

Supplementary Information

**Substituents Effect in Magnesium Tetraethynylporphyrin with Two
Diketopyrrolopyrrole Units for Bulk Heterojunction Organic Solar
Cells**

Keisuke Ogumi,^{a§} Takafumi Nakagawa,^{b§} Hiroshi Okada,^b Ryohei Sakai,^c Huan Wang,^d
Yutaka Matsuo.^{*,b,d}

^a Tokyo Metropolitan Industrial Technology Research Institute, 2-4-10, Aomi, Koto-ku,
Tokyo 135-0064, Japan

^b Department of Mechanical Engineering, School of Engineering, The University of
Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

^c Fujipream Corporation, 38-1 Shikisai, Himeji, Hyogo 671-2216, Japan

^d Hefei National Laboratory for Physical Science at the Microscale, University of Science
and technology of China, Hefei, Anhui 230026, China

[§] These authors were contributed equally.

E-mail: matsuo@photon.t.u-tokyo.ac.jp / matsuo@ustc.edu.cn

– Table of Contents –

NMR spectra	S2
UV-vis absorption spectra	S11
Electrochemical data	S13
Photoelectron yield spectra	S16
Thermal analysis data	S19
Theoretical calculation data	S20
AFM images and appearance of the devices	S54
Hole mobility data	S58
Additional device data	S59

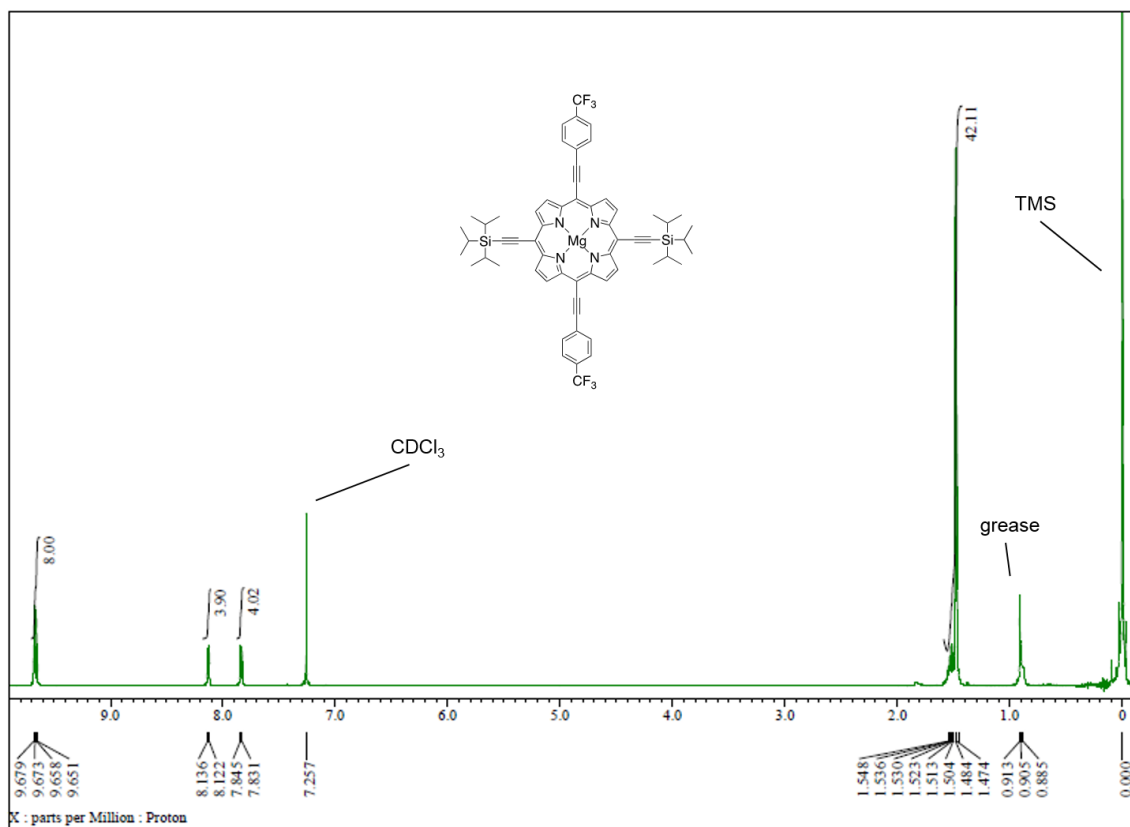


Figure S1. ¹H NMR spectrum for **1c**.

¹H NMR (600 MHz, CDCl₃): δ 1.46–1.55 (m, 42H, TIPS), 7.84 (d, *J* = 8.4 Hz, 4H, C₆H₄), 8.13 (d, *J* = 8.4 Hz, 4H, C₆H₄), 9.67 (dd, *J* = 9.0 Hz, *J* = 4.2 Hz, 8H, Porphyrin).

