Syntheses, photophysical, electroluminescence and computational studies of rhenium(I) diimine triarylamine-containing alkynyl complexes

Wai-Kin Chung,[a] Keith Man-Chung Wong,[a] Wai Han Lam,[a] Xiuling Zhu,[b] Nianyong Zhu,[a] Hoi-Sing Kwok[b] and Vivian Wing-Wah Yam*[a]

[a] *Institute of Molecular Functional Materials (Areas of Excellence Scheme, University Grants Committee, Hong Kong) and Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong.*

Fax: +(852) 2857-1586; Tel: +(852) 2859-2153; E-mail: wwyam@hku.hk

[b] *Department of Electrical & Electronic Engineering, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong.*

Supplementary Information

Table S1 Selected structural parameters of the PBE0 optimized geometries for **1**, **2**, **5**, **9** and **12**[a]

	1	**2**	**2**[b]	**5**	**9**	**12**
Re–C(1)	2.106	2.106	(2.182)	2.107	2.106	2.106
Re–N(1)	2.184	2.184	(2.177)	2.185	2.191	2.232
Re–N(2)	2.184	2.184	(2.178)	2.185	2.191	2.232
$Re–CO_{trans\ to\ C(1)}$	1.965	1.966	(1.991)	1.964	1.965	1.962
$Re–CO_{trans\ to\ N(2)}$	1.922	1.922	(1.900)	1.921	1.921	1.915
$Re–CO_{trans\ to\ N(1)}$	1.922	1.922	(1.938)	1.921	1.921	1.915
C(1)–C(2)	1.230	1.230	(1.108)	1.230	1.230	1.230
C(2)–C(3)	1.423	1.423	(1.469)	1.423	1.423	1.423
N–C[c]	1.412	1.411	(1.425)	1.412	1.412	1.412
ϕ_{NPh}[d]	39.8	39.6	(43.4)	39.8	39.8	39.9

[a]The atomic numbering is shown in Figure S1. Bond distances and angles are in Å and °, respectively

[b]The structural parameters in parentheses are from X-ray crystallographic data

[c]Average N–C distances of the triarylamine ligand

[d]Average interplanar angles between the NC_3 plane of the triarylamine ligand and the phenyl rings.

Table S2 Selected singlet excited states (S_n) of the complexes computed by TDDFT/CPCM (CH_2Cl_2)

Complex	S_n	Excitation[a] (Coefficient)[b]	Vertical excitation wavelength (nm)	*f*[c]	Character[d]
1	S_1	H → L (0.68)	572	0.001	LLCT
	S_2	H–2 → L (0.66)	433	0.053	MLCT/LLCT
	S_3	H–1 → L (0.63)	417	0.007	MLCT/LLCT
	S_4	H → L+1 (0.69)	389	0.002	LLCT
	S_5	H → L+2 (0.68)	374	0.096	LLCT
	S_6	H → L+3 (0.65)	363	0.704	IL/LLCT
	S_7	H–3 → L (0.70)	359	0.018	MLCT
2	S_1	H → L (0.67)	543	0.001	LLCT
	S_2	H–2 → L (0.68)	430	0.057	MLCT/LLCT
	S_3	H–1 → L (0.64)	414	0.005	MLCT/LLCT
	S_4	H → L+1 (0.68)	375	0.004	LLCT
	S_5	H → L+2 (0.43)	367	0.866	LLCT
		H → L+4 (0.50)			IL/LLCT
	S_6	H → L+3 (0.66)	360	0.551	IL
	S_7	H–3 → L (0.62)	359	0.088	MLCT
5	S_1	H → L (0.68)	562	0.001	LLCT
	S_2	H–2 → L (0.65)	431	0.057	MLCT/LLCT
	S_3	H–1 → L (0.62)	413	0.010	MLCT/LLCT
	S_4	H → L+1 (0.69)	378	0.004	LLCT
	S_5	H → L+2 (0.52)	366	0.583	LLCT
		H → L+3 (–0.41)			IL/LLCT
	S_6	H → L+2 (0.44)	359	0.220	LLCT
		H → L+3 (0.51)			IL/LLCT
	S_7	H–3 → L (0.70)	357	0.007	MLCT
9	S_1	H → L (0.68)	564	0.001	LLCT
	S_2	H → L+1 (0.69)	515	0.001	LLCT
	S_3	H–2 → L (0.69)	428	0.066	MLCT/LLCT
	S_4	H–1 → L (0.66)	413	0.002	MLCT/LLCT
	S_5	H–2 → L+1 (0.70)	398	0.016	MLCT/LLCT
	S_6	H–1 → L+1 (0.68)	385	0.011	MLCT/LLCT
	S_7	H → L+2 (0.66)	365	0.799	IL/LLCT
12	S_1	H → L (0.68)	544	0.001	LLCT
	S_2	H → L+1 (0.69)	478	0.007	LLCT
	S_3	H–2 → L (0.69)	411	0.056	MLCT/LLCT
	S_4	H–1 → L (0.67)	402	0.001	MLCT/LLCT
	S_5	H–2 → L+1 (0.69)	369	0.022	MLCT/LLCT
	S_6	H–1 → L+1 (0.64)	363	0.075	MLCT/LLCT
	S_7	H → L+2 (0.62)	360	0.745	IL/LLCT

[a]The orbitals involved in the excitations (H = HOMO and L = LUMO)

[b]The coefficients in the configuration interaction (CI) expansion that are less than absolute value of 0.3 are not listed

[c]Oscillator strengths

[d]Character of the transition

Table S3 Mulliken percentage compositions[a] of selected molecular orbitals (H = HOMO and L = LUMO) in the complexes

MOs	%				%			
	1				**2**			
	Re	CO	N^N	C≡CR	Re	CO	N^N	C≡CR
L+4	13	48	2	37	11	19	11	58
L+3	18	34	6	42	0	0	0	100
L+2	3	3	93	1	3	5	86	5
L+1	1	2	97	0	1	2	97	0
L	2	3	94	1	2	3	94	1
H	5	3	0	92	6	3	0	91
H–1	25	12	1	62	23	11	1	65
H–2	37	17	4	42	38	17	4	41
H–3	67	31	2	0	67	31	2	0
	5				**9**			
	Re	CO	N^N	C≡CR	Re	CO	N^N	C≡CR
L+4	12	46	2	40	1	3	0	96
L+3	16	31	12	41	1	2	96	0
L+2	4	5	87	4	19	35	3	42
L+1	2	2	96	0	1	1	99	0
L	2	3	95	1	2	3	94	1
H	5	3	0	92	5	3	0	92
H–1	25	12	1	61	24	11	1	63
H–2	37	17	4	42	37	17	5	41
H–3	67	31	2	0	68	31	2	0
	12							
	Re	CO	N^N	C≡CR				
L+4	0	0	0	99				
L+3	1	4	94	1				
L+2	16	29	6	49				
L+1	0	1	99	0				
L	2	3	95	1				
H	5	3	0	92				
H–1	24	11	1	63				
H–2	35	16	8	41				
H–3	55	26	15	3				

