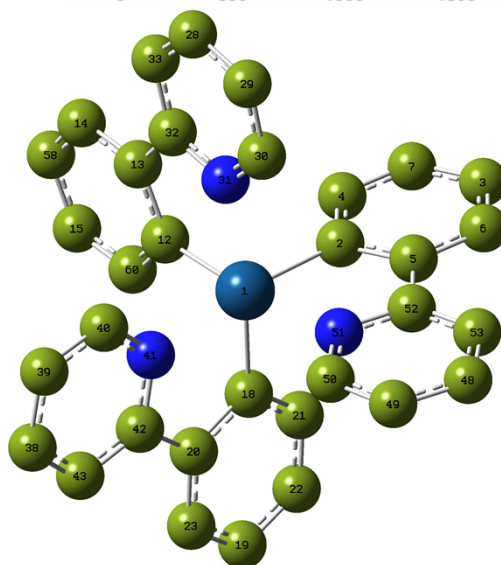


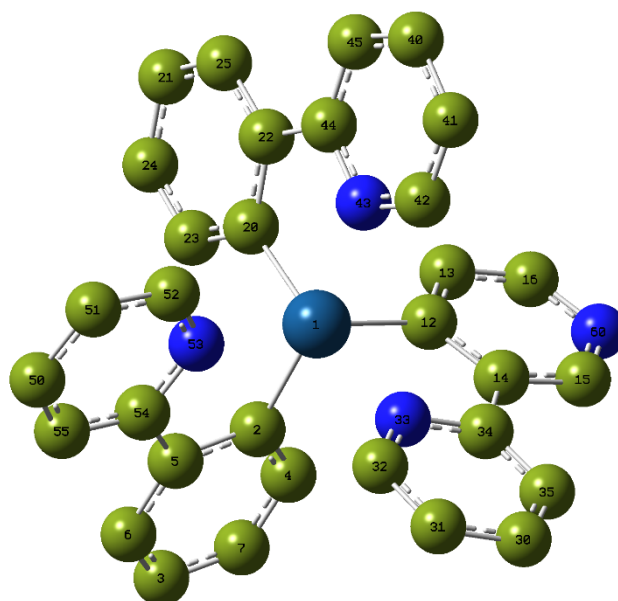
Figure. S1 The calculated Huang-Rhys factors versus the normal mode wavenumber at the ground state for **complexes 1, 2, 5, 6, 7, 8, 10**.

Table S1. The selected bond lengths (Å), angles (°) and dihedral angles (°) of the S_0 and T_1 states and the corresponding modification between the two states for **1**.



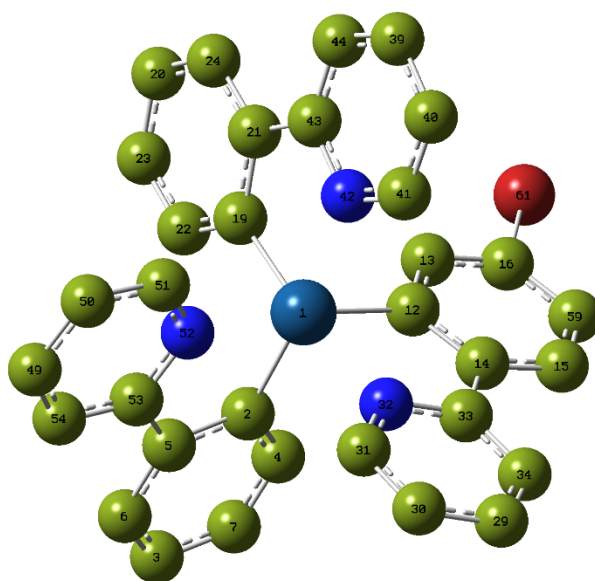
	S ₀	T ₁	Δ (T ₁ -S ₀)
L(Ir1-C2)	2.026	2.023	-0.003
L(Ir1-C12)	2.027	1.983	-0.044
L(Ir1-C18)	2.027	2.041	0.014
L(Ir1-N31)	2.190	2.156	-0.034
L(Ir1-N41)	2.189	2.205	0.016
L(Ir1-N51)	2.190	2.213	0.023
A(Ir1-C2-N51)	53.33	53.89	0.56
A(Ir1-N41-N51)	41.87	42.61	0.74
D(Ir1-C2-C5-C52)	0.580	0.78	0.2
D(C2-C5-C52-N51)	-1.420	-1.09	0.33
Benzene ligands			
C6-C5	1.41	1.41	0.00
C5-C2	1.43	1.43	0.00
C2-C4	1.41	1.41	0.00
C4-C7	1.39	1.39	0.00
C7-C3	1.40	1.40	0.00
C3-C6	1.39	1.39	0.00
C5-C52	1.46	1.46	0.00
Pyridine ligands			
C48-C49	1.40	1.40	0.00
C49-C50	1.39	1.39	0.00
C50-N51	1.34	1.34	0.00
N51-C52	1.36	1.36	0.00
C52-C53	1.41	1.41	0.00
C53-C48	1.39	1.39	0.00

Table S2. The selected bond lengths (Å), angles (°) and dihedral angles (°) of the S₀ and T₁ states and the corresponding modification between the two states for **2**.



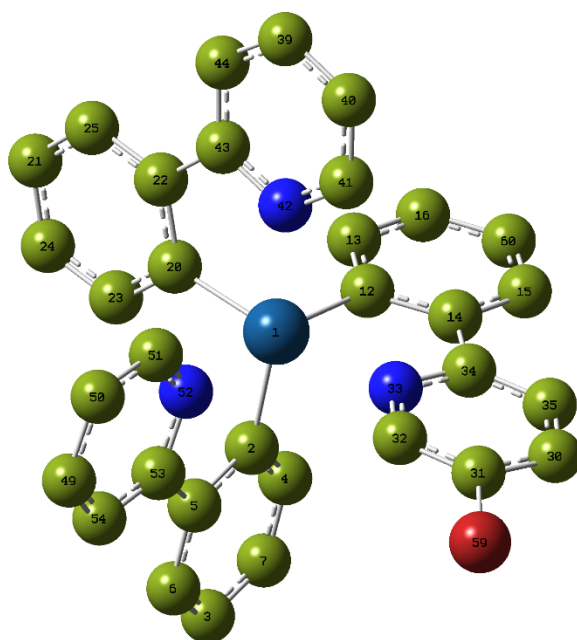
	S_0	T_1	$\Delta (T_1-S_0)$
L(Ir1-C2)	2.028	2.041	0.013
L(Ir1-C12)	2.015	2.023	0.008
L(Ir1-C20)	2.027	1.983	-0.044
L(Ir1-N33)	2.197	2.213	0.016
L(Ir1-N43)	2.193	2.156	-0.037
L(Ir1-N53)	2.188	2.205	0.017
A(Ir1-C12-N33)	53.63	53.35	0.28
A(Ir1-N53-N33)	41.91	43.37	1.46
D(Ir1-C12-C14-C33)	0.58	0.60	0.02
D(C12-C14-C34-N33)	-1.55	-1.52	0.03
N-substituted benzene ligands			
C15-C14	1.40	1.40	0.00
C14-C12	1.43	1.42	0.01
C12-C13	1.41	1.40	0.01
C13-C16	1.39	1.39	0.00
C16-N60	1.35	1.34	0.01
N60-C15	1.33	1.33	0.00
C14-C34	1.46	1.47	0.01