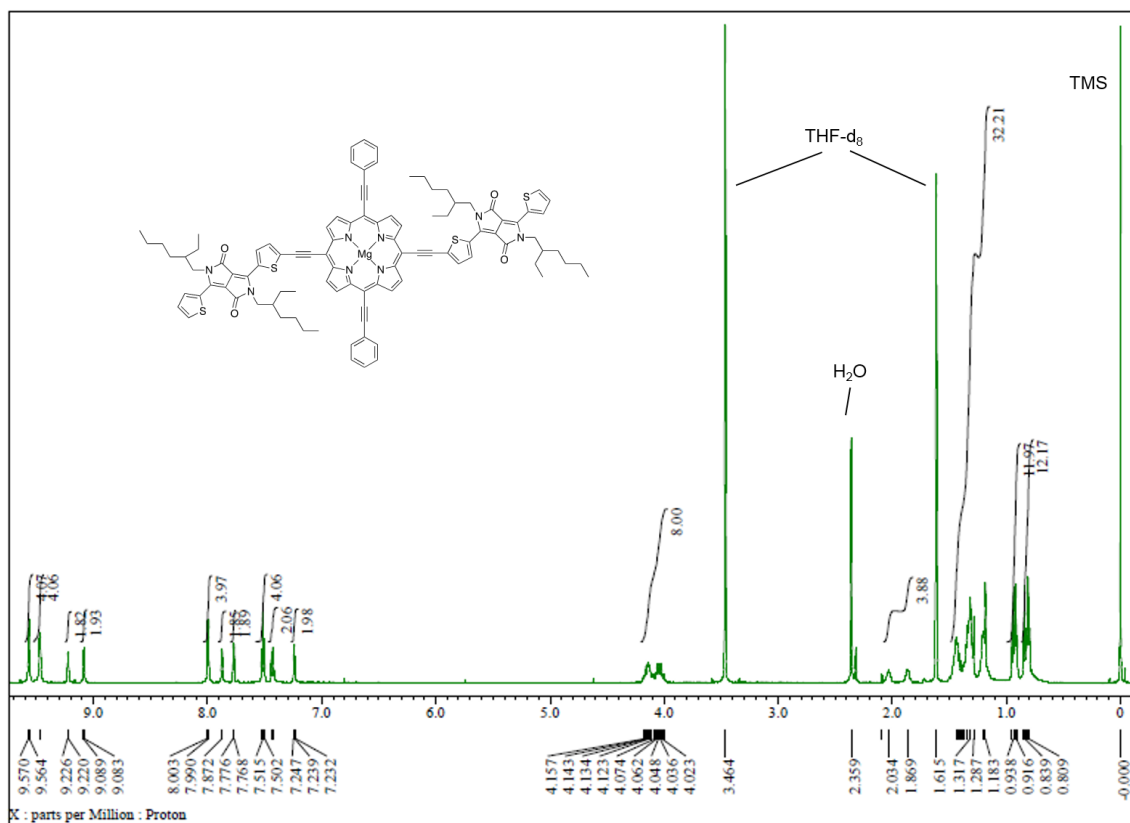


Figure S2. ¹H NMR spectrum for **2a**.

¹H NMR (600 MHz, THF-*d*₈): δ 0.80–0.85 (m, 12H, CH₃), 0.90–0.95 (m, 12H, CH₃), 1.13–1.44 (m, 32H, CH₂), 1.87–2.03 (br, 4H, CH), 4.00–4.18 (m, 8H, CH₂), 7.24 (t, $J = 4.5$ Hz, 2H, C₄SH₃), 7.43 (t, $J = 7.2$ Hz, 2H, C₆H₅), 7.52 (t, $J = 7.8$ Hz, 4H, C₆H₅), 7.77 (d, $J = 4.8$ Hz, 2H, C₄SH₃), 7.88 ($J = 3.6$ Hz, 2H, C₄SH₂), 8.00 (d, $J = 7.8$ Hz, 4H, C₆H₅), 9.09 (d, $J = 3.6$ Hz, 2H, C₄SH₃), 9.22 (d, $J = 3.6$ Hz, 2H, C₄SH₂), 9.47 (d, $J = 4.2$ Hz, 4H, Porphyrin), 9.57 (d, $J = 3.6$ Hz, 4H, Porphyrin).

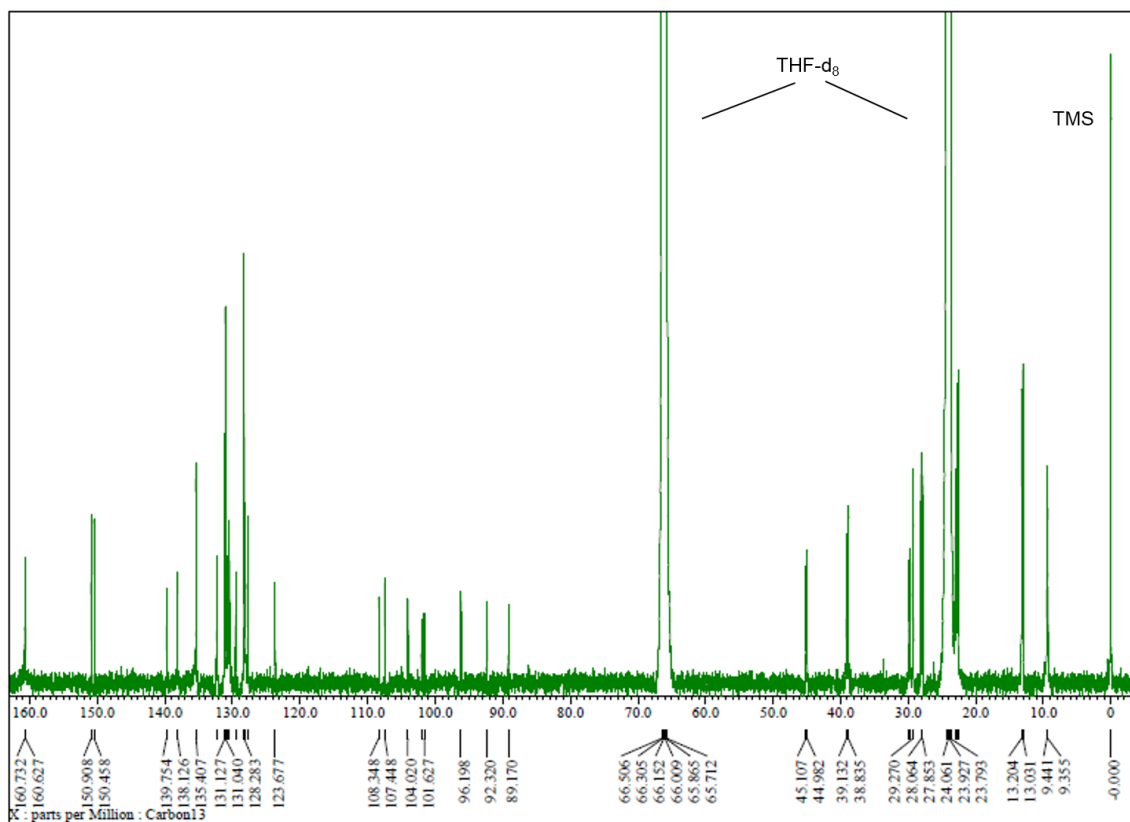


Figure S3. ^{13}C NMR spectrum for **2a**.

