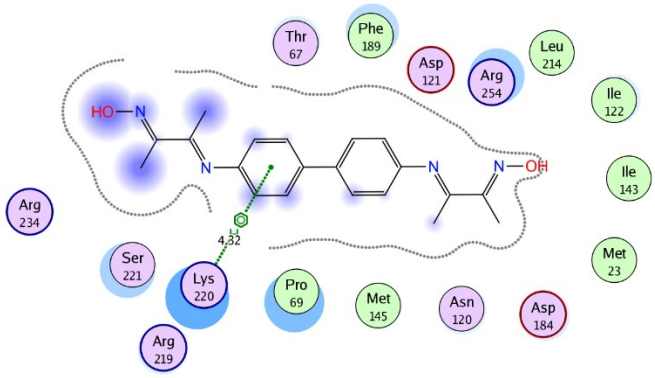
Figure. 6SI 2D interaction of benzidinedioxime and bis-benzidinedioxime complexes with DHFR pocket, (D - F) 2D interaction of complex of palladium(II), platinum(IV), and benzidinedioxime with DHBR pocket respectively



(I)



(J)



(K)

Figure. 7SI: 2D interaction of benzidinedioxime and bis-benzidinedioxime complexes with DHBS pocket, (I - K) 2D interaction of complex of palladium(II), platinum(IV), and benzidinedioxime with DHBR pocket respectively

Table 1SI Bonds distance of bis-benzidinedioxime nickel(II)

Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance
C-C	C1	C2	1.41	C-H	C21	H68	1.01	C-N	C40	N41	1.31
C-C	C1	C3	1.62	C-H	C21	H69	1.11	C-C	C40	C46	1.58
C-H	C1	H59	1.12	C-H	C22	H70	1.11	N-O	N41	O51	1.34
C-C	C2	C4	1.41	C-H	C22	H71	1.11	N-Ni	N41	Ni53	1.89
C-H	C2	H60	1.12	C-H	C22	H72	1.11	N-C	N42	C43	1.33
C-C	C3	C5	1.45	C-H	C23	H73	1.11	N-Ni	N42	Ni52	1.83
C-N	C3	N13	1.37	C-H	C23	H74	1.11	C-C	C43	C44	1.48
C-C	C4	C6	1.40	C-H	C23	H75	1.11	C-C	C43	C48	1.71
C-C	C4	C7	1.60	C-H	C24	H76	1.11	C-N	C44	N45	1.31
C-C	C5	C6	1.41	C-H	C24	H77	1.11	C-C	C44	C49	1.59
C-H	C5	H61	1.05	C-H	C24	H78	1.11	N-O	N45	O50	1.35
C-H	C6	H62	1.13	O-H	O25	H79	1.03	N-Ni	N45	Ni52	1.82
C-C	C7	C8	1.41	C-C	C26	C27	1.41	C-H	C46	H88	1.11
C-C	C7	C9	1.40	C-C	C26	C28	1.40	C-H	C46	H89	1.11
C-C	C8	C10	1.41	C-H	C26	H80	1.13	C-H	C46	H90	1.11
C-H	C8	H63	1.12	C-C	C27	C29	1.41	C-H	C47	H91	1.11
C-C	C9	C11	1.40	C-H	C27	H81	1.12	C-H	C47	H92	1.11

Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance
C-C	C10	C12	1.40	C-N	C28	N38	1.54	C-H	C48	H94	1.09
C-H	C10	H65	1.13	C-C	C29	C31	1.40	C-H	C48	H95	1.14
C-C	C11	C12	1.39	C-C	C29	C32	1.59	C-H	C48	H96	0.98
C-H	C11	H66	1.24	C-C	C30	C31	1.40	C-H	C49	H97	1.11
C-N	C12	N17	1.54	C-H	C30	H82	1.14	C-H	C49	H98	1.11
N-C	N13	C14	1.33	C-H	C31	H83	1.12	C-H	C49	H99	1.11
N-Ni	N13	Ni52	1.83	C-C	C32	C33	1.40	O-H	O50	H100	1.02
C-C	C14	C15	1.48	C-C	C32	C34	1.41	O-H	O51	H101	1.03
C-C	C14	C22	1.58	C-C	C33	C35	1.41	Ni-O	Ni52	O57	1.86
C-N	C15	N16	1.31	C-H	C33	H84	1.13	Ni-O	Ni52	O58	1.86
C-C	C15	C21	1.59	C-C	C34	C36	1.41	Ni-O	Ni53	O54	1.86
N-Ni	N16	Ni52	1.82	C-H	C34	H85	1.12	Ni-O	Ni53	O55	1.86
N-O	N16	O56	1.39	C-C	C35	C37	1.40	O-H	O54	H102	1.02
N-C	N17	C18	1.32	C-H	C35	H86	1.13	O-H	O54	H103	1.02
N-Ni	N17	Ni53	1.91	C-C	C36	C37	1.39	O-H	O55	H104	1.02
C-C	C18	C19	1.51	C-H	C36	H87	1.12	O-H	O55	H105	1.02
C-C	C18	C23	1.59	C-N	C37	N42	1.56	O-H	O56	H106	1.02
C-N	C19	N20	1.32	N-C	N38	C39	1.32	O-H	O57	H107	1.02
C-C	C19	C24	1.57	N-Ni	N38	Ni53	1.91	O-H	O57	H108	1.02
N-O	N20	O25	1.35	C-C	C39	C40	1.50	O-H	O58	H109	1.02
N-Ni	N20	Ni53	1.89	C-C	C39	C47	1.58	O-H	O58	H110	1.02

Type	Angle	Type	Angle	Type	Angle	Type	Angle
C2-C1-C3	124.51	N16-C15-C21	122.43	C28-C26-H80	118.02	C40-C46-H90	110.15
C2-C1-H59	120.29	C15-N16-Ni52	116.54	C26-C28-C30	118.39	O51-N41-Ni53	120.77
C1-C2-C4	121.84	C15-N16-O56	118.19	C26-C28-N38	121.66	N41-O51-H101	112.88
C1-C2-H60	118.81	C15-C21-H67	110.62	C29-C27-H81	119.08	N41-Ni53-O54	99.12
C3-C1-H59	114.58	C15-C21-H68	109.14	C27-C29-C31	117.04	N41-Ni53-O55	90.41
C1-C3-C5	102.26	C15-C21-H69	115.73	C27-C29-C32	122.77	C43-N42-Ni52	115.17
C1-C3-N13	121.12	Ni52-N16-O56	125.01	C30-C28-N38	119.89	N42-C43-C44	111.71
C4-C2-H60	119.35	N16-Ni52-N42	160.31	C28-C30-C31	120.84	N42-C43-C48	124.54
C2-C4-C6	116.96	N16-Ni52-N5	88.99	C28-C30-H82	127.91	N42-Ni52-N45	83.8
C2-C4-C7	121.33	N16-Ni52-O57	85.83	C28-N38-C39	120	N42-Ni52-O57	77.69
C5-C3-N13	128.12	N16-Ni52-O58	101.76	C28-N38-Ni53	124.83	N52-Ni52-O58	96
C3-C5-C6	130.54	N16-O56-H106	116.51	C31-C29-C32	120.18	C44-C43-C48	123.49
C3-C5-H61	119.36	C18-N17-Ni53	115.37	C29-C31-C30	121.87	C43-C44-N45	110.91
C3-N13-C14	123.9	N17-C18-C19	112.63	C29-C31-H83	119.77	C43-C44-C49	123.9
C3-N13-Ni52	120.07	N17-C18-C23	123.67	C29-C32-C33	121.52	C43-C48-H94	103.36
C6-C4-C7	121.68	N17-Ni53-N20	82.8	C29-C33-C34	121.34	C43-C48-H95	103.1
C4-C6-C5	120.97	N17-Ni53-N38	111.98	C31-C30-H82	110.17	C43-C48-H96	109.83
C4-C6-H62	119.38	N17-Ni53-N41	162.69	C30-C31-H83	118.36	N45-C44-C49	125.03
C4-C7-C8	122.97	N17-Ni53-O54	92.76	C33-C32-C34	117.13	C44-N45-O50	119.81
C4-C7-C9	120.09	N17-Ni53-O55	79.98	C32-C33-C35	121	C44-N45-Ni52	117.26
C6-C5-H61	108.88	C18-C19-C23	123.66	C32-C33-H84	119.32	C44-C49-H97	110.09
C5-C6-H62	119.65	C18-C19-N20	111.99	C32-C34-C36	121.6	C44-C49-H98	109.64

Table 2SI Bond angles of bis-benzidinedioxime of nickel(II)