Table S3. The selected bond lengths (\AA), angles ($^\circ$) and dihedral angles ($^\circ$) of the S_0 and T_1 states and the corresponding modification between the two states for **3**.



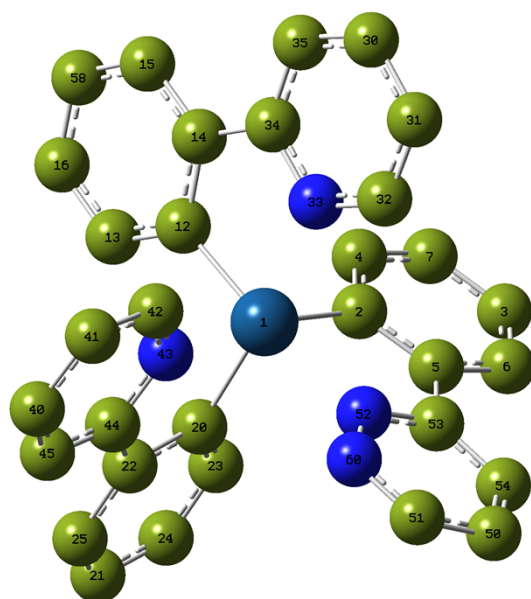
	S_0	T_1	$\Delta (T_1-S_0)$
L(Ir1-C2)	2.027	1.984	-0.043
L(Ir1-C12)	2.024	2.038	0.014
L(Ir1-C19)	2.027	2.024	-0.003
L(Ir1-N32)	2.192	2.206	0.014
L(Ir1-N42)	2.191	2.213	0.022
L(Ir1-N52)	2.183	2.150	-0.033
A(Ir1-C12-N32)	53.44	53.42	-0.020
A(Ir1-N52-N32)	41.99	43.57	1.580
D(Ir1-C12-C14-C33)	1.302	0.290	-1.012
D(C12-C14-C33-N32)	-1.667	-1.447	0.220
Br-substituted benzene ligands			
C15-C14	1.406	1.406	0.00
C14-C12	1.427	1.426	-0.001
C12-C13	1.410	1.408	-0.002
C13-C16	1.388	1.389	0.001
C16-C59	1.395	1.394	-0.001
C59-C15	1.389	1.390	0.001
C14-C33	1.466	1.468	0.002
C16-Br51	1.982	1.980	-0.002

Table S4. The selected bond lengths (\AA), angles ($^\circ$) and dihedral angles ($^\circ$) of the S_0 and T_1 states and the corresponding modification between the two states for **4**.



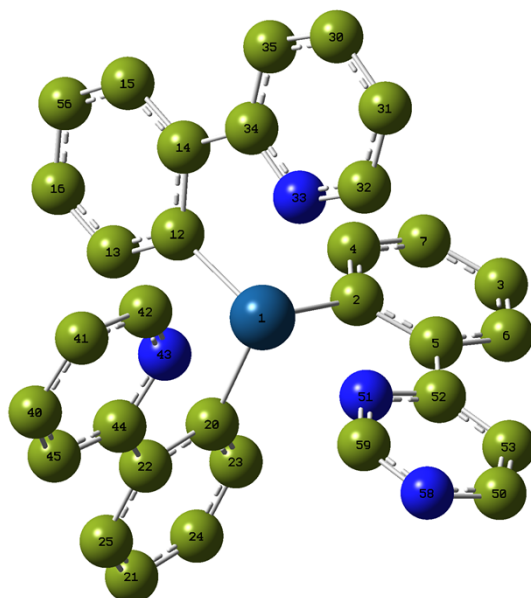
	S_0	T_1	$\Delta (T_1-S_0)$
L(Ir1-C2)	2.028	2.024	-0.004
L(Ir1-C12)	2.026	1.984	-0.042
L(Ir1-C20)	2.026	2.039	0.013
L(Ir1-N33)	2.192	2.156	-0.036
L(Ir1-N42)	2.190	2.204	0.014
L(Ir1-N52)	2.188	2.213	0.025
A(Ir1-C12-N33)	53.40	52.32	-1.08
A(Ir1-N52-N33)	41.94	41.72	-0.22
D(Ir1-C12-C14-C34)	1.233	-1.312	-2.545
D(C12-C14-C34-N33)	-1.587	0.916	2.503
Br-substituted pyridine ligands			
C30-C31	1.394	1.430	0.036
C31-C32	1.386	1.382	-0.004
C32-N33	1.343	1.341	-0.002
N33-C34	1.365	1.420	0.055
C34-C35	1.407	1.426	0.019
C35-C30	1.387	1.370	-0.017
C34-C14	1.463	1.413	-0.050
C31-Br59	1.961	1.961	0.000

Table S5. The selected bond lengths (\AA), angles ($^\circ$) and dihedral angles ($^\circ$) of the S_0 and T_1 states and the corresponding modification between the two states for **5**.