^{13}C NMR (150 MHz, THF- d_8): δ 9.34, 9.44, 9.46, 13.03, 13.20, 22.62, 22.73, 22.88, 23.04, 23.06, 27.84, 27.86, 28.06, 29.26, 29.34, 29.68, 29.72, 29.85, 29.87, 38.83, 39.13, 44.98, 45.11, 89.17, 92.32, 96.20, 101.64, 102.04, 104.03, 107.45, 108.35, 123.68, 124.51, 127.79, 128.14, 128.28, 129.52, 120.45, 130.59, 130.82, 131.05, 131.14, 132.34, 135.41, 138.13, 139.75, 150.46, 150.91, 160.63, 160.73.

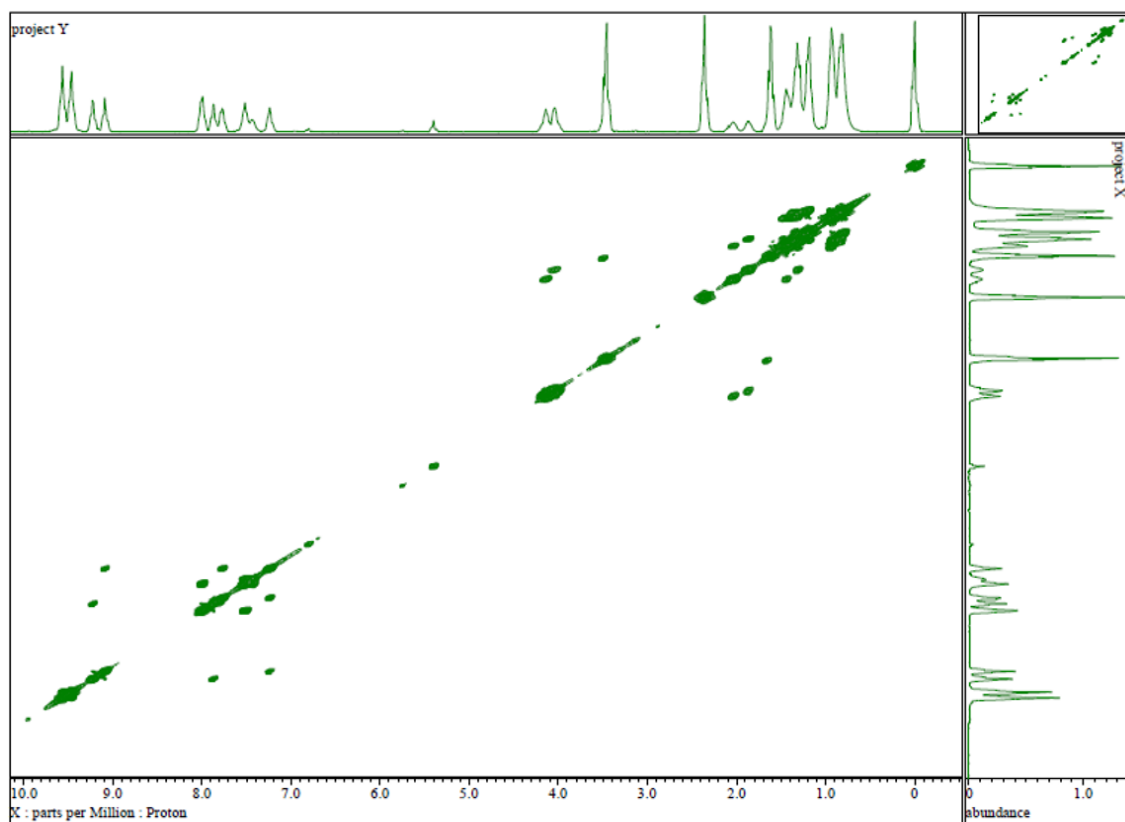


Figure S4. ^1H - ^1H COSY spectrum for **2a**.