[a]The compositions were expressed in terms of contributions from the Re atom (Re), three carbonyl ligands (CO), diimine ligand (N^N), and triphenylamine alkynyl ligand (C≡C–C_6H_4-R)

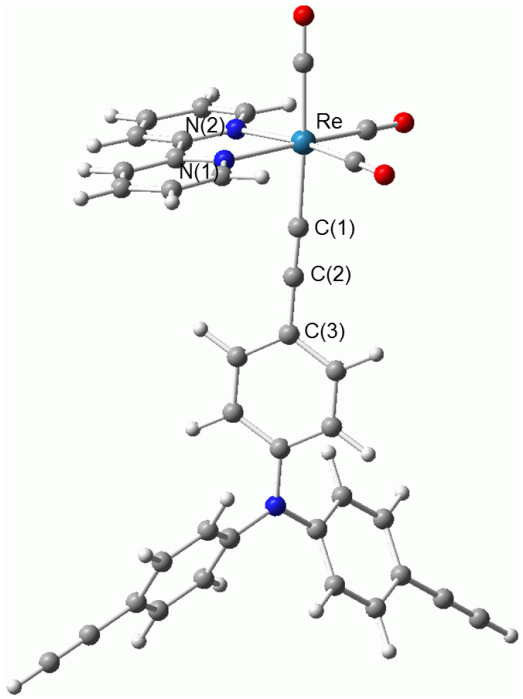

Figure S1 Optimized geometry of **2**.

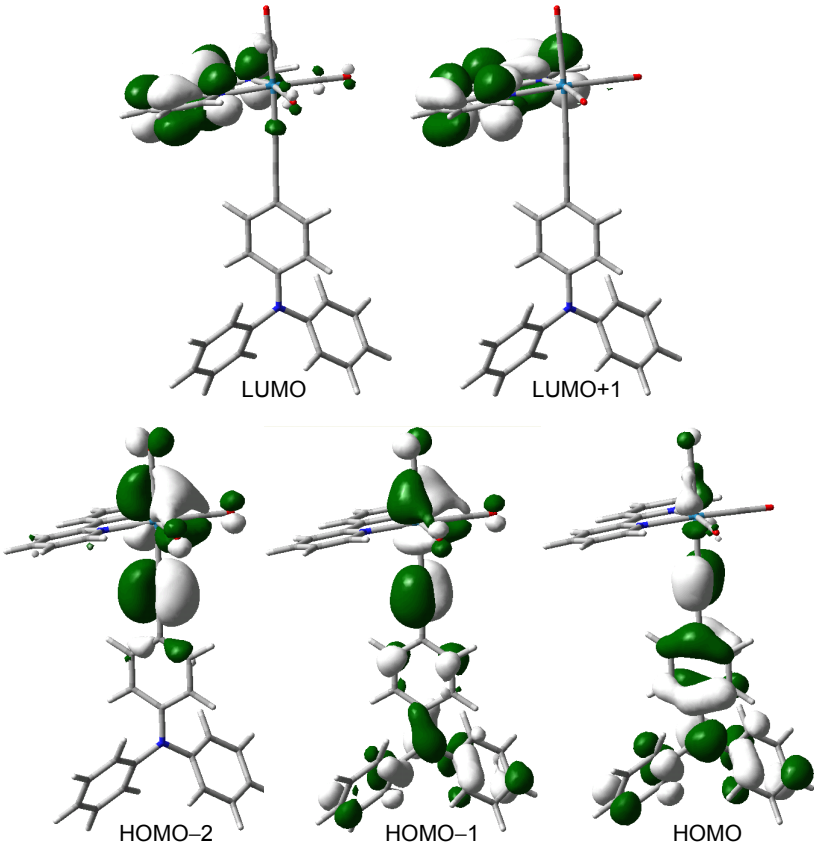

Figure S2 Spatial plots (isovalue = 0.03 au) of selected frontier molecular orbitals of **1** obtained from PBE0/CPCM calculation.

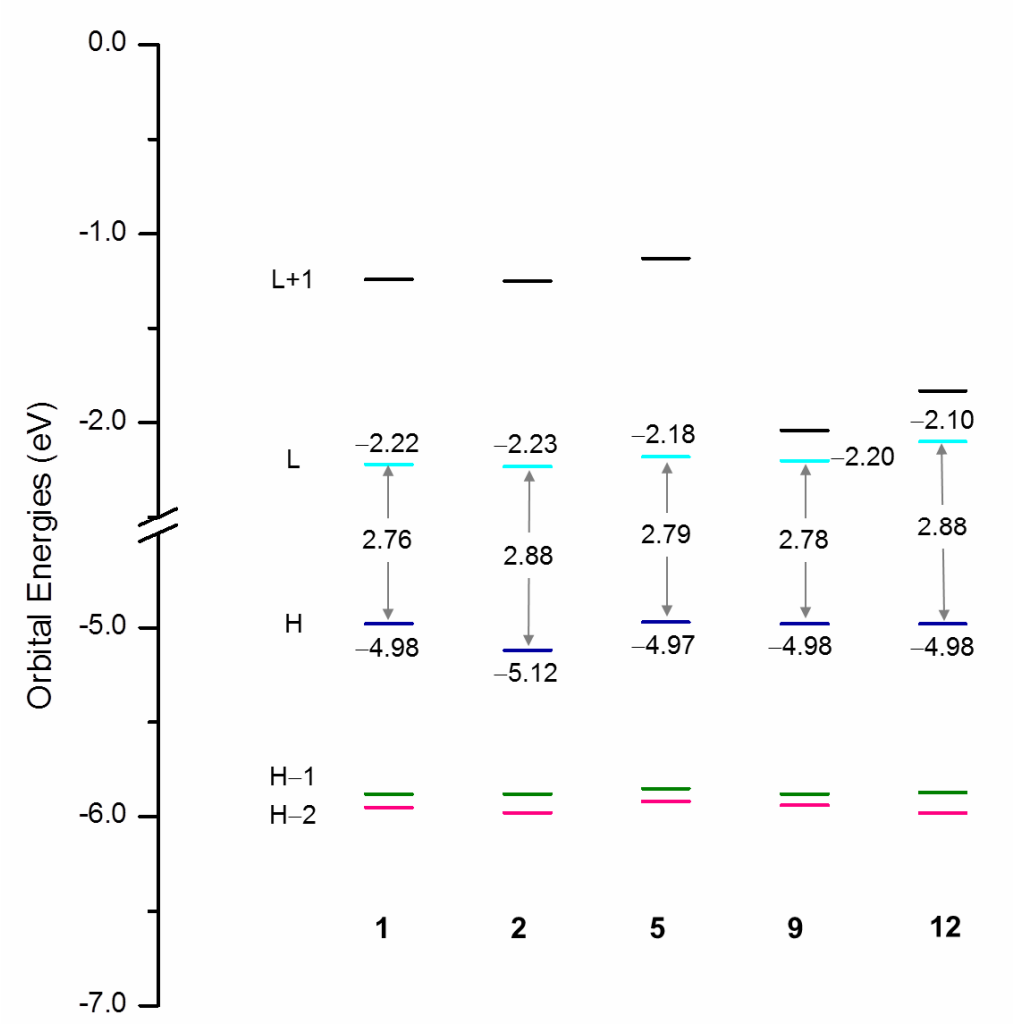

Figure S3 Orbital energy diagram of the frontier molecular orbitals (H = HOMO and L = LUMO) in **1**, **2**, **5** and **9** and **12**.