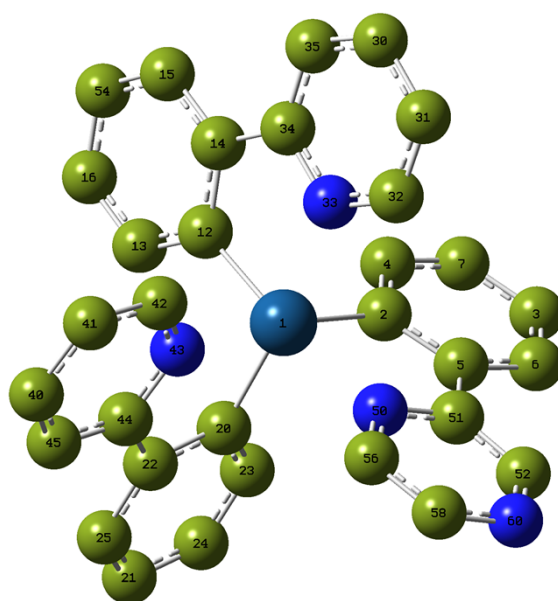
	S_0	T_1	$\Delta (T_1-S_0)$
L(Ir1-C2)	2.025	2.041	0.016
L(Ir1-C12)	2.031	2.068	0.037
L(Ir1-C20)	2.029	1.991	-0.038
L(Ir1-N33)	2.187	2.279	0.092
L(Ir1-N43)	2.182	2.203	0.021
L(Ir1-N52)	2.157	2.058	-0.099
A(Ir1-C2-N52)	52.72	50.12	-2.60
A(Ir1-N43-N52)	42.17	40.73	-1.44
D(Ir1-C2-C5-C53)	-0.14	-0.39	-0.25
D(C2-C5-C53-N52)	-2.08	-10.03	-7.95
N-substituted pyridine ligands			
C50-C51	1.40	1.41	0.01
C51-N60	1.33	1.32	0.01
N60-N52	1.33	1.38	0.05
N52-C53	1.36	1.41	0.05
C53-C54	1.41	1.38	0.03
C54-C50	1.38	1.41	0.03
C53-C5	1.46	1.46	0.00

Table S6. The selected bond lengths (\AA), angles ($^\circ$) and dihedral angles ($^\circ$) of the S_0 and T_1 states and the corresponding modification between the two states for **6**.



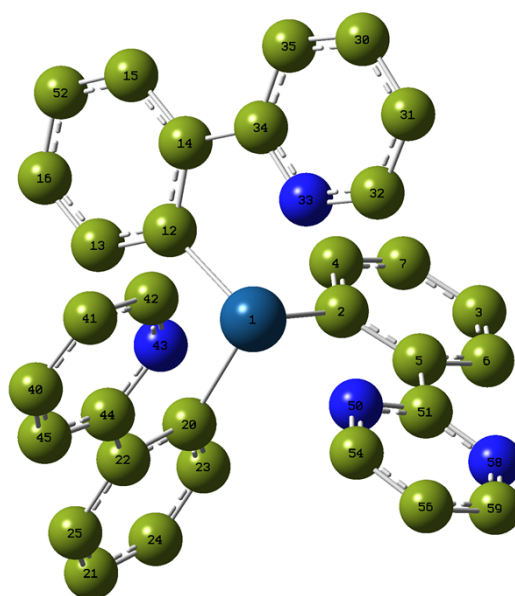
	S_0	T_1	$\Delta (T_1-S_0)$
L(Ir1-C2)	2.025	1.978	-0.047
L(Ir1-C12)	2.026	2.040	0.014
L(Ir1-C20)	2.029	2.026	-0.003
L(Ir1-N33)	2.192	2.202	0.01
L(Ir1-N43)	2.187	2.222	0.035
L(Ir1-N51)	2.190	2.162	-0.028
A(Ir1-C2-N51)	53.45	52.43	-1.02
A(Ir1-N43-N51)	41.87	41.70	-0.17
D(Ir1-C2-C5-C52)	0.863	-1.17	-2.033
D(C2-C5-C52-N51)	-1.44	0.74	2.18
N-substituted pyridine ligands			
C50-N58	1.35	1.38	0.03
N58-C59	1.33	1.33	0.00
C59-N51	1.34	1.34	0.00
N51-C52	1.37	1.41	0.04
C52-C53	1.41	1.43	0.02
C53-C50	1.38	1.37	0.01
C52-C5	1.46	1.42	0.04

Table S7. The selected bond lengths (\AA), angles ($^\circ$) and dihedral angles ($^\circ$) of the S_0 and T_1 states and the corresponding modification between the two states for **7**.



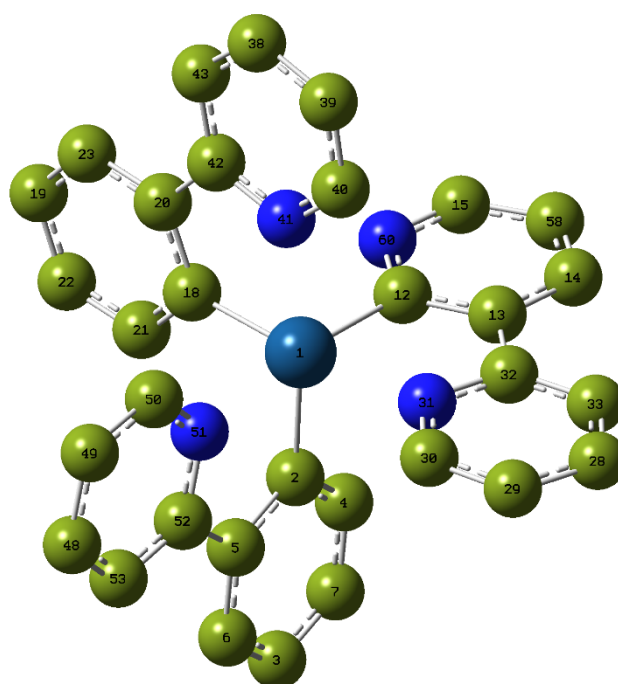
	S ₀	T ₁	Δ (T ₁ -S ₀)
L(Ir1-C2)	2.027	1.985	-0.042
L(Ir1-C12)	2.028	2.044	0.016
L(Ir1-C20)	2.030	2.022	-0.008
L(Ir1-N33)	2.190	2.208	0.018
L(Ir1-N43)	2.191	2.211	0.02
L(Ir1-N50)	2.177	2.139	-0.038
A(Ir1-C2-N50)	53.02	52.09	-0.93
A(Ir1-N43-N50)	41.80	41.49	-0.31
D(Ir1-C2-C5-C51)	1.27	-1.51	-2.78
D(C2-C5-C51-N50)	-1.35	1.00	2.35
N-substituted pyridine ligands			
N60-C58	1.34	1.39	0.05
C58-C56	1.39	1.38	0.01
C56-N50	1.34	1.34	0.00
N50-C51	1.36	1.42	0.06
C51-C52	1.41	1.42	0.01
C52-N60	1.33	1.32	0.01
C51-C5	1.46	1.42	0.04

Table S8. The selected bond lengths (Å), angles (°) and dihedral angles (°) of the S₀ and T₁ states and the corresponding modification between the two states for **8**.