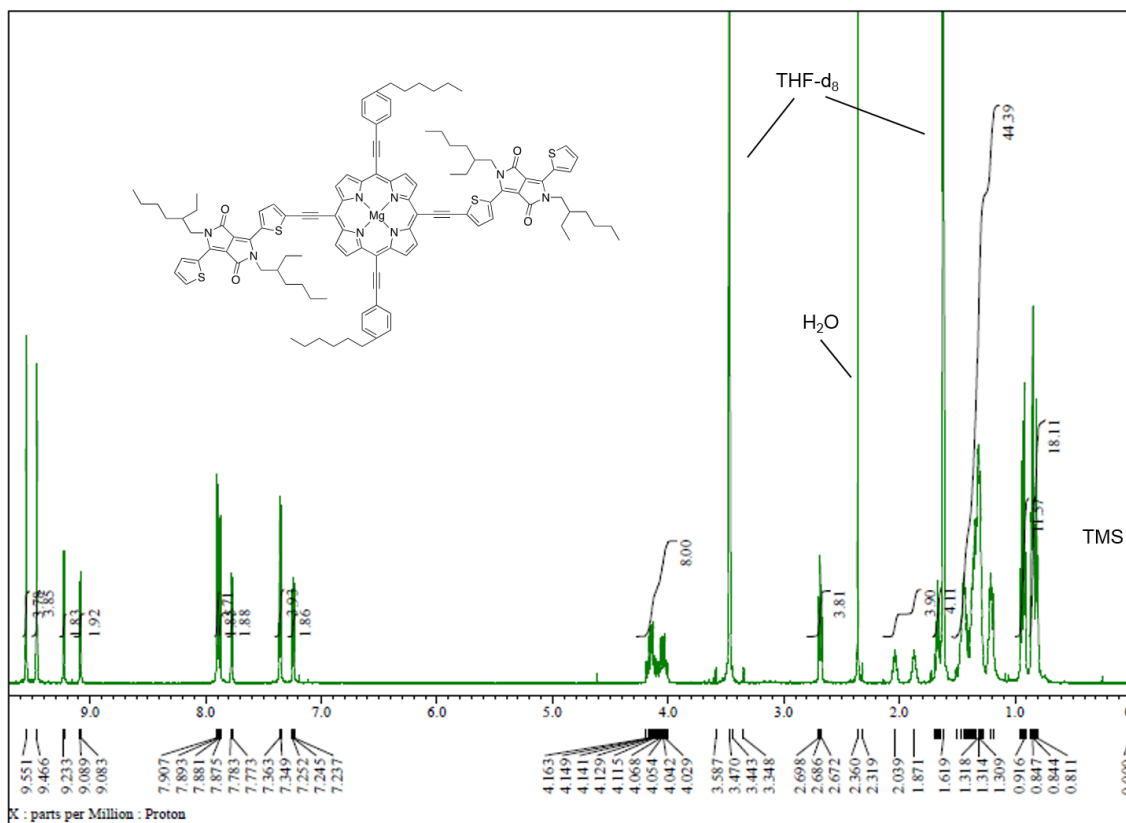


Figure S5. ^1H NMR spectrum for **2b**.

^1H NMR (600 MHz, THF-d_8): δ 0.80–0.86 (m, 18H, CH_3), 0.91–0.95 (m, 12H, CH_3), 1.18–1.47 (m, 44H, CH_2), 1.70 (quin, $J = 7.8$ Hz, 4H, CH_2), 1.85–2.07 (br, 4H, CH), 4.00–4.19 (m, 8H, CH_2), 7.25 (t, $J = 4.2$ Hz, 2H, C_4SH_3), 7.36 (d, $J = 8.4$ Hz, 4H, C_6H_4), 7.77–7.78 (m, 2H, C_4SH_3), 7.88 (d, $J = 3.6$ Hz, 2H, C_4SH_2), 7.90 (d, $J = 8.4$ Hz, 4H, C_6H_4), 9.09 (d, $J = 3.6$ Hz, 2H, C_4SH_3), 9.23 (d, $J = 4.2$ Hz, 2H, C_4SH_2), 9.63 (d, $J = 3.6$ Hz, 4H, Porphyrin), 9.56 (d, $J = 4.8$ Hz, 4H, Porphyrin).

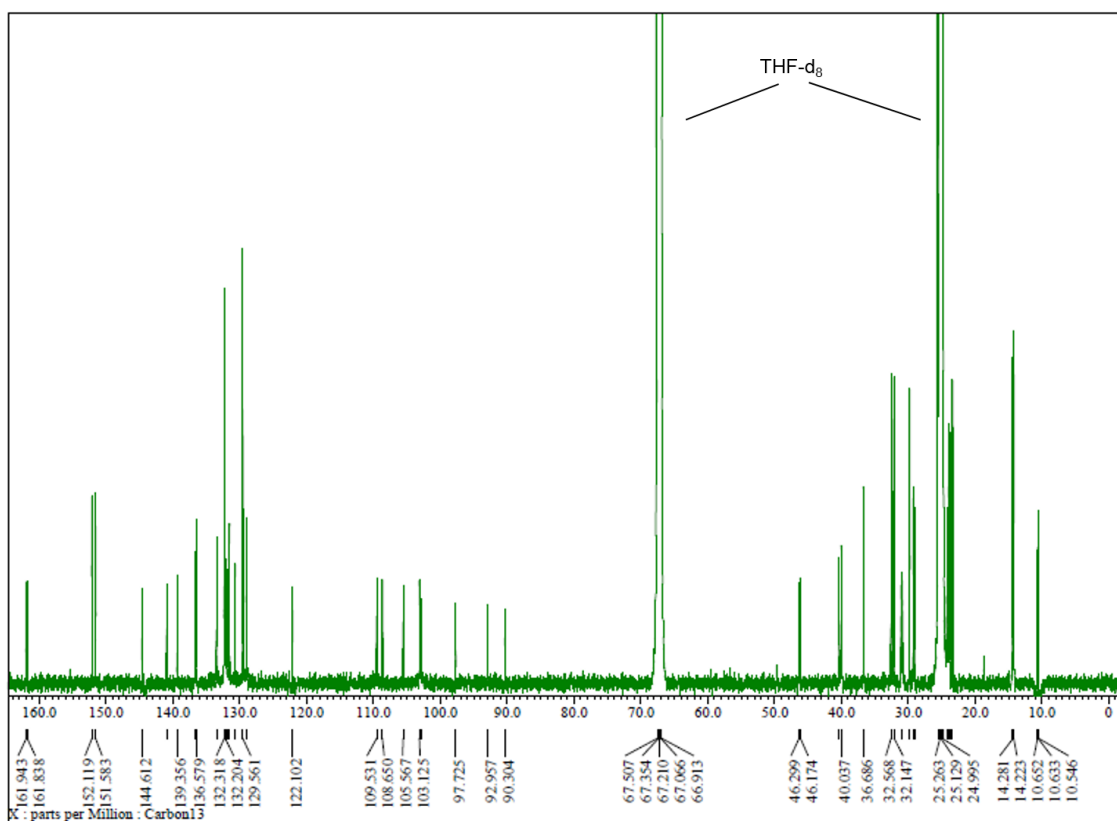


Figure S6. ^{13}C NMR spectrum for **2b**.