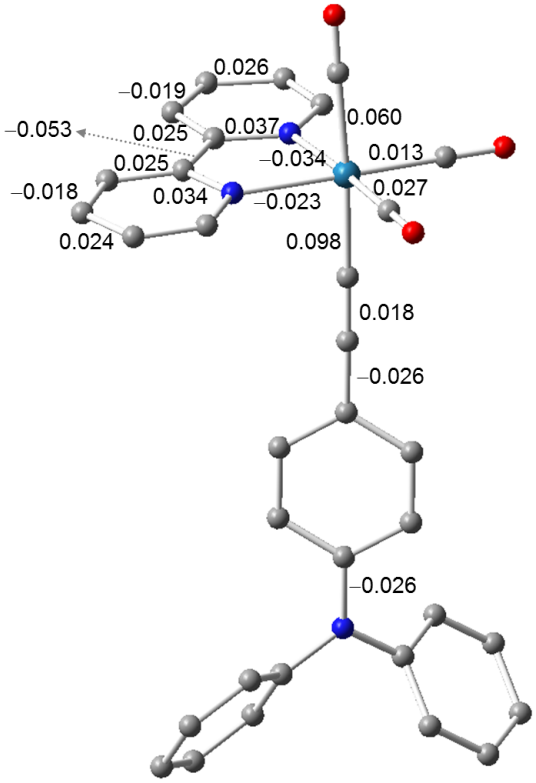

Figure S4 The change in bond distances (in Å) in triplet-excited state of **1** relative to the ground state. Only difference in bond distances larger than 0.013 Å were shown. The positive and negative values indicate bond elongation and contraction in the excited state, respectively. For clarity, all hydrogen atoms are omitted

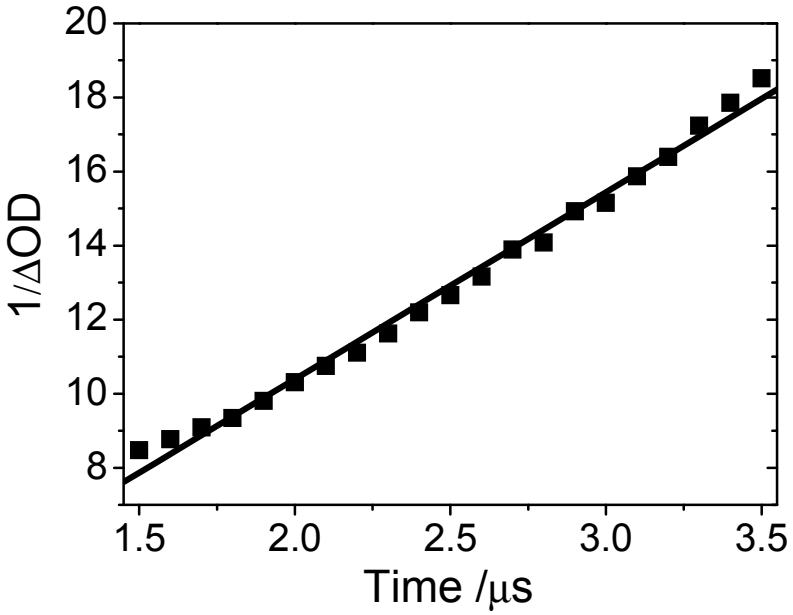

Figure S5 A plot of 1/ΔOD versus time monitored at 640 nm (■) after laser flash of **11** and triphenylamine (2.01×10^{-2} M) in degassed dichloromethane solution (0.1 M $^{n}Bu_4NPF_6$) and its theoretical fit (—).

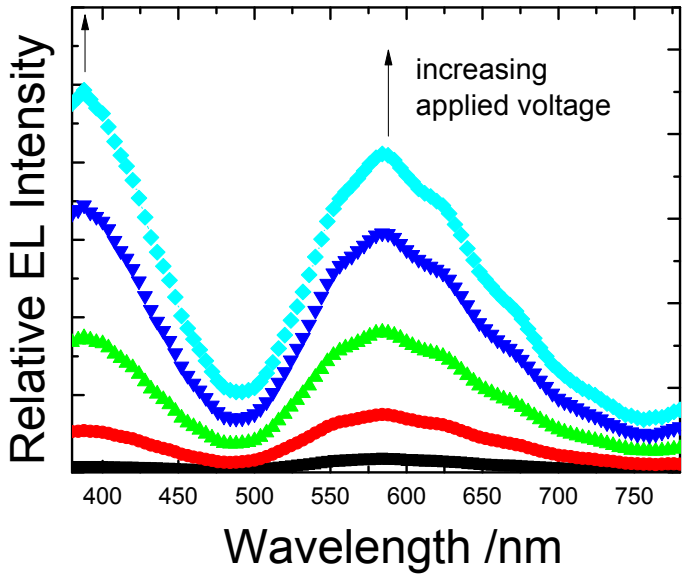

Figure S6 Electroluminescence spectra of **3** at different DC voltages applied (from bottom to top: 8, 10, 12, 14 and 16 V). The device structure was ITO/MoO_x (2.5 nm)/MCP (8 wt% **3**) (20 nm)/TPBi (50 nm)/LiF (1 nm)/Al (80 nm).

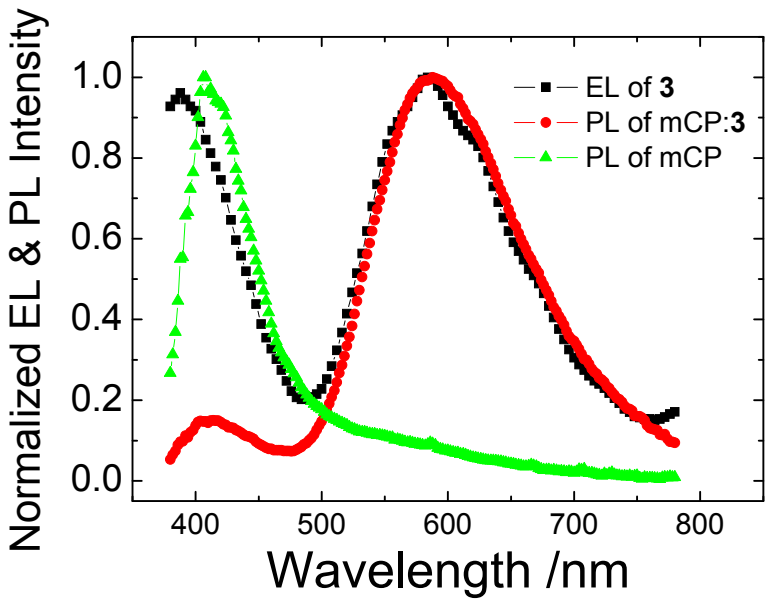

Figure S7 Electroluminescence spectra of **3** and the photoluminescence spectra of 50 nm thin-film MCP and 60 nm thin-film MCP with 8wt% **3** as dopant.