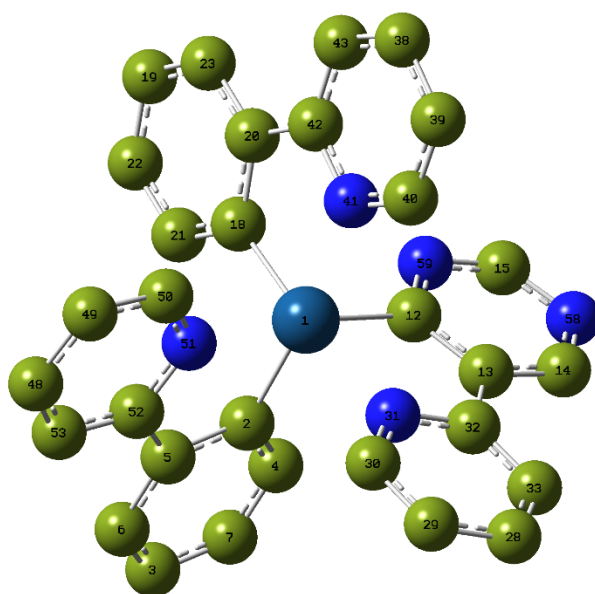
	S_0	T_1	$\Delta (T_1-S_0)$
L(Ir1-C2)	2.029	1.982	-0.047
L(Ir1-C12)	2.028	2.038	0.01
L(Ir1-C20)	2.028	2.026	-0.002
L(Ir1-N33)	2.190	2.201	0.011
L(Ir1-N43)	2.190	2.220	0.03
L(Ir1-N50)	2.193	2.164	-0.029
A(Ir1-C2-N50)	53.33	52.28	-1.05
A(Ir1-N43-N50)	42.02	41.84	-0.18
D(Ir1-C2-C5-C51)	1.53	-0.29	-1.82
D(C2-C5-C51-N50)	-1.41	0.48	1.89
N-substituted pyridine ligands			
C59-C56	1.40	1.43	0.03
C56-C54	1.39	1.39	0.00
C54-N50	1.34	1.34	0.00
N50-C51	1.37	1.41	0.04
C51-N58	1.34	1.37	0.03
N58-C59	1.33	1.32	0.01
C51-C5	1.46	1.41	0.05

Table S9. The selected bond lengths (\AA), angles ($^\circ$) and dihedral angles ($^\circ$) of the S_0 and T_1 states and the corresponding modification between the two states for **9**.



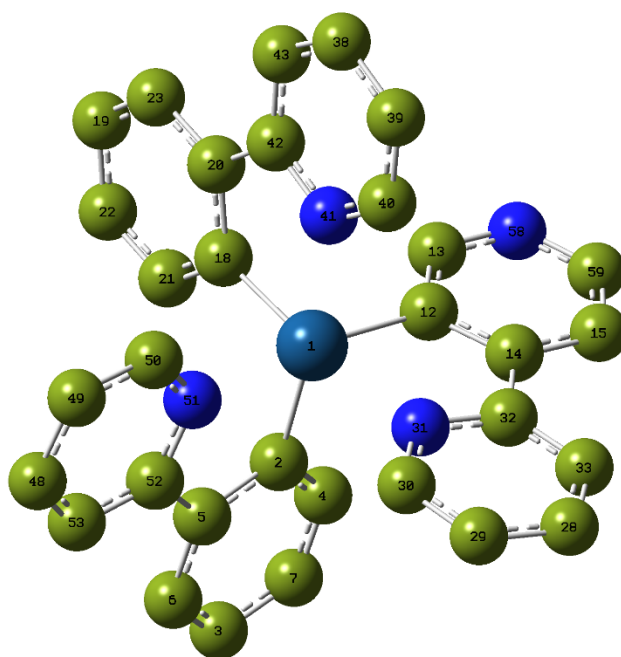
	S_0	T_1	$\Delta (T_1-S_0)$
L(Ir1-C2)	2.029	2.022	0.007
L(Ir1-C12)	2.009	1.980	-0.029
L(Ir1-C18)	2.025	2.037	0.012
L(Ir1-N31)	2.196	2.154	-0.042
L(Ir1-N41)	2.188	2.200	0.012
L(Ir1-N51)	2.199	2.228	0.029
A(Ir1-C12-N31)	53.54	52.15	-1.39
A(Ir1-N51-N31)	42.06	41.52	-0.54
D(Ir1-C12-C13-C32)	0.311	-2.256	-2.567
D(C12-C13-C32-N31)	-1.621	-1.542	3.163
N-substituted benzene ligands			
C14-C13	1.400	1.437	0.037
C13-C12	1.436	1.490	0.054
C12-N60	1.351	1.332	-0.019
N60-C15	1.336	1.344	0.008
C15-C58	1.398	1.422	0.024
C58-C14	1.389	1.372	-0.017
C13-C32	1.463	1.402	-0.061

Table S10. The selected bond lengths (\AA), angles ($^\circ$) and dihedral angles ($^\circ$) of the S_0 and T_1 states and the corresponding modification between the two states for **10**.



	S ₀	T ₁	Δ (T ₁ -S ₀)
L(Ir1-C2)	2.031	1.984	-0.047
L(Ir1-C12)	1.997	2.013	0.016
L(Ir1-C18)	2.025	2.023	-0.002
L(Ir1-N31)	2.205	2.220	0.015
L(Ir1-N41)	2.191	2.211	0.02
L(Ir1-N51)	2.198	2.164	-0.034
A(Ir1-C12-N31)	53.89	53.87	-0.02
A(Ir1-N51-N31)	42.22	43.75	1.53
D(Ir1-C12-C13-C32)	-0.41	-1.04	-0.63
D(C12-C13-C32-N31)	-1.87	-1.65	0.22
2N-substituted benzene ligands			
C14-C13	1.39	1.40	0.01
C13-C12	1.43	1.43	0.00
C12-N59	1.35	1.35	0.00
N59-C15	1.33	1.33	0.00
C15-N58	1.34	1.34	0.00
N58-C14	1.34	1.34	0.00
C13-C32	1.46	1.46	0.00

Table S11. The selected bond lengths (Å), angles (°) and dihedral angles (°) of the S₀ and T₁ states and the corresponding modification between the two states for **11**.