Type	Angle	Type	Angle	Type	Angle	Type	Angle
C8-C7-C9	116.93	C18-C19-C24	124.23	C32-C34-H85	119.43	C44-C49-H99	116.82
C7-C8-C18	120.98	C18-C23-H73	113.53	C35-C33-H84	119.68	O50-N45-Ni52	122.88
C7-C8-H63	119.1	C18-C23-H74	109.61	C33-C35-C37	121.41	N45-O50-H100	115.89
C7-C9-C11	121.89	C18-C23-H75	113.28	C33-C35-H86	120.37	N45-Ni52-O57	101.27
C7-C9-H64	119.74	N20-C19-C24	123.76	C36-C34-H85	118.96	N45-Ni52-O58	85.96
C10-C8-H63	119.92	C19-N20-O25	123.13	C34-C36-C37	120.99	H88-C46-H89	104.4
C8-C10-C12	120.89	C19-N20-Ni53	116.62	C34-C36-H87	119.99	H88-C46-H90	108.33
C8-C10-H65	121.07	C19-C24-H76	110.44	C37-C35-H86	118.22	H89-C46-H90	108.58
C11-C9-H64	118.37	C19-C24-H77	109.85	C35-C37-C36	117.74	H91-C47-H92	109.68
C9-C11-C12	120.89	C19-C24-H78	114.68	C35-C37-N42	118.41	H91-C47-H93	106.56
C9-C11-H66	123.84	O25-N20-Ni53	120.25	C37-C36-H87	119.02	H92-C47-H93	104.46
C12-C10-H65	118.04	N20-O25-H79	113.06	C36-C37-N42	123.79	H94-C48-H95	102.79
C10-C12-C11	118.35	N20-Ni53-N38	162.24	C37-N42-C43	117.44	H94-C48-H96	119.35
C10-C12-N17	121.86	N20-Ni53-N41	84.57	C37-N42-Ni52	127.38	H95-C48-H96	116.49
C12-C11-H66	114.89	N20-Ni53-O54	90.28	C39-N38-Ni53	115.11	H97-C49-H98	110.11
C11-C12-N17	119.73	N20-Ni53-O55	99.15	N38-C39-C40	112.84	H97-C49-H99	104.25
C12-N17-C18	119.47	H67-C21-H68	96.47	N38-C39-C47	125.05	H98-C49-H99	105.67
C12-N17-Ni53	125.01	H67-C21-H69	104.32	N38-Ni53-N41	82.72	O57-Ni52-O58	169.69
C14-N13-Ni52	115.17	H68-C21-H69	118.5	N38-Ni53-O54	79.57	Ni52-O57-H107	117.65
N13-C14-C15	111.54	H70-C22-H71	110.96	N38-Ni53-O55	93.32	Ni52-O57-H108	118.45

Type	Angle	Type	Angle	Type	Angle	Type	Angle
N13-C14-C22	125.62	H70-C22-H72	106.19	C40-C39-C47	122.05	Ni52-O58-H109	118
N13-Ni52-N16	84.25	H71-C22-H72	103.93	C39-C40-N41	112.06	Ni52-O58-H110	118.8
N13-Ni52-N2	108.05	H73-C23-H74	109.04	C39-C40-C46	124.39	O54-Ni53-O55	167.21
N13-Ni52-N45	160.5	H73-C23-H75	103.26	C39-C47-H91	110.05	N53i-O54-H102	115.33
N13-Ni52-O57	96.48	H74-C23-H75	107.8	C39-C47-H92	110.87	Ni53-O54-H103	116.44
N13-Ni52-O58	77.58	H76-C24-H77	110.58	C39-C47-H93	114.95	Ni53-O55-H104	116.25
C15-C14-C22	122.81	H76-C24-H78	106.09	N41-C40-C46	123.52	Ni53-O55-H105	115.28
C14-C15-N16	111.24	H77-C24-H78	105.03	C40-N41-O51	122.72	H102-O54-H103	106.08
C14-C15-C21	126.17	C27-C26-C28	120.89	C40-N41-Ni53	116.5	H104-O55-H105	106.64
C14-C22-H70	110.65	C27-C26-H80	121.09	C40-C46-H88	112.08	H107-O57-H108	110.22
C14-C22-H71	109.4	C26-C27-C29	120.91	C40-C46-H89	113.04	H109-O58-H110	110.23
C14-C22-H72	115.51	C26-C27-H81	120.01				