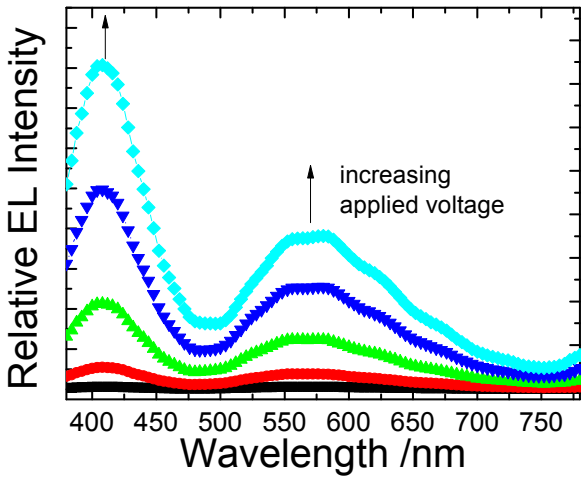

Figure S8 Electroluminescence spectra of **4** at different DC voltages applied (from bottom to top: 8, 10, 12, 14, 16 V). The device structure was ITO/MoO_x (2.5 nm)/NPB (50 nm)/MCP (8 wt% **4**) (25 nm)/TPBi (50 nm)/LiF (1 nm)/Al (80 nm).

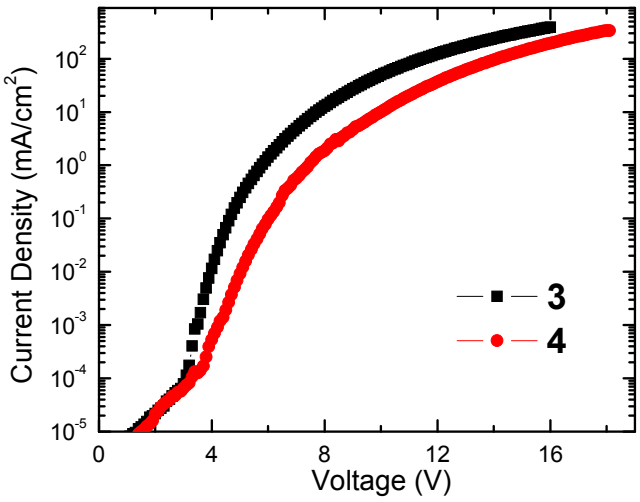

Figure S9 Current density-voltage curve for **3** and **4**.

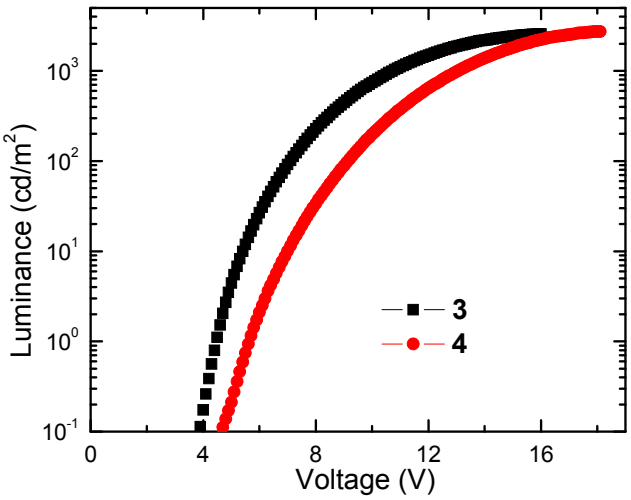

Figure S10 Luminance-voltage relationship curve for **3** and **4**.

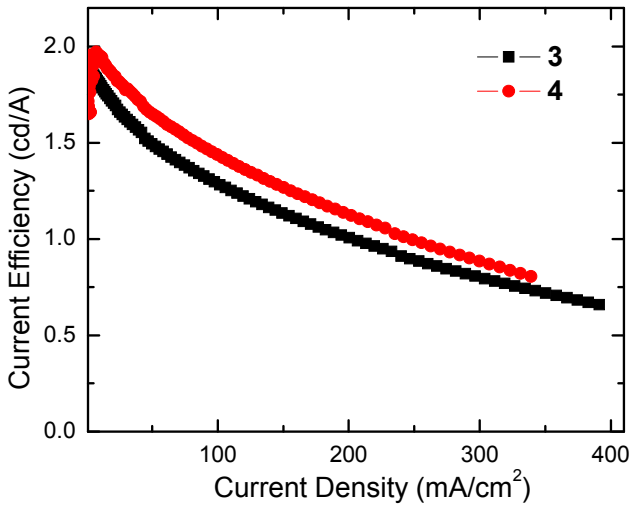

Figure S11 Current efficiency-current density relationship curve for **3** and **4**.

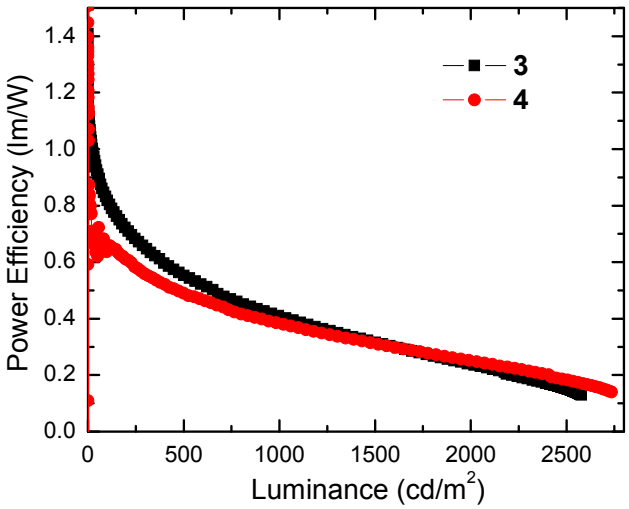

Figure S12 Power efficiency versus luminance for **3** and **4**.