	S_0	T_1	$\Delta (T_1-S_0)$
L(Ir1-C2)	2.029	2.027	-0.002
L(Ir1-C12)	2.023	1.968	-0.055
L(Ir1-C18)	2.026	2.039	0.013
L(Ir1-N31)	2.197	2.175	-0.022
L(Ir1-N41)	2.192	2.200	0.008
L(Ir1-N51)	2.185	2.223	0.038
A(Ir1-C12-N31)	53.67	52.99	-0.068
A(Ir1-N51-N31)	42.00	41.93	-0.07
D(Ir1-C12-C14-C32)	1.175	-2.095	-3.27
D(C12-C14-C32-N31)	-1.493	0.964	2.457
N-substituted benzene ligands			
C15-C14	1.404	1.422	0.018
C14-C12	1.420	1.480	0.06
C12-C13	1.412	1.416	0.004
C13-N58	1.338	1.336	-0.002
N58-C59	1.343	1.370	0.027
C59-C15	1.388	1.378	-0.01
C14-C32	1.468	1.411	-0.057

Table S12. Selected reorganization energy E_r (cm^{-1}) and the vibrational normal mode frequencies ω (cm^{-1}) for **1-11**.

1		2		3		4		5		6		7	
ω	E_r	ω	E_r	ω	E_r	ω	E_r	ω	E_r	ω	E_r	ω	E_r
42	11	41	9	31	13	20	5	31	17	30	9	33	7
50	5	50	6	37	11	37	2	32	54	31	7	42	13
85	7	162	11	51	1	46	22	42	52	41	17	43	8
162	6	204	10	155	4	112	7	49	22	50	13	50	10
163	8	228	12	163	7	170	11	81	64	85	10	85	5
205	10	229	21	191	3	179	27	117	70	147	19	118	8
230	29	259	37	232	13	218	3	118	435	160	28	123	7
260	42	271	20	262	71	238	23	148	68	162	5	162	6
271	26	302	16	303	34	275	16	163	264	203	9	205	20
303	33	303	17	382	12	288	58	164	118	228	14	205	6
376	14	378	16	444	9	325	16	187	33	229	60	227	35
455	9	453	11	447	3	466	13	204	159	258	70	260	59
643	7	644	9	643	5	672	18	204	62	271	44	270	13
644	5	653	22	650	5	682	22	229	288	272	9	272	14
653	10	653	6	653	14	686	83	262	34	302	32	304	41
654	16	679	44	679	38	742	2	271	180	304	14	376	15
678	10	682	26	683	44	777	12	276	42	376	10	463	25
679	28	690	19	699	10	782	87	278	91	452	6	486	6
684	52	775	43	749	2	1024	31	286	48	492	13	491	7
776	52	777	23	776	45	1030	45	303	464	639	9	519	6
778	9	1024	5	777	18	1036	25	305	86	670	80	525	14
1025	62	1026	27	1026	92	1039	2	376	14	682	7	640	99
1026	47	1026	74	1051	128	1040	8	376	29	713	19	659	16
1039	23	1039	21	1055	45	1051	71	428	108	784	10	691	36
1040	7	1040	6	1064	17	1052	36	442	257	1025	19	797	114
1051	70	1051	114	1086	33	1061	25	454	25	1025	76	1033	15
1051	77	1057	87	1087	4	1081	3	485	40	1047	32	1038	17
1061	40	1085	44	1088	14	1083	4	489	172	1050	102	1048	63
1086	39	1131	14	1130	14	1112	43	490	30	1051	6	1051	40
1131	23	1133	14	1193	86	1153	34	519	19	1061	16	1051	24
1135	8	1155	5	1272	10	1166	52	521	99	1084	19	1061	24
1185	20	1185	21	1300	2	1192	40	588	31	1088	8	1109	53
1193	87	1193	88	1316	12	1269	16	683	22	1110	9	1153	18
1271	9	1270	8	1333	73	1334	29	763	17	1153	15	1190	29
1317	13	1316	16	1335	18	1335	26	784	27	1193	12	1272	79
1335	84	1333	73	1346	77	1341	91	786	36	1208	45	1274	7
1337	8	1335	6	1347	37	1410	33	1019	118	1346	19	1305	54
1347	111	1346	128	1460	45	1471	102	1026	17	1347	17	1336	7
1459	8	1459	49	1478	10	1482	152	1030	13	1363	81	1338	28
1460	37	1479	13	1490	222	1508	220	1051	31	1430	85	1359	107
1479	7	1490	165	1491	2	1515	8	1058	55	1467	124	1440	94
1489	153	1490	40	1511	35	1587	307	1081	14	1482	83	1470	20

1490	57	1513	208	1514	158	1604	2	1089	11	1511	87	1487	125
1513	132	1516	73	1516	81	1632	34	1144	15	1514	50	1512	121
1516	138	1597	99	1597	184	1640	28	1213	45	1581	128	1516	36
1597	86	1598	133	1598	42	1641	28	1244	67	1634	87	1517	5
1597	122	1615	16	1614	5			1301	20	1642	20	1565	372
1615	27	1616	40	1615	30			1348	64			1629	16
1615	11	1639	50	1616	21			1407	210			1640	14
1616	22	1641	50	1639	55			1476	52			1642	13
1639	55	1653	44	1641	44			1478	15				
1642	41	1654	23	1653	14			1490	17				
1652	35							1597	12				
1653	28							1602	35				
								1634	305				

Table S12 (continued). Selected reorganization energy E_r (cm⁻¹) and the vibrational normal mode frequencies ω (cm⁻¹) for **1-11**.

7		9		10		11	
ω	E_r	ω	E_r	ω	E_r	ω	E_r
34	5	29	4	30	10	30	15
43	15	30	3	158	10	40	10
50	8	40	13	203	5	50	7
84	7	48	5	227	19	85	11
117	5	82	7	232	23	115	9
146	9	119	8	257	39	147	11
160	23	160	14	272	9	161	13
205	13	198	4	275	6	203	14
226	43	227	14	300	35	227	82
259	60	258	37	304	5	260	84
269	25	272	15	379	13	270	55
274	11	385	5	451	10	303	64
302	54	519	9	643	5	376	8
377	7	637	13	644	7	454	9
445	5	653	18	653	20	593	20
499	13	692	112	654	8	641	50
679	92	775	3	680	51	722	103
680	28	793	30	683	22	776	5
684	35	820	2	695	12	781	2
777	6	1022	66	776	48	975	4
788	64	1025	13	777	21	1025	14
1022	109	1026	12	1026	29	1029	82
1048	97	1033	63	1027	75	1046	56
1051	21	1040	4	1039	25	1055	41
1053	9	1057	13	1052	143	1062	37
1060	7	1077	87	1058	63	1090	25
1078	32	1084	34	1086	20	1116	20