^{13}C NMR (150 MHz, THF- d_8): δ 10.55 (two peaks, overlapped), 10.63, 10.65, 14.22, 14.28, 14.41, 23.39, 23.82, 23.93, 24.08, 24.24 (two peaks, overlapped), 29.06, 29.27, 29.81, 30.88, 30.92, 31.05, 31.08, 32.15, 32.57, 36.69, 40.04, 40.33, 46.17, 16.30, 90.30, 92.96, 97.73, 102.93, 103.13, 105.57, 108.65, 109.53, 122.10, 128.98, 129.56 (two peaks, overlapped), 130.72, 131.55, 131.74, 132.00, 132.20 (two peaks, overlapped), 132.32, 133.50, 136.58, 136.64, 139.36, 140.94, 144.61, 151.58, 152.12, 161.84, 161.94.

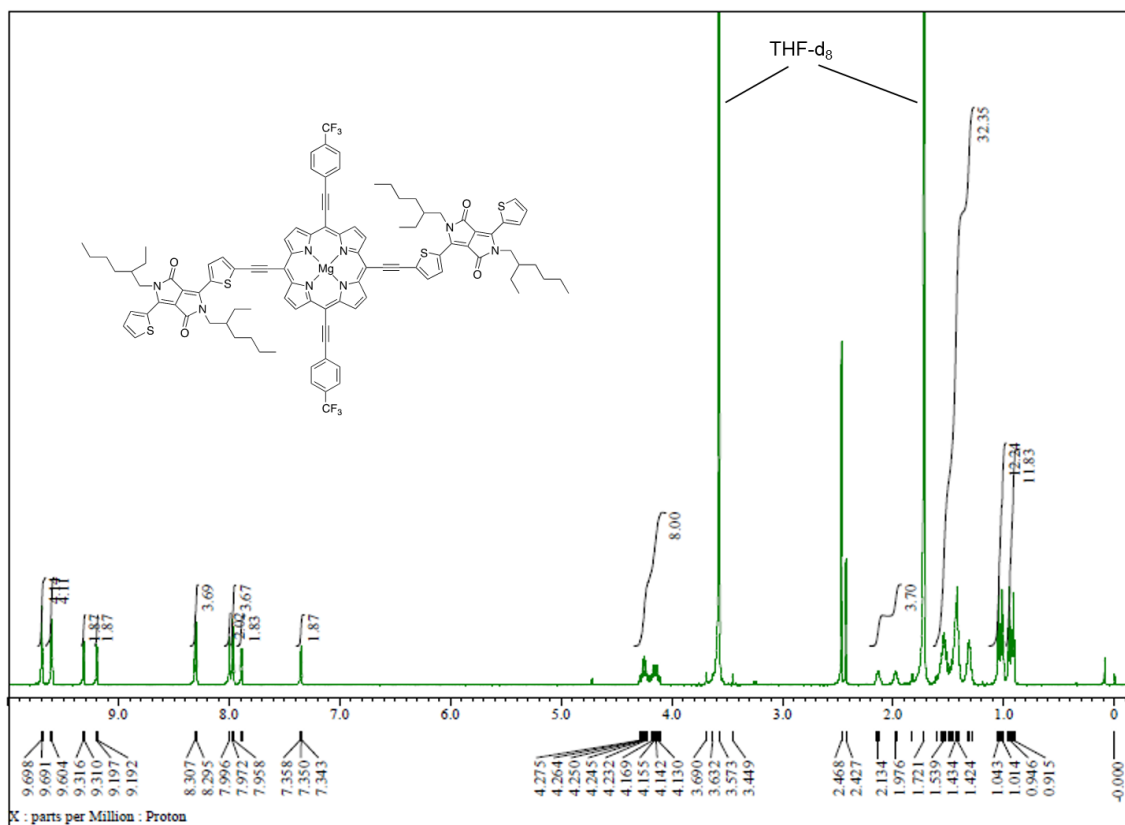


Figure S7. ^1H NMR spectrum for **2c**.

^1H NMR (600 MHz, THF-d_8): δ 0.90–0.96 (m, 12H, CH_3), 1.00–1.06 (m, 12H, CH_3), 1.29–1.61 (m, 32H, CH_2), 1.97–2.15 (br, 4H, CH), 4.10–4.29 (m, 8H, CH_2), 7.35 (t, $J = 4.8$ Hz, 2H, C_4SH_3), 7.89 (d, $J = 4.8$ Hz, 2H, C_4SH_3), 7.97 (d, $J = 8.4$ Hz, 4H, C_6H_4), 8.00 (d, $J = 4.2$ Hz, 2H, C_4SH_3), 8.30 (d, $J = 7.2$ Hz, 4H, C_6H_4), 9.19 (d, $J = 3.0$ Hz, 2H, C_4SH_3), 9.31 (d, $J = 3.6$ Hz, 2H, C_4SH_3), 9.60–9.61 (m, 4H, Porphyrin), 9.69–9.70 (m, 4H, Porphyrin).