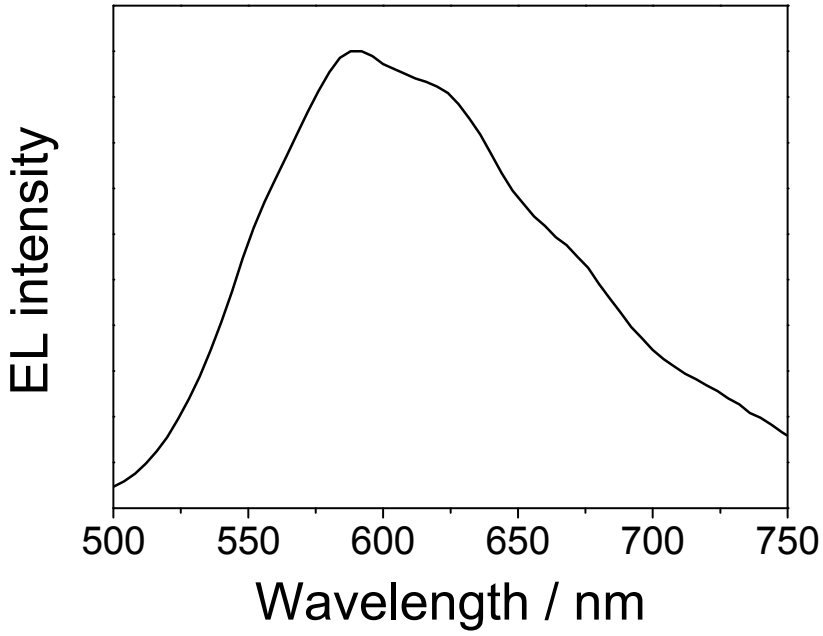

Figure S13 Electroluminescence spectrum of complex **11** at bias voltage 10 V. The device structure was ITO/MoO_x (2.5 nm)/NPB (50 nm)/MCP (8 wt% **11**) (20 nm)/TPBi (50 nm)/LiF (1 nm)/Al (80 nm).

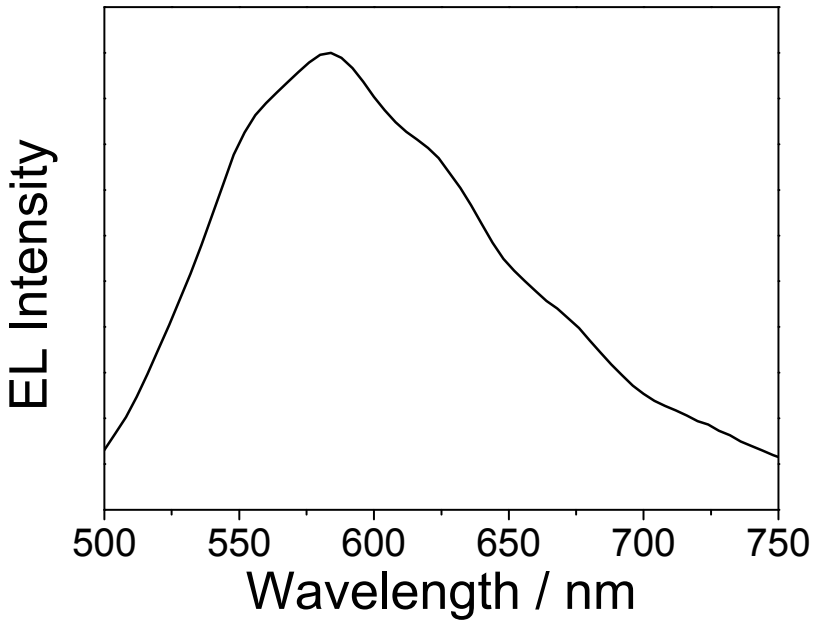

Figure S14 Electroluminescence spectrum of **12** at bias voltage 10 V. The device structure was ITO/MoO_x (2.5 nm)/NPB (50 nm)/MCP (8wt% **12**)/TPBi (50 nm)/LiF (1 nm)/Al (80 nm)

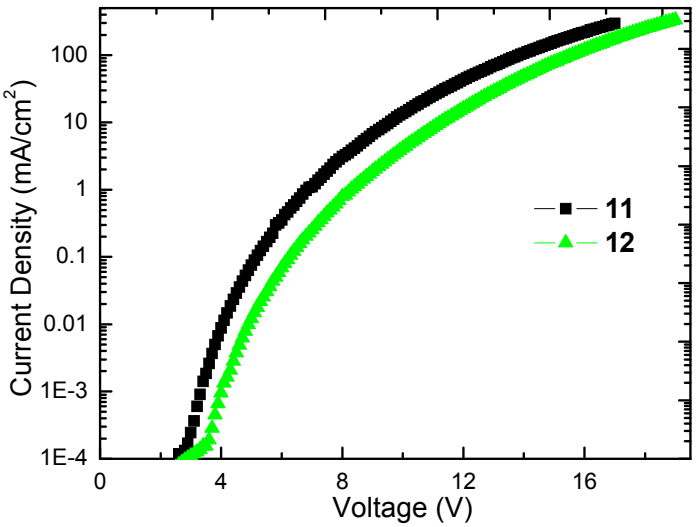

Figure S15 Current density-voltage relationship curve for **11** and **12**.

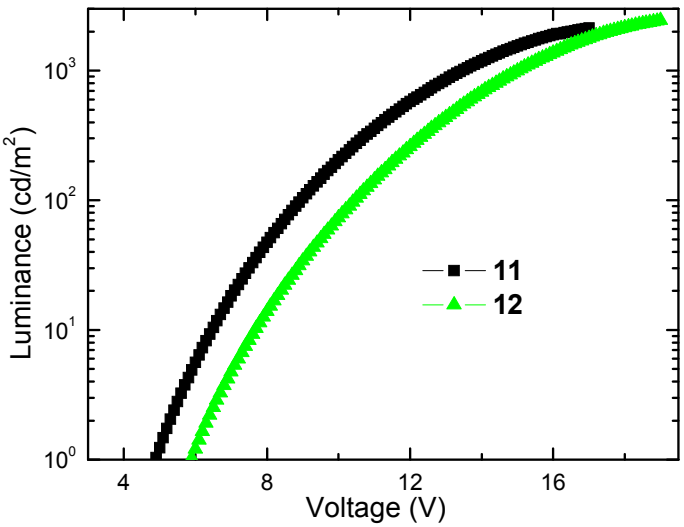

Figure S16 Luminance-voltage relationship curve for **11** and **12**.

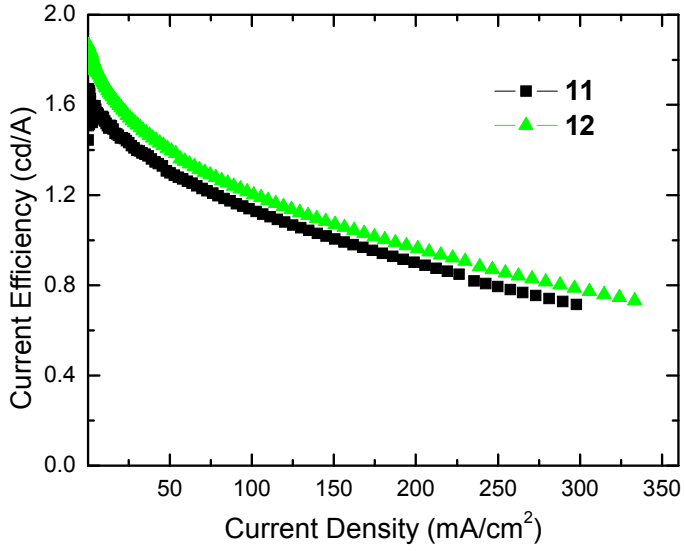

Figure S17 Current efficiency versus current density for **11** and **12**.