1108	29	1102	35	1087	27	1132	18
1124	32	1132	8	1131	19	1136	29
1151	6	1137	15	1132	6	1187	49
1187	16	1155	28	1155	8	1199	48
1248	25	1158	13	1185	24	1283	33
1275	16	1188	75	1195	90	1334	15
1277	11	1267	16	1276	15	1344	132
1291	32	1312	11	1317	13	1434	33
1372	21	1327	10	1333	83	1465	68
1447	194	1343	188	1345	123	1493	186
1471	18	1410	32	1461	7	1510	231
1490	9	1479	46	1461	33	1513	31
1491	19	1513	41	1478	15	1575	99
1494	296	1516	313	1491	35	1615	87
1589	221	1581	209	1491	199	1653	22
1633	120	1615	115	1513	209		
		1633	247	1514	37		
		1651	84	1516	32		
		1654	27	1598	38		
				1599	195		
				1615	6		
				1616	48		
				1640	95		
				1643	12		
				1653	59		
				1654	7		

Table S13. Relative Energy Gaps (in kcal/mol) Between the Stationary Points along the MLCT \rightarrow 3 MC \rightarrow 1 GS Channels and the 3 MLCT State for **1-7**.

Complex	MLCT	TS	MC	MECP
1	0.00	7.18	6.13	6.21
2	0.00	8.71	2.35	2.45
3	0.00	12.61	7.57	7.64
4	0.00	10.22	4.45	15.89
5	0.00	14.33	13.45	13.54
6	0.00	9.84	9.44	9.88
7-1	0.00	11.00	9.96	10.03
7-2	0.00	13.01	12.92	13.29
8	0.00	-	7.05	7.52
9	0.00	26.04	8.12	8.14
10-1	0.00	6.98	5.46	5.58
10-2	0.00	8.86	8.77	9.29
11	0.00	23.37	16.45	19.57

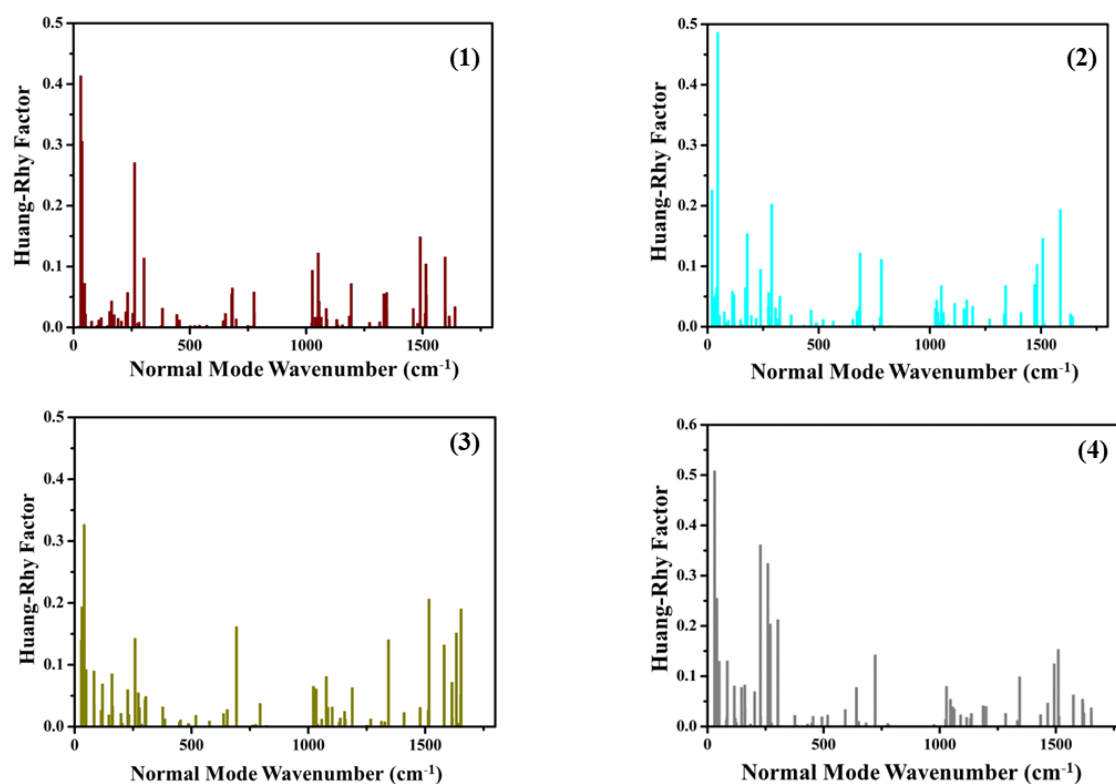


Figure. S2 The calculated Huang-Rhys factors versus the normal mode wavenumber at the ground state for **complexes 3, 4, 9 and 11.**