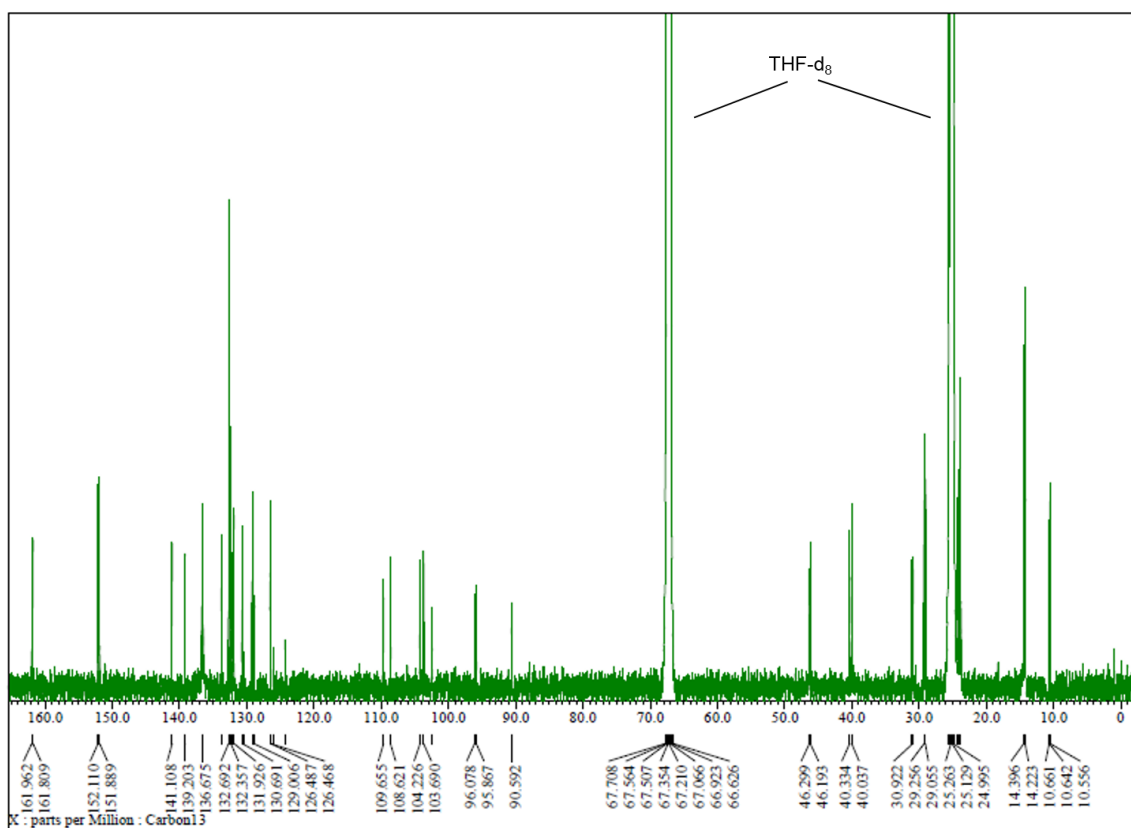


Figure S8. ^{13}C NMR spectrum for **2c**.

^{13}C NMR (150 MHz, THF-d_8): δ 10.56, 10.64, 10.66, 14.22, 14.40, 23.82, 23.92, 24.09, 24.26, 24.87, 25.00, 25.13, 25.26, 25.33, 25.40, 25.46, 25.60, 29.06, 29.26, 30.88, 30.92, 31.04, 31.07, 40.04, 40.33, 46.19, 46.30, 90.59, 95.87, 96.08, 102.43, 103.69, 104.23, 108.62, 109.66, 124.28, 126.08, 126.47, 126.49, 128.86, 129.01, 129.20, 130.46, 130.69, 131.93, 132.00, 132.36, 132.69, 133.73 (two peaks, overlapped), 136.49, 136.68, 139.20, 141.11, 151.89, 152.11, 161.81, 161.96.

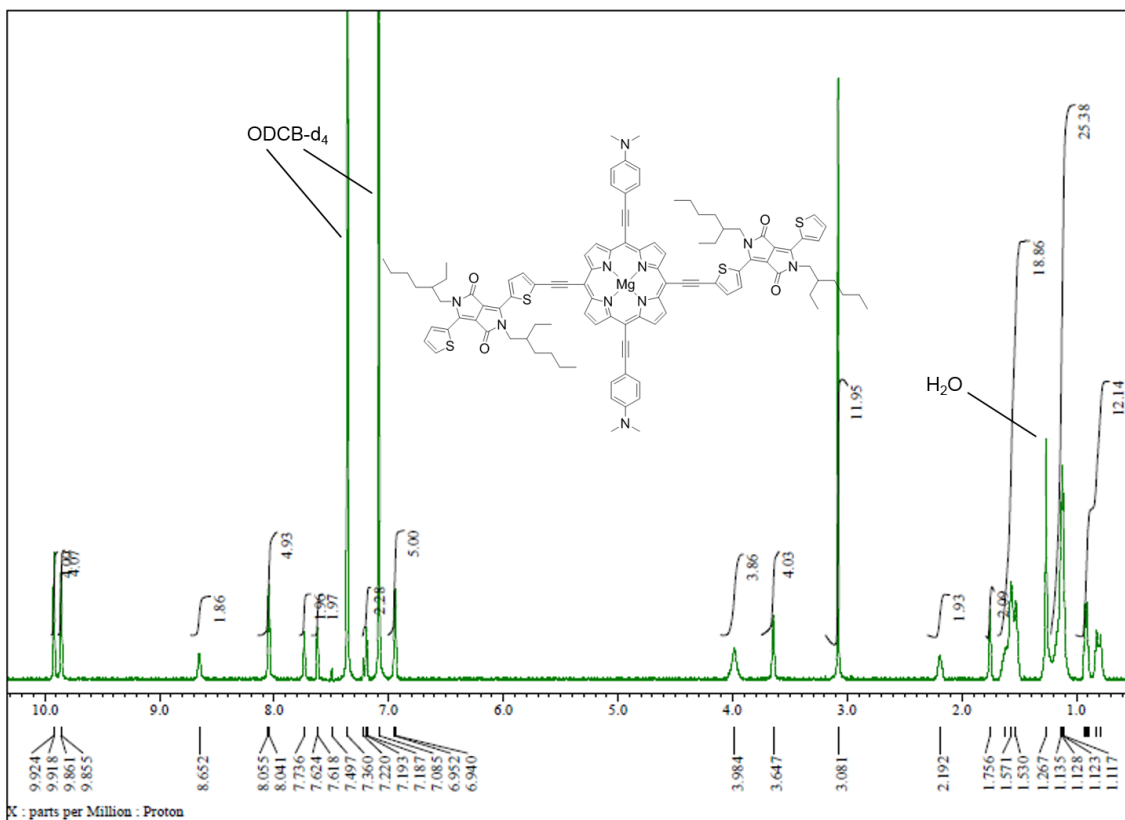


Figure S9. ¹H NMR spectrum for **2d**.