Cartesian coordinates for the optimized geometries

1 (S_0)

1	C	7.496385	-1.375128	-0.525935
2	C	6.271880	-1.204796	0.133986
3	C	5.818668	-2.215963	0.991656
4	C	6.572044	-3.369343	1.176341
5	C	7.794183	-3.531463	0.527565
6	C	8.250373	-2.524556	-0.320346
7	N	5.503114	-0.038362	-0.065913
8	C	6.132165	1.218813	-0.183458
9	C	7.236157	1.543449	0.616701
10	C	7.853808	2.782343	0.491612
11	C	7.376281	3.726248	-0.415049
12	C	6.272765	3.409840	-1.204524
13	C	5.658334	2.167521	-1.099694
14	C	4.094094	-0.130053	-0.150588
15	C	3.278001	0.805605	0.497415
16	C	1.897444	0.720015	0.405628
17	C	1.273929	-0.311692	-0.319203
18	C	2.105379	-1.250330	-0.957675
19	C	3.486390	-1.157432	-0.883444
20	C	-0.143520	-0.406012	-0.406314
21	C	-1.366653	-0.504051	-0.493178
22	Re	-3.468085	-0.613111	-0.586653
23	C	-3.398077	-2.533606	-0.580792
24	O	-3.338923	-3.690300	-0.527319
25	N	-3.375979	1.550319	-0.302236
26	C	-3.384318	2.431420	-1.312236
27	C	-3.253080	3.797497	-1.118009
28	C	-3.102823	4.274897	0.179405
29	C	-3.089030	3.367071	1.227511
30	C	-3.224791	2.003955	0.962112
31	C	-3.221122	0.970385	2.009491
32	N	-3.367614	-0.300491	1.572984
33	C	-3.368890	-1.298777	2.467303
34	C	-3.234777	-1.085915	3.830324
35	C	-3.089659	0.218387	4.290180
36	C	-3.083451	1.254474	3.368600
37	H	-2.995164	5.337626	0.373595
38	H	-2.980114	0.427101	5.349949
39	C	-5.433140	-0.633956	-0.594705
40	O	-6.592962	-0.650341	-0.603496
41	C	-3.411303	-0.631418	-2.507773
42	O	-3.361474	-0.592485	-3.665392
43	H	1.276683	1.453311	0.912809
44	H	3.737873	1.603954	1.072884
45	H	4.108563	-1.885936	-1.395323
46	H	1.647085	-2.051002	-1.530531
47	H	4.871592	-2.090211	1.507617
48	H	6.203076	-4.142795	1.845037
49	H	8.382622	-4.431811	0.679159
50	H	9.197047	-2.638704	-0.842222
51	H	7.850008	-0.600939	-1.200224
52	H	7.604751	0.817041	1.334741
53	H	8.708958	3.015043	1.121092
54	H	7.858172	4.695560	-0.505475
55	H	5.891690	4.131224	-1.922884
56	H	4.806460	1.921222	-1.726313
57	H	-3.476611	-2.297606	2.060468
58	H	-3.240871	-1.931979	4.508953
59	H	-2.967603	2.277419	3.706792
60	H	-2.968816	3.718942	2.245330
61	H	-3.265296	4.464857	-1.972929
62	H	-3.495357	2.011194	-2.305136

2 (S_0)

1	C	4.980292	2.255154	-0.900501
2	C	5.533051	1.235885	-0.110533
3	C	6.675155	1.522030	0.652992
4	C	7.250077	2.781704	0.617346
5	C	6.698484	3.805764	-0.169016
6	C	5.550407	3.517152	-0.923954
7	N	4.940374	-0.038792	-0.076470
8	C	5.726015	-1.201793	0.023757
9	C	5.275218	-2.301662	0.768397
10	C	6.038717	-3.454012	0.856561
11	C	7.284075	-3.546285	0.215065
12	C	7.731749	-2.442078	-0.527538
13	C	6.964526	-1.293314	-0.629097
14	C	8.071452	-4.729271	0.312559
15	C	8.740883	-5.734117	0.395710
16	C	7.287030	5.102527	-0.198858
17	C	7.787012	6.204527	-0.223810
18	C	3.527153	-0.152978	-0.138191
19	C	2.924335	-1.075585	-1.000545
20	C	1.543852	-1.191182	-1.052944
21	C	0.712880	-0.377647	-0.260005
22	C	1.333950	0.550454	0.595938
23	C	2.714590	0.655832	0.663876
24	C	-0.703593	-0.492044	-0.325001
25	C	-1.926445	-0.604650	-0.396810
26	Re	-4.027171	-0.732636	-0.478559
27	C	-3.953240	-2.626419	-0.156854
28	O	-3.892474	-3.758312	0.085824
29	N	-3.936867	-0.068963	1.600216
30	C	-3.937770	-0.906506	2.646730
31	C	-3.810793	-0.471577	3.956663
32	C	-3.673379	0.891316	4.196117
33	C	-3.667940	1.761738	3.116616
34	C	-3.798788	1.257362	1.822264
35	C	-3.804176	2.104978	0.619359
36	N	-3.946014	1.448848	-0.553985
37	C	-3.956034	2.152227	-1.694912
38	C	-3.835018	3.532630	-1.726978
39	C	-3.694135	4.217518	-0.525002
40	C	-3.679254	3.494106	0.657975
41	C	-5.992513	-0.761125	-0.491594
42	O	-7.151859	-0.782777	-0.502765
43	C	-3.960902	-1.066519	-2.370285
44	O	-3.904330	-1.218387	-3.518182
45	H	-4.039732	-1.959206	2.409624
46	H	-3.816691	-1.194466	4.765236
47	H	-3.569686	1.272125	5.207504
48	H	-3.558602	2.826996	3.282391
49	H	-3.566883	4.009294	1.604626
50	H	-3.594775	5.298475	-0.507436
51	H	-3.848002	4.050653	-2.679800
52	H	-4.060310	1.574074	-2.605769
53	H	1.085138	-1.909882	-1.725242
54	H	3.548624	-1.704049	-1.629423
55	H	3.176257	1.369911	1.340113
56	H	0.712071	1.182741	1.223116
57	H	4.318648	-2.244080	1.278175
58	H	5.678948	-4.296622	1.439200
59	H	8.686391	-2.500829	-1.041526
60	H	7.319393	-0.456543	-1.222740
61	H	9.329939	-6.620598	0.467741
62	H	7.106756	0.747970	1.279917
63	H	8.131255	2.989921	1.216696
64	H	5.115353	4.294558	-1.544782
65	H	4.099078	2.045846	-1.498749
66	H	8.229961	7.174697	-0.247269