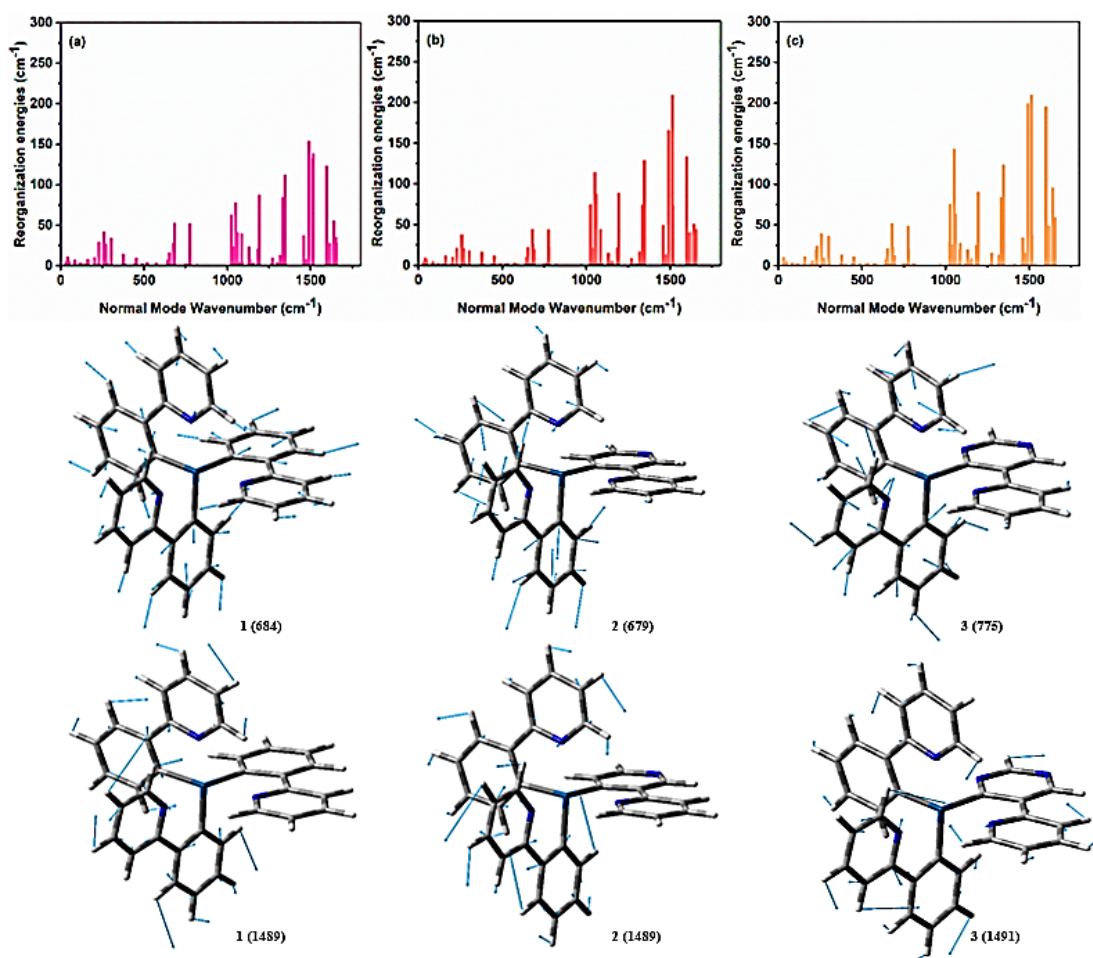


Figure S3. Positive mode displacement vectors with maximum reorganization energy and regularized mode frequencies for complexes **1 (a)**, **2 (b)** and **10 (c)**.

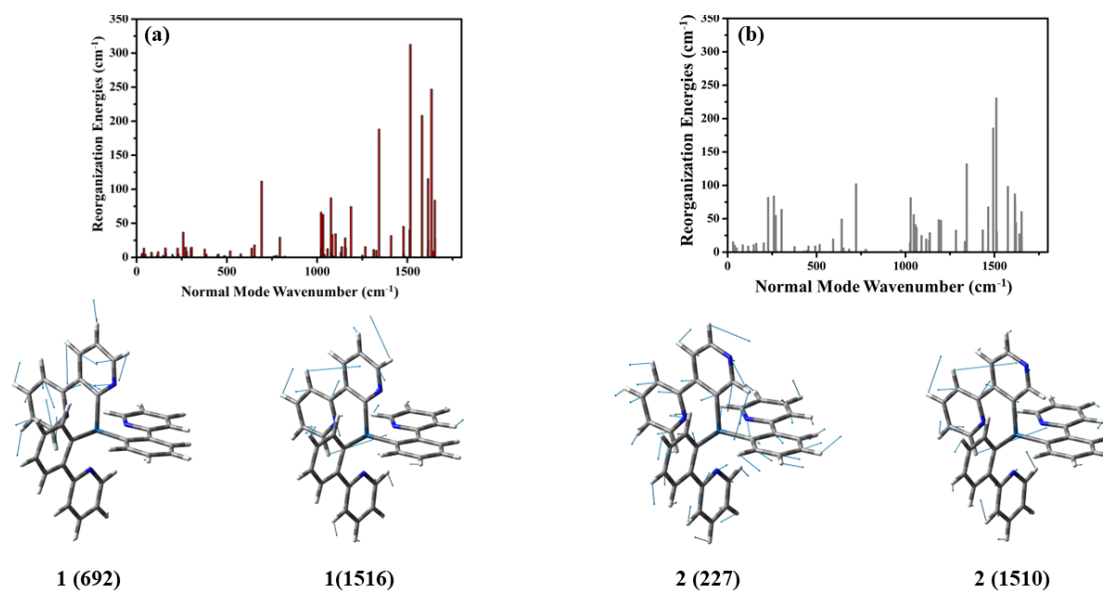


Figure S4. Positive mode displacement vectors with maximum reorganization energy and regularized mode frequencies for complexes **9 (a)** and **11 (b)**.