Table 3SI Bonds distance of bis-benzidinedioxime palladium(II)

Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance
C-C	C1	C2	1.3971	C-N	C20	N22	1.30467	C-C	C36	C38	1.3955
C-C	C1	C3	1.39461	C-C	C20	C23	1.58557	C-H	C36	H83	1.1267
C-H	C1	H55	1.13005	O-N	O21	N22	1.34211	C-C	C37	C38	1.3919
C-C	C2	C4	1.39792	O-H	O21	H64	1.02614	C-H	C37	H84	1.1322
C-H	C2	H56	1.12017	N-Pd	N22	Pd53	1.76112	C-N	C38	N39	1.5193
C-C	C3	C5	1.398	C-H	C23	H65	1.11305	N-C	N39	C40	1.3357
C-N	C3	N18	1.52322	C-H	C23	H66	1.11024	N-Pd	N39	Pd53	1.8124
C-C	C4	C6	1.40069	C-H	C23	H67	1.10953	C-C	C40	C42	1.484
C-C	C4	C7	1.56481	C-H	C24	H68	1.11038	C-C	C40	C51	1.5957
C-C	C5	C6	1.41167	C-H	C24	H69	1.11088	O-N	O41	N43	1.3426
C-H	C5	H57	1.12516	C-H	C24	H70	1.10928	O-H	O41	H85	1.0267
C-H	C6	H58	1.12613	C-H	C25	H71	1.11276	C-N	C42	N43	1.3049
C-C	C7	C8	1.40405	C-H	C25	H72	1.11437	C-C	C42	C52	1.5796
C-C	C7	C9	1.39218	C-H	C25	H73	1.1093	N-Pd	N43	Pd53	1.7718
C-C	C8	C10	1.41351	C-H	C26	H74	1.11296	N-C	N44	C45	1.3319
C-H	C8	H59	1.12291	C-H	C26	H75	1.11006	N-Pd	N44	Pd54	2.0315
C-C	C9	C11	1.38971	C-H	C26	H76	1.11254	C-C	C45	C46	1.5804
C-H	C9	H60	1.10466	C-C	C27	C28	1.41353	C-C	C45	C50	1.5802
C-C	C10	C12	1.39805	C-C	C27	C29	1.39638	C-N	C46	N48	1.3243

Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance
C-H	C10	H61	1.12352	C-H	C27	H77	1.12423	C-C	C46	C49	1.5701
C-C	C11	C12	1.38694	C-C	C28	C30	1.40516	O-N	O47	N48	1.3357
C-H	C11	H62	1.13612	C-H	C28	H78	1.12763	O-H	O47	H86	1.0142
C-N	C12	N13	1.50778	C-C	C29	C31	1.38927	N-Pd	N48	Pd54	2.0147
N-C	N13	C14	1.32842	C-N	C29	N44	1.50601	C-H	C49	H87	1.1149
N-Pd	N13	Pd54	2.02559	C-C	C30	C32	1.39425	C-H	C49	H88	1.1131
C-C	C14	C16	1.5896	C-C	C30	C33	1.56761	C-H	C49	H89	1.1102
C-C	C14	C25	1.57414	C-C	C31	C32	1.38842	C-H	C50	H90	1.1128
O-N	O15	N17	1.33439	C-H	C31	H79	1.13557	C-H	C50	H91	1.1106
O-H	O15	H63	1.01307	C-H	C32	H80	1.10777	C-H	C50	H92	1.1128
C-N	C16	N17	1.32854	C-C	C33	C34	1.40546	C-H	C51	H93	1.1107
C-C	C16	C26	1.57109	C-C	C33	C35	1.40004	C-H	C51	H94	1.1147
N-Pd	N17	Pd54	2.0075	C-C	C34	C36	1.40969	C-H	C51	H95	1.1091
N-C	N18	C19	1.33829	C-H	C34	H81	1.12536	C-H	C52	H96	1.1123
N-Pd	N18	Pd53	1.81437	C-C	C35	C37	1.3943	C-H	C52	H97	1.107
C-C	C19	C20	1.49286	C-H	C35	H82	1.12017	C-H	C52	H98	1.1146
C-C	C19	C24	1.59992								

Table 4SI Bond angles of bis-benzidinedioxime palladium(II)