5 (S_0)

1	C	-3.035628	1.071431	3.142469
2	C	-3.140948	0.768532	1.785036
3	N	-3.253373	-0.507658	1.359600
4	C	-3.252286	-1.488929	2.273421
5	C	-3.148702	-1.251347	3.631797
6	C	-3.035247	0.061129	4.098724
7	C	-3.144491	1.789745	0.724343
8	N	-3.261912	1.316118	-0.534346
9	C	-3.267387	2.192266	-1.549483
10	C	-3.166002	3.558874	-1.363929
11	C	-3.047357	4.075330	-0.070578
12	C	-3.040179	3.157922	0.975094
13	Re	-3.303530	-0.852260	-0.797771
14	C	-3.209337	-0.892244	-2.716433
15	O	-3.138459	-0.865984	-3.873721
16	C	-1.206713	-0.695519	-0.662133
17	C	0.011691	-0.567405	-0.549910
18	C	1.423735	-0.436407	-0.431245
19	C	2.004680	0.648667	0.250114
20	C	3.380074	0.771550	0.372679
21	C	4.233490	-0.179755	-0.199562
22	C	3.669083	-1.260754	-0.888137
23	C	2.292882	-1.389848	-0.993334
24	N	5.638087	-0.049512	-0.083944
25	C	6.241352	1.210400	-0.278266
26	C	7.318818	1.619281	0.519666
27	C	7.909818	2.861186	0.318735
28	C	7.431250	3.725714	-0.663434
29	C	6.353766	3.326007	-1.451069
30	C	5.766393	2.079426	-1.270018
31	C	6.424258	-1.180504	0.221041
32	C	7.675134	-1.366550	-0.383190
33	C	8.444988	-2.481774	-0.074222
34	C	7.979945	-3.440050	0.823751
35	C	6.732023	-3.263171	1.417211
36	C	5.961815	-2.142682	1.128904
37	C	-3.195157	-2.769954	-0.765752
38	O	-3.114162	-3.924883	-0.695844
39	C	-5.266204	-0.912083	-0.842296
40	O	-6.425475	-0.951249	-0.872372
41	C	-2.926358	5.549767	0.171682
42	C	-2.909962	0.359521	5.562446
43	H	1.353970	1.394554	0.697937
44	H	3.807077	1.611753	0.912963
45	H	4.321263	-2.002166	-1.340848
46	H	1.867855	-2.231808	-1.531587
47	H	4.994149	-2.005133	1.601800
48	H	6.355156	-3.998608	2.123376
49	H	8.581183	-4.314335	1.056141
50	H	9.411892	-2.608554	-0.554469
51	H	8.036686	-0.631735	-1.096190
52	H	7.687963	0.955709	1.295890
53	H	8.744619	3.159582	0.947850
54	H	7.892306	4.697800	-0.813273
55	H	5.972273	3.984349	-2.227431
56	H	4.934962	1.767900	-1.895037
57	H	-3.333206	-2.497415	1.884202
58	H	-3.152318	-2.091228	4.320100
59	H	-2.947705	2.103475	3.463925
60	H	-2.947181	3.518246	1.993776
61	H	-3.175198	4.214870	-2.229245
62	H	-3.351556	1.765082	-2.542203
63	H	-2.885674	5.781752	1.239419
64	H	-2.017867	5.946020	-0.296499
65	H	-3.775877	6.088651	-0.262740
66	H	-2.897235	1.435639	5.755720
67	H	-3.742102	-0.079031	6.124401
68	H	-1.984999	-0.068223	5.966465

9 (S_0)

1	C	-3.062550	2.040944	2.670477
2	C	-3.175587	1.282096	1.487067
3	N	-3.271559	-0.072134	1.486565
4	C	-3.245536	-0.706397	2.653983
5	C	-3.136069	-0.034284	3.877999
6	C	-3.045724	1.340987	3.891141
7	C	-3.190893	1.938329	0.217277
8	N	-3.299942	1.153578	-0.885219
9	C	-3.302823	1.739185	-2.078077
10	C	-3.210679	3.127461	-2.239667
11	C	-3.107100	3.934622	-1.127243
12	C	-3.093308	3.343710	0.149817
13	Re	-3.338294	-1.002498	-0.496360
14	C	-3.256374	-1.581929	-2.326333
15	O	-3.191772	-1.886646	-3.443023
16	C	-1.241631	-0.815737	-0.424217
17	C	-0.022699	-0.663959	-0.357651
18	C	1.390245	-0.508461	-0.287056
19	C	1.974105	0.660503	0.233948
20	C	3.350431	0.806392	0.313222
21	C	4.201288	-0.207366	-0.144435
22	C	3.633260	-1.372524	-0.674926
23	C	2.256601	-1.522321	-0.736019
24	N	5.606235	-0.057845	-0.070315
25	C	6.199816	1.172196	-0.422239
26	C	7.285184	1.677472	0.306689
27	C	7.867788	2.888041	-0.049720
28	C	7.372953	3.626525	-1.122456
29	C	6.287568	3.131601	-1.842290
30	C	5.708367	1.913968	-1.505069
31	C	6.404144	-1.138740	0.361525
32	C	7.643653	-1.397026	-0.239248
33	C	8.425648	-2.461008	0.194806
34	C	7.983571	-3.296991	1.217856
35	C	6.746826	-3.048899	1.809216
36	C	5.964981	-1.976983	1.394931
37	C	-3.227573	-2.829221	0.088188
38	O	-3.144649	-3.915480	0.484784
39	C	-5.301925	-1.071205	-0.508831
40	O	-6.461031	-1.115771	-0.518436
41	H	-3.032269	5.014456	-1.223318
42	H	-2.957946	1.887975	4.826002
43	H	1.325777	1.454697	0.593457
44	H	3.779797	1.712469	0.731244
45	H	4.283111	-2.163483	-1.038206
46	H	1.828967	-2.430587	-1.150086
47	H	5.006363	-1.782199	1.866170
48	H	6.388304	-3.688275	2.611819
49	H	8.594125	-4.132327	1.548471
50	H	9.383618	-2.645746	-0.284524
51	H	7.986788	-0.758456	-1.047699
52	H	7.667029	1.113334	1.152277
53	H	8.708910	3.262647	0.528098
54	H	7.827460	4.575000	-1.394090
55	H	5.893344	3.690637	-2.687132
56	H	4.870712	1.526699	-2.077230
57	H	-3.309443	-1.788201	2.612606
58	H	-3.120155	-0.609915	4.797283
59	C	-2.966843	3.466385	2.574263
60	C	-2.981660	4.090723	1.366280
61	H	-3.218464	3.544468	-3.241036
62	H	-3.376661	1.079058	-2.935340
63	H	-2.906234	5.172825	1.303377
64	H	-2.879340	4.041751	3.491807