¹H NMR (600 MHz, ODCB-*d*₄, 120 °C): δ 0.79–0.94 (m, 12H), 1.12–1.14 (m, 25H), 1.53–1.62 (m, 19H), 1.76 (m, 2H), 2.19 (br, 2H), 3.08 (s, 12H), 3.65 (s, 4H), 3.98 (br, 4H), 6.95 (d, *J* = 7.2 Hz, 5H), 7.19–7.22 (m, 2H), 7.62 (d, *J* = 3.6 Hz, 2H), 7.74 (br, 2H), 8.05 (d, *J* = 8.4 Hz, 5H), 8.65 (br, 2H), 9.86 (d, *J* = 3.6 Hz, 4H, Porphyrin), 9.92 (d, *J* = 3.6 Hz, 4H, Porphyrin).

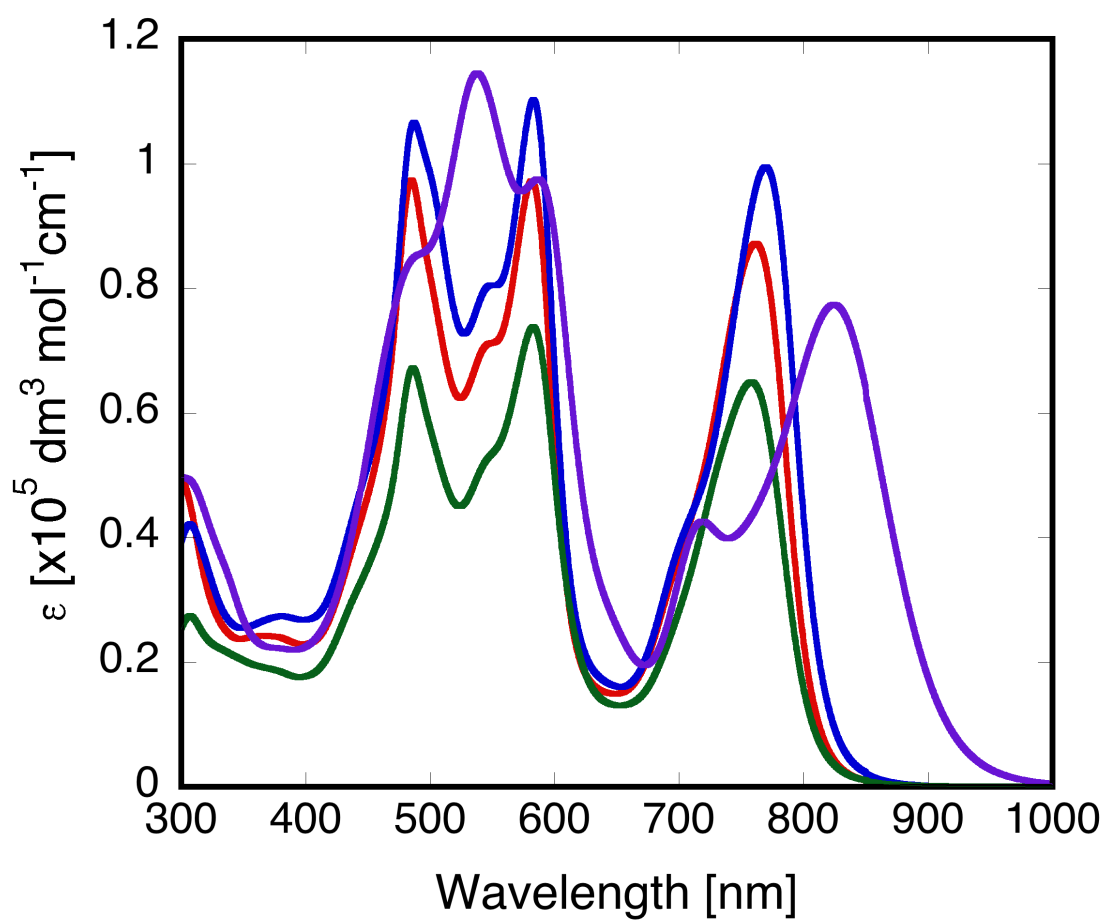


Figure S10. UV-vis absorption spectra of **2a** (red line), **2b** (blue line), **2c** (green line), and **2d** (purple line) in CH_2Cl_2 .