Type	Angle	Type	Angle	Type	Angle	Type	Angle
C2-C1-C3	120.04	C8-C7-C9	118.35	N13-Pd54-N44	125.74	N18-Pd53-N39	91.64
C2-C1-H55	121.1	C7-C8-C10	120	N13-Pd54-N48	127.76	N18-Pd53-N43	174.05
C1-C2-C4	121.15	C7-C8-H59	118.82	C16-C14-C255	121.96	C20-C19-C24	119.23
C1-C2-H56	119.66	C7-C9-C11	121.89	C14-C16-N17	115.75	C19-C20-N22	111.22
C3-C1-H55	118.85	C7-C9-H60	118.82	C14-C16-C26	121.92	C19-C20-C23	123.43
C1-C3-C5	119.54	C10-C8-H59	121.14	C14-C25-H71	113.85	C19-C24-H68	110.38
C1-C3-N18	117.48	C8-C10-C12	119.89	C14-C25-H72	109.21	C19-C24-H69	109.18
C4-C2-H56	119.19	C8-C10-H61	121.93	C14-C25-H73	112.17	C19-C24-H70	117.89
C2-C4-C6	118.72	C11-C9-H60	119.28	N17-O15-H63	111.69	N22-C20-C23	125.16
C2-C4-C7	117.2	C9-C11-C12	119.69	O15-N17-C16	126.39	C20-N22-O21	122.88
C5-C3-N18	122.71	C9-C11-H62	120.79	O15-N17-Pd54	122.2	C20-N22-Pd53	114.44
C3-C5-C6	120.19	C12-C10-H61	118.17	N17-C16-C26	122.24	C20-C23-H65	109.07
C3-C5-H57	118.1	C10-C12-C11	119.94	C16-N17-Pd54	110.87	C20-C23-H66	114.58
C3-N18-C19	113.76	C10-C12-N13	125.84	C16-C26-H74	109.72	C20-C23-H67	112.92
C3-N18-Pd53	132.12	C12-C11-H62	119.5	C16-C26-H75	110.01	N22-O21-H64	112.71
C6-C4-C7	123.88	C11-C12-N13	114.22	C16-C26-H76	115.45	O21-N22-Pd53	120.36
C4-C6-C5	120.2	C12-N13-C14	121.12	N17-Pd54-N44	126.59	N22-Pd53-N39	174.15
C4-C6-H58	118.91	C12-N13-Pd54	122.5	N17-Pd54-N48	109.67	N22-Pd53-N43	90.69
C4-C7-C8	125.19	C14-N13-Pd54	110.49	C19-N18-Pd53	109.58	H65-C23-H66	106.59
C4-C7-C9	116.24	N13-C14-C16	115.94	N18-C19-C20	113.41	H65-C23-H67	108.1
C6-C5-H57	121.71	N13-C14-C25	121.78	N18-C19-C24	127.28	H66-C23-H67	105.21
C5-C6-H58	120.89	N13-Pd54-N17	85.96	N18-Pd53-N22	89.45	H68-C24-H69	110.46