12 (S_0)				
1	C	-2.154743	1.691097	2.892904
2	C	-2.616270	1.143049	1.676837
3	N	-3.117844	-0.120439	1.578888
4	C	-3.253662	-0.847469	2.692787
5	C	-2.813673	-0.357712	3.940288
6	C	-2.246884	0.886295	4.041976
7	C	-2.615447	1.958794	0.496652
8	N	-3.116334	1.421108	-0.651293
9	C	-3.249926	2.206397	-1.725200
10	C	-2.808862	3.546122	-1.707306
11	C	-2.243158	4.080416	-0.578760
12	C	-2.152956	3.289711	0.580192
13	Re	-3.320187	-0.799108	-0.538302
14	C	-3.262887	-1.234684	-2.402158
15	O	-3.200428	-1.527812	-3.522704
16	C	-1.216106	-0.717361	-0.483496
17	C	0.008566	-0.619995	-0.420407
18	C	1.425510	-0.508284	-0.349068
19	C	2.040591	0.561008	0.327424
20	C	3.420569	0.667349	0.404276
21	C	4.243609	-0.284586	-0.210393
22	C	3.644045	-1.349867	-0.893929
23	C	2.263727	-1.463050	-0.953530
24	N	5.652132	-0.170960	-0.141206
25	C	6.262952	1.086590	-0.327889
26	C	7.370494	1.465702	0.442989
27	C	7.969540	2.704926	0.249479
28	C	7.469860	3.595874	-0.697955
29	C	6.362862	3.225565	-1.458568
30	C	5.766755	1.982034	-1.285087
31	C	6.436998	-1.316444	0.110291
32	C	7.660193	-1.503339	-0.547618
33	C	8.429557	-2.632186	-0.291213
34	C	7.990333	-3.602643	0.606669
35	C	6.769499	-3.424519	1.253689
36	C	6.000775	-2.290730	1.018019
37	C	-3.262016	-2.696344	-0.286198
38	O	-3.198490	-3.848073	-0.163622
39	C	-5.282067	-0.774851	-0.521357
40	O	-6.443335	-0.771832	-0.519174
41	H	-1.886689	5.106993	-0.561302
42	H	-1.891058	1.264979	4.996552
43	H	1.413810	1.306704	0.808902
44	H	3.874951	1.494691	0.941979
45	H	4.272001	-2.091814	-1.378753
46	H	1.811418	-2.293191	-1.487918
47	H	5.054736	-2.152104	1.532574
48	H	6.413505	-4.169410	1.960732
49	H	8.590758	-4.487356	0.798056
50	H	9.374930	-2.759683	-0.812358
51	H	8.000753	-0.758389	-1.260466
52	H	7.756578	0.781139	1.192268
53	H	8.827793	2.980157	0.857200
54	H	7.937517	4.565672	-0.842010
55	H	5.964721	3.904811	-2.208109
56	H	4.912166	1.693258	-1.889482
57	H	-2.927923	-0.990683	4.814105
58	C	-1.637746	3.022011	2.929644
59	C	-1.636881	3.793991	1.812834
60	H	-2.921540	4.139993	-2.608350
61	H	-1.260789	4.813031	1.838415
62	H	-1.262286	3.405733	3.874271
63	C	-3.874371	1.672244	-2.972530
64	H	-3.154035	1.083321	-3.550184
65	H	-4.723967	1.024787	-2.741459
66	H	-4.216576	2.496506	-3.604528
67	C	-3.879403	-2.202477	2.632948
68	H	-4.727715	-2.214434	1.943965
69	H	-3.159207	-2.951779	2.287588
70	H	-4.223725	-2.501842	3.626809

1 (T_1)				
1	C	7.477361	-1.334826	-0.569590
2	C	6.323545	-1.157016	0.200099
3	C	5.991693	-2.100211	1.178521
4	C	6.799544	-3.215465	1.369755
5	C	7.950173	-3.392735	0.604363
6	C	8.286238	-2.446062	-0.361122
7	N	5.509077	-0.010535	0.002564
8	C	6.146513	1.254330	-0.098199
9	C	7.147843	1.605976	0.812355
10	C	7.787285	2.835254	0.700471
11	C	7.430373	3.727444	-0.308427
12	C	6.431494	3.376867	-1.214285
13	C	5.795887	2.143985	-1.119308
14	C	4.127064	-0.123403	-0.086826
15	C	3.289737	0.948355	0.293589
16	C	1.920622	0.832943	0.206532
17	C	1.310259	-0.355072	-0.266820
18	C	2.160627	-1.422602	-0.647191
19	C	3.530184	-1.312822	-0.559494
20	C	-0.079143	-0.467785	-0.354196
21	C	-1.321929	-0.559160	-0.417606
22	Re	-3.337115	-0.664899	-0.569275
23	C	-3.283368	-2.594775	-0.444424
24	O	-3.235908	-3.748591	-0.346554
25	N	-3.328168	1.493135	-0.461178
26	C	-3.168017	2.323809	-1.507096
27	C	-3.163844	3.696667	-1.401902
28	C	-3.338443	4.263480	-0.116854
29	C	-3.494123	3.438482	0.965018
30	C	-3.484009	2.026921	0.808207
31	C	-3.613373	1.097247	1.871415
32	N	-3.568205	-0.247925	1.527280
33	C	-3.666552	-1.177884	2.498544
34	C	-3.817838	-0.878596	3.831634
35	C	-3.871938	0.487755	4.204332
36	C	-3.769252	1.451350	3.237474
37	H	-3.348837	5.342078	0.012755
38	H	-3.992744	0.769883	5.246384
39	C	-5.356401	-0.631037	-0.711231
40	O	-6.500827	-0.626957	-0.817278
41	C	-3.177503	-0.861567	-2.501865
42	O	-3.083752	-0.965596	-3.650461
43	H	1.283502	1.654941	0.518023
44	H	3.733327	1.861893	0.675388
45	H	4.161064	-2.138076	-0.872572
46	H	1.711656	-2.334804	-1.027881
47	H	5.103226	-1.951481	1.785281
48	H	6.533674	-3.942248	2.132290
49	H	8.582073	-4.262108	0.760851
50	H	9.179292	-2.577060	-0.965843
51	H	7.731552	-0.599927	-1.327593
52	H	7.417415	0.912198	1.603082
53	H	8.562366	3.100508	1.414121
54	H	7.929073	4.688842	-0.389787
55	H	6.152669	4.060639	-2.011213
56	H	5.028771	1.861682	-1.834492
57	H	-3.616521	-2.208996	2.162753
58	H	-3.891733	-1.675523	4.562648
59	H	-3.806615	2.499915	3.512572
60	H	-3.626376	3.862490	1.954593
61	H	-3.033432	4.309513	-2.286491
62	H	-3.039073	1.840364	-2.470775