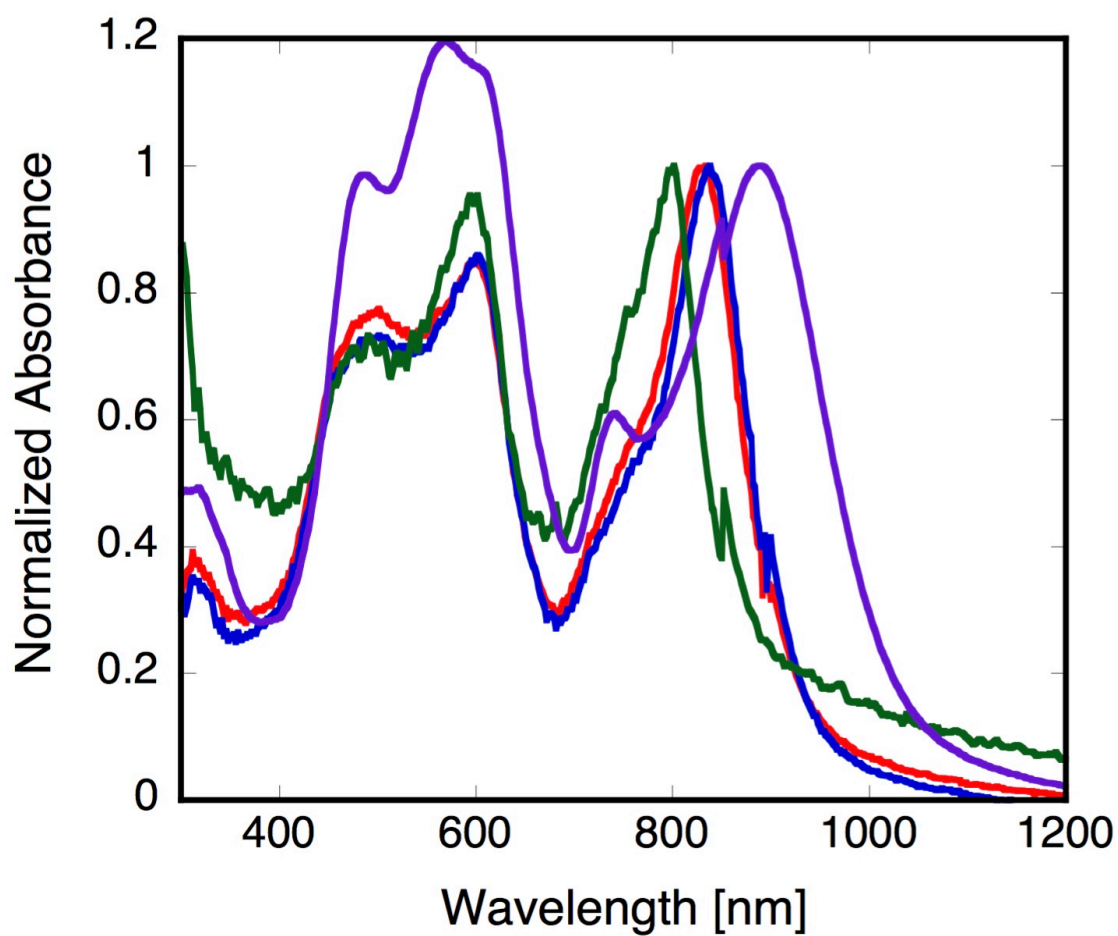


Figure S11. UV-vis absorption spectra of thin films for **2a** (red line), **2b** (blue line), **2c** (green line), and **2d** (purple line) which were fabricated on a PEDOT:PSS spin-coated glasses. The spikes around 850–900 nm were caused by lamp switching.

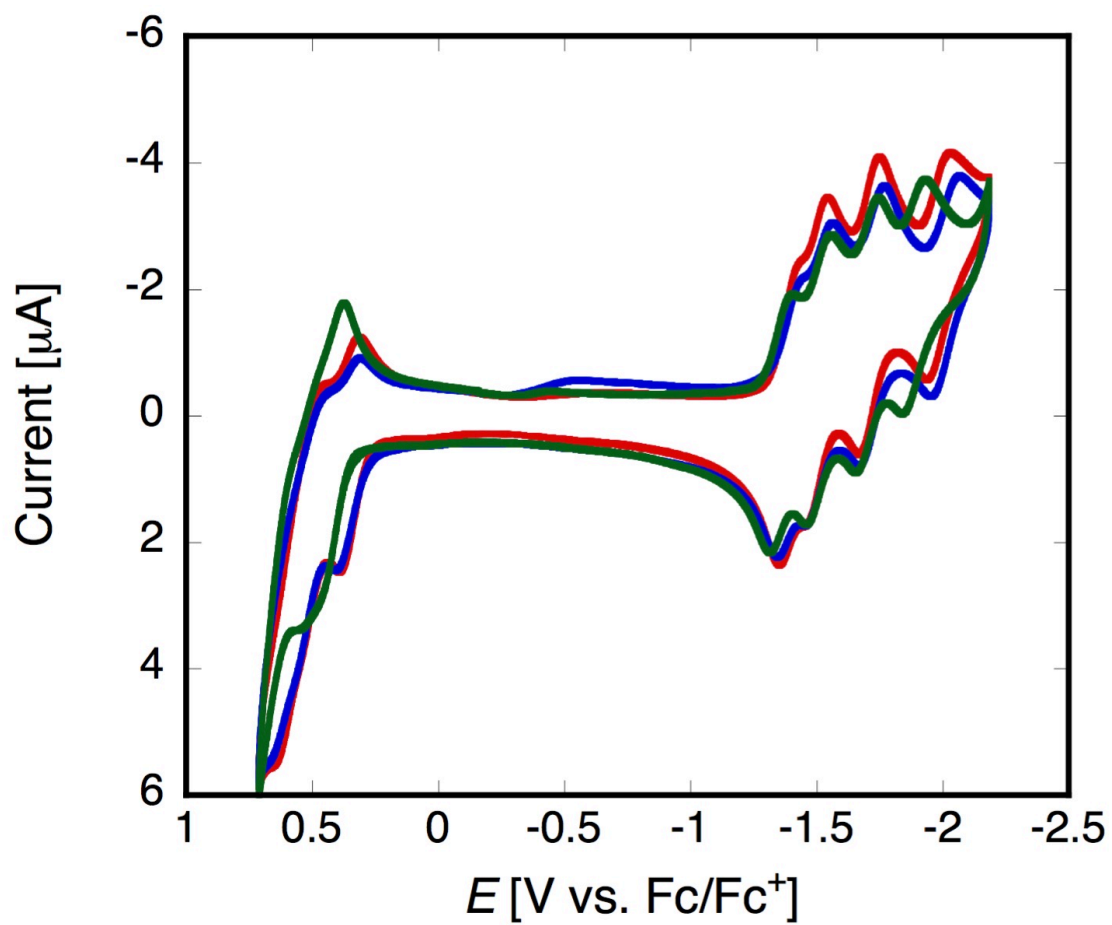


Figure S12. Cyclic voltammetry curves of **2a** (red line), **2b** (blue line), and **2c** (green line) in THF.