Type	Angle	Type	Angle	Type	Angle	Type	Angle
H68-C24-H70	104.95	C29-N44-Pd54	121.85	C38-C37-H84	119.1	C45-N44-Pd54	111.08
H69-C24-H70	103.67	C32-C30-C33	116.58	C37-C38-N39	116.79	N44-C45-C46	115.69
H71-C25-H72	108.33	C30-C32-C31	121.98	C38-N39-C40	113.29	N44-C45-C50	122.91
H71-C25-H73	103.84	C30-C32-H80	119.1	C38-N39-Pd53	132.16	N44-Pd54-N48	84.98
H72-C25-H73	109.22	C30-C33-C34	123.74	C40-N39-Pd39	109.93	C46-C45-C50	121.15
H74-C26-H75	110.08	C30-C33-C35	117.62	N39-C40-C42	112.95	C45-C46-N48	115.49
H74-C26-H76	105.13	C32-C31-H79	120.86	N39-C40-C51	125.78	C45-C46-C49	123.24
H75-C26-H76	106.25	C31-C32-H80	118.92	N39-Pd53-N43	88.82	C45-C50-H90	110.53
C28-C27-C29	119.97	C34-C33-C35	118.44	C42-C40-C51	121.17	C45-C50-H91	109.32
C28-C27-H77	121.97	C33-C34-C36	120.35	C40-C42-N43	111.01	C45-C50-H92	115.97
C27-C28-C30	120.2	C33-C34-H81	119.11	C40-C2-C52	126.06	N48-C46-C49	121.18
C27-C28-H78	120.75	C33-C35-C37	121.04	C40-C51-H93	115.06	C46-N48-O47	125.61
C29-C27-H77	118.05	C33-C35-H82	119.52	C40-C51-H94	110.45	C46-N48-Pd54	111.55
C27-C29-C31	119.76	C36-C34-H81	120.54	C40-C51-H95	112.29	C46-C49-H87	110.01
C27-C29-N44	125.71	C34-C36-C38	120	N43-O41-H85	113.87	C46-C49-H88	112.66
C30-C28-H78	119.03	C34-C36-H83	121.76	O41-N-43C42	121.51	C46-C49-H89	112.59
C28-C30-C32	118.07	C37-C35-H82	119.44	O41-N43-Pd53	121.4	N48-O47-H86	111.58
C28-C30-C33	125.14	C35-C37-C38	120.21	N43-C42-C52	122.83	O47-N48-Pd54	122.26
C31-C29-N44	114.53	C35-C37-H84	120.68	C42-N43-Pd53	114.11	H87-C49-H88	108.61
C29-C31-C32	119.83	C38-C36-H83	118.24	C42-C52-H96	111.15	H87-C49-H89	107.74
C29-C31-H79	119.3	C36-C38-C37	119.73	C42-C52-H97	113.65	H88-C49-H89	104.96
C29-N44-C45	121.73	C36-C38-N39	123.21	C42-C52-H98	111.21	H90-C50-H91	110.29

Type	Angle	Type	Angle	Type	Angle	Type	Angle
H90-C50-H92	104.51	H93-C51-H94	108.64	H94-C51-H95	108.68	H96-C52-H98	108.16
H91-C50-H92	106.01	H93-C51-H95	101.23	H96-C52-H97	108.58	H97-C52-H98	103.71

Table 5SI Bonds distance of bis-benzidinedioxime of platinum(IV)

Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance
C-C	C1	C2	1.31623	C-H	C12	H63	1.0736	C-H	C24	H73	1.1308
C-C	C1	C6	1.34595	C-C	C13	C14	1.3743	C-H	C24	H74	1.1011
C-H	C1	H59	1.07414	C-H	C13	H64	1.0606	C-H	C24	H75	1.1026
C-C	C2	C3	1.37877	C-C	C14	C15	1.3918	C-H	C25	H76	1.0774
C-H	C2	H60	1.06702	C-N	C14	N17	1.3347	C-H	C25	H77	1.0827
C-C	C3	C4	1.37551	C-C	C15	C16	1.3247	C-H	C25	H78	1.1301
C-C	C3	C8	1.30072	C-H	C15	H65	1.0771	O-Pt	O26	Pt54	1.8685
C-C	C4	C5	1.32825	C-H	C16	H66	1.0563	Pt-N	Pt27	N34	2.1544
C-H	C4	H61	1.08839	N-C	N17	C18	1.2612	Pt-O	Pt27	O48	1.8577
C-C	C5	C6	1.3946	N-Pt	N17	Pt54	2.0103	Pt-Cl	Pt27	Cl57	2.3947
C-H	C5	H62	1.08513	C-C	C18	C19	1.4966	Pt-Cl	Pt27	Cl58	2.3452
C-N	C6	N7	1.28816	C-C	C18	C24	1.5588	C-C	C28	C29	1.335
N-C	N7	C11	1.28951	C-N	C19	N20	1.2872	C-C	C28	C33	1.4321
N-Pt	N7	Pt27	1.93236	C-C	C19	C25	1.5105	C-H	C28	H79	1.0799
C-C	C8	C12	1.35852	N-O	N20	O26	1.2623	C-C	C29	C30	1.3742
C-C	C8	C16	1.36445	O-Pt	O21	Pt27	1.9296	C-H	C29	H80	1.0886
N-C	N9	C10	1.27976	C-H	C22	H67	1.0958	C-C	C30	C31	1.3581
N-O	N9	O21	1.30618	C-H	C22	H68	1.0938	C-C	C30	C35	1.31
C-C	C10	C11	1.45581	C-H	C22	H69	1.0966	C-C	C31	C32	1.2989
C-C	C10	C22	1.46117	C-H	C23	H70	1.0933	C-H	C31	H81	1.0594
C-C	C11	C23	1.49662	C-H	C23	H71	1.0971	C-C	C32	C33	1.3395
C-C	C12	C13	1.31237	C-H	C23	H72	1.0908	C-H	C32	H82	1.0203

Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance	Type	Atom 1	Atom 2	Distance
C-N	C33	N34	1.37028	C-N	C41	N44	1.3459	C-H	C49	H89	1.1069
N-C	N34	C38	1.30259	C-C	C42	C43	1.3358	C-H	C50	H90	1.0769
C-C	C35	C39	1.372	C-H	C42	H85	1.0713	C-H	C50	H91	1.0945
C-C	C35	C43	1.375	C-H	C43	H86	1.0853	C-H	C50	H92	1.102
N-C	N36	C37	1.26276	N-C	N44	C45	1.2899	C-H	C51	H93	1.0912
N-O	N36	O48	1.27114	N-Pt	N44	Pt54	2.0352	C-H	C51	H94	1.1082
C-C	C37	C38	1.44333	C-C	C45	C46	1.4852	C-H	C51	H95	1.1016
C-C	C37	C49	1.42642	C-C	C45	C51	1.5072	C-H	C52	H96	1.0978
C-C	C38	C50	1.54902	C-N	C46	N47	1.2683	C-H	C52	H97	1.1042
C-C	C39	C40	1.29343	C-C	C46	C52	1.4396	C-H	C52	H98	1.078
C-H	C39	H83	1.07789	N-O	N47	O53	1.2705	O-Pt	O53	Pt54	1.8753
C-C	C40	C41	1.34549	C-H	C49	H87	1.084	Pt-Cl	Pt54	Cl55	2.4225
C-H	C40	H84	1.02447	C-H	C49	H88	1.0933	Pt-Cl	Pt54	Cl56	2.3616
C-C	C41	C42	1.41447								

Table 6SI Bond angles of bis-benzidinedioxime platinum(IV)

Type	Angle	Type	Angle	Type	Angle	Type	Angle
C2-C1-C6	117.19	C11-N7-Pt27	124.88	C11-C23-H70	112.57	N17-Pt54-Cl55	85.86
C2-C1-H59	121.84	N7-C11-C10	121.58	C11-C23-H71	110.87	N17-Pt54-Cl56	89.54
C1-C2-C3	117.64	N7-C11-C23	120.45	C11-C23-H72	105.27	C19-C18-C24	119.21
C1-C2-H60	118.87	N7-Pt27-O21	86.48	C13-C12-H63	120.56	C18-C19-N20	124.17
C6-C1-H59	120.96	N7-Pt27-N34	103.93	C12-C13-C14	119.35	C18-C19-C25	112.12
C1-C6-C5	126.28	N7-Pt27-O48	171.57	C12-C13-H64	119.14	C18-C24-H73	117.53
C1-C6-N7	115.77	N7-Pt27-Cl57	81.12	C14-C13-H64	121.5	C18-C24-H74	112.14
C3-C2-H60	123.41	N7-Pt27-Cl58	92.14	C13-C14-C15	122.56	C18-C24-H75	103.37
C2-C3-C4	125.52	C12-C8-C16	124.86	C13-C14-N17	116.35	N20-C19-C25	122.14
C2-C3-C8	117.73	C8-C12-C13	117.1	C15-C14-N17	119.58	C19-N20-O26	119.23
C4-C3-C8	116.74	C8-C12-H63	122.31	C14-C15-C16	117.1	C19-C25-H76	99.71
C3-C4-C5	116.63	C8-C16-C15	118.42	C14-C15-H65	122.82	C19-C25-H77	115.94
C3-C4-H61	120.89	C8-C16-H66	120.29	C14-N17-C18	117.46	C19-C25-H78	124.91
C3-C8-C12	117.8	C10-N9-O21	121.52	C14-N17-Pt54	124.82	N20-O26-Pt54	114.53
C3-C8-C16	117.3	N9-C10-C11	123.09	C16-C15-H65	120.05	O21-Pt27-N34	167.65
C5-C4-H61	122.46	N9-C10-C22	119.14	C15-C16-H66	121.29	O21-Pt27-O48	85.73
C4-C5-C6	116.64	N9-O21-Pt27	120.73	C18-N17-Pt54	117.32	O21-Pt27-Cl57	91.95
C4-C5-H62	120.47	C11-C10-C22	117.76	N17-C18-C19	119.79	O21-Pt27-Cl58	96.16
C6-C5-H62	122.88	C10-C11-C23	117.96	N17-C18-C24	120.58	H67-C22-H68	103.72
C5-C6-N7	117.83	C10-C22-H67	104.92	N17-Pt54-O26	88.39	H67-C22-H69	116.67
C6-N7-C11	119.35	C10-C22-H68	111.57	N17-Pt54-N44	97.01	H68-C22-H69	109.92
C6-N7-Pt27	115.4	C10-C22-H69	109.85	N17-Pt54-O53	174.61	H70-C23-H71	104.42