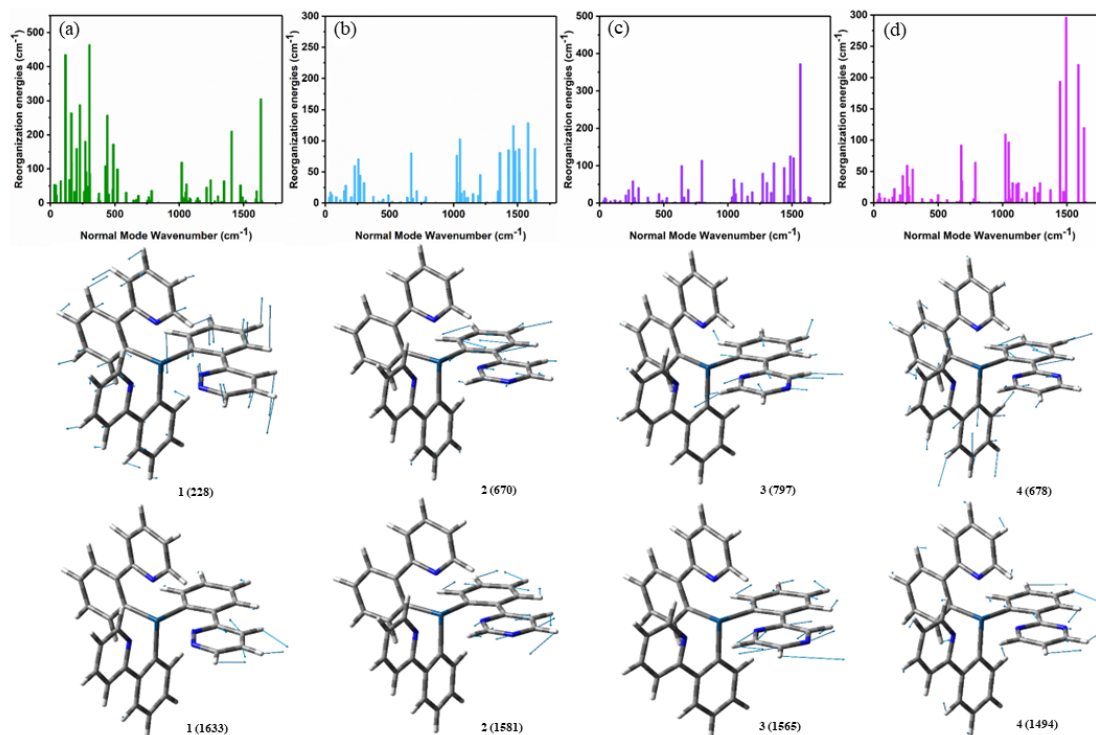


Figure S5. Positive-mode displacement vectors with maximum reorganization energy and regularized mode frequencies for complexes **5 (a)**, **6 (b)**, **7 (c)** and **8 (d)**.

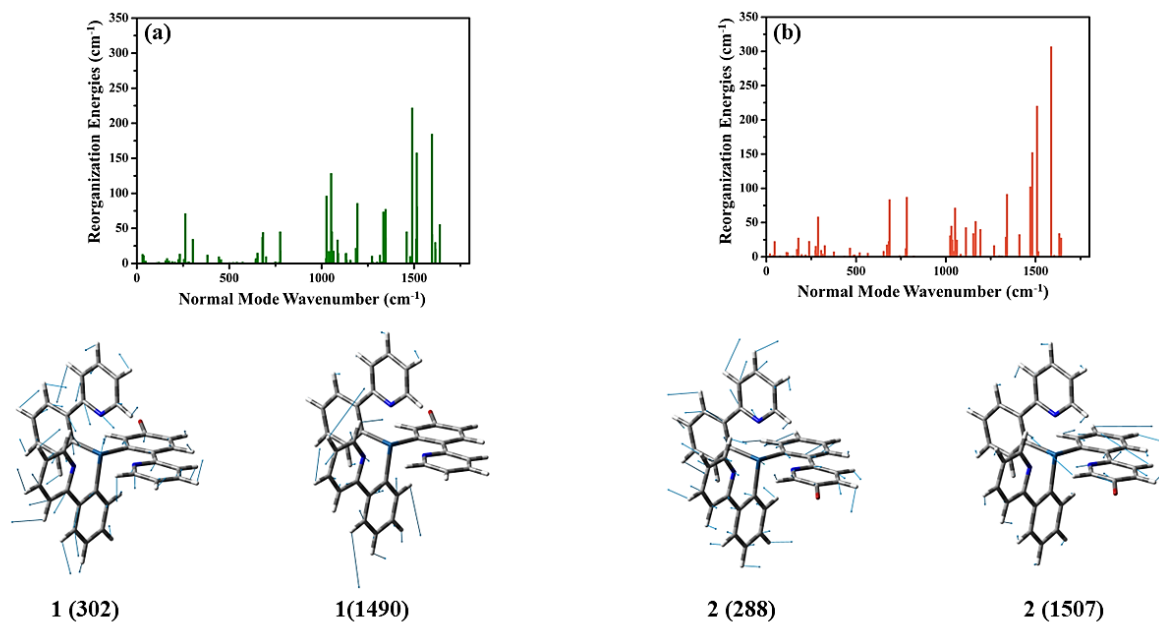


Figure S6. Positive-mode displacement vectors with maximum reorganization energy and regularized mode frequencies for complexes **3 (a)** and **4 (b)**.

Table S14. Important structural parameters calculated separately in the S₀ state using vacuum and solvent models.

	Vacuum	CH ₂ Cl ₂	Δ (Vacuum - CH ₂ Cl ₂)
L(Ir1-C2)	2.026	2.028	0.002
L(Ir1-C12)	2.027	2.027	0.000
L(Ir1-C18)	2.027	2.028	0.001
L(Ir1-N31)	2.190	2.189	-0.001
L(Ir1-N41)	2.189	2.189	0.000
L(Ir1-N51)	2.190	2.188	-0.002
A(Ir1-C2-N51)	53.33	53.33	0.000
A(Ir1-N41-N51)	41.87	41.87	0.000
D(Ir1-C2-C5-C52)	0.580	1.306	0.726
D(C2-C5-C52-N51)	-1.420	-1.435	-0.015
Benzene ligands			
C6-C5	1.41	1.41	0.000
C5-C2	1.43	1.43	0.000
C2-C4	1.41	1.41	0.000
C4-C7	1.39	1.39	0.000
C7-C3	1.40	1.40	0.000
C3-C6	1.39	1.39	0.000
C5-C52	1.46	1.47	0.010
Pyridine ligands			
C48-C49	1.40	1.40	0.000
C49-C50	1.39	1.39	0.000
C50-N51	1.34	1.34	0.000
N51-C52	1.36	1.36	0.000
C52-C53	1.41	1.41	0.000
C53-C48	1.39	1.39	0.000

Table S15. Important structural parameters calculated separately in the T₁ state using vacuum and solvent models.

	Vacuum	CH ₂ Cl ₂	Δ (Vacuum - CH ₂ Cl ₂)
L(Ir1-C2)	2.041	2.040	-0.001
L(Ir1-C12)	2.023	2.027	0.004
L(Ir1-C18)	1.983	1.984	0.001
L(Ir1-N31)	2.213	2.217	0.004
L(Ir1-N41)	2.156	2.158	0.002
L(Ir1-N51)	2.205	2.198	-0.007
A(Ir1-C2-N51)	53.35	53.20	-0.15
A(Ir1-N41-N51)	43.37	43.20	-0.17
D(Ir1-C2-C5-C52)	0.60	0.26	-0.34
D(C2-C5-C52-N51)	-1.52	-0.45	1.07
Benzene ligands			
C6-C5	1.41	1.41	0.000
C5-C2	1.43	1.43	0.000
C2-C4	1.41	1.41	0.000
C4-C7	1.39	1.39	0.000
C7-C3	1.40	1.40	0.000
C3-C6	1.39	1.39	0.000
C5-C52	1.46	1.47	0.010
Pyridine ligands			
C48-C49	1.40	1.40	0.000
C49-C50	1.39	1.39	0.000
C50-N51	1.34	1.34	0.000
N51-C52	1.36	1.36	0.000
C52-C53	1.41	1.41	0.000
C53-C48	1.39	1.39	0.000