Type	Angle	Type	Angle	Type	Angle	Type	Angle
H70-C23-H72	111.89	C29-C28-H79	116.53	C39-C35-C43	124.58	C42-C41-N44	119.59
H71-C23-H72	111.99	C28-C29-C30	116.64	C35-C39-C40	118.26	C41-C42-C43	118.04
H73-C24-H74	97.76	C28-C29-H80	121.7	C35-C39-H83	124.48	C41-C42-H85	124.21
H73-C24-H75	115.08	C33-C28-H79	125	C35-C43-C42	116.57	C41-N44-C45	119.34
H74-C24-H75	111.23	C28-C33-C32	121.12	C35-C43-H86	121.67	C41-N44-Pt54	122.06
H76-C25-H77	99.37	C28-C33-N34	121.73	C37-N36-O48	120.35	C43-C42-H85	117.73
H76-C25-H78	75.64	C30-C29-H80	121.63	N36-C37-C38	125.12	C42-C43-H86	121.74
H77-C25-H78	118.99	C29-C30-C31	124.35	N36-C37-C49	116.2	C45-N44-Pt54	118.35
O26-Pt54-N44	172.24	C29-C30-C35	118.47	C38-C37-C49	118.66	N44-C45-C46	120.64
O26-Pt54-O53	87.5	C31-C30-C35	117.02	C37-C38-C50	114.5	N44-C45-C51	122.06
O26-Pt54-Cl55	92.58	C30-C31-C32	118.8	C37-C49-H87	102.6	N44-Pt54-O53	86.75
O26-Pt54-Cl56	91.75	C30-C31-H81	123.93	C37-C49-H88	106.64	N44-Pt54-Cl55	82.3
N34-Pt27-O48	83.45	C30-C35-C39	115.69	C37-C49-H89	110.63	N44-Pt54-Cl56	93.86
N34-Pt27-Cl57	83.27	C30-C35-C43	119.7	C38-C50-H90	119.9	C46-C45-C51	117.2
N34-Pt27-Cl58	90.15	C32-C31-H81	117.22	C38-C50-H91	111.47	C45-C46-N47	125.21
Pt27-N34-C33	128.07	C31-C32-C33	120.47	C38-C50-H92	111.03	C45-C46-C52	120.07
Pt27-N34-C38	116.96	C31-C32-H82	117.14	C40-C39-H83	117.26	C45-C51-H93	104.07
O48-Pt27-Cl57	95.91	C33-C32-H82	122.37	C39-C40-C41	119.93	C45-C51-H94	113.36
O48-Pt27-Cl58	91.91	C32-C33-N34	116.79	C39-C40-H84	117.4	C45-C51-H95	113.45
Pt27-O48-N36	116.55	C33-N34-C38	114.86	C41-C40-H84	122.64	N47-C46-C52	114.54
Cl57-Pt27-Cl58	169.13	N34-C38-C37	120.1	C40-C41-C42	122.5	C46-N47-O53	119.91
C29-C28-C33	118.4	N34-C38-C50	125.39	C40-C41-N44	117.88	C46-C52-H96	111.54

Type	Angle	Type	Angle	Type	Angle	Type	Angle
C46-C52-H97	107.72	H88-C49-H89	117.43	H93-C51-H95	110.71	H97-C52-H98	107.5
C46-C52-H98	103.41	H90-C50-H91	102.38	H94-C51-H95	108.33	O53-Pt54-Cl55	90.85
N47-O53-Pt54	118.68	H90-C50-H92	107.23	H96-C52-H97	109.21	O53-Pt54-Cl56	94.07
H87-C49-H88	112.21	H91-C50-H92	103.28	H96-C52-H98	116.96	Cl55-Pt54-Cl56	173.59
H87-C49-H89	106.37	H93-C51-H94	106.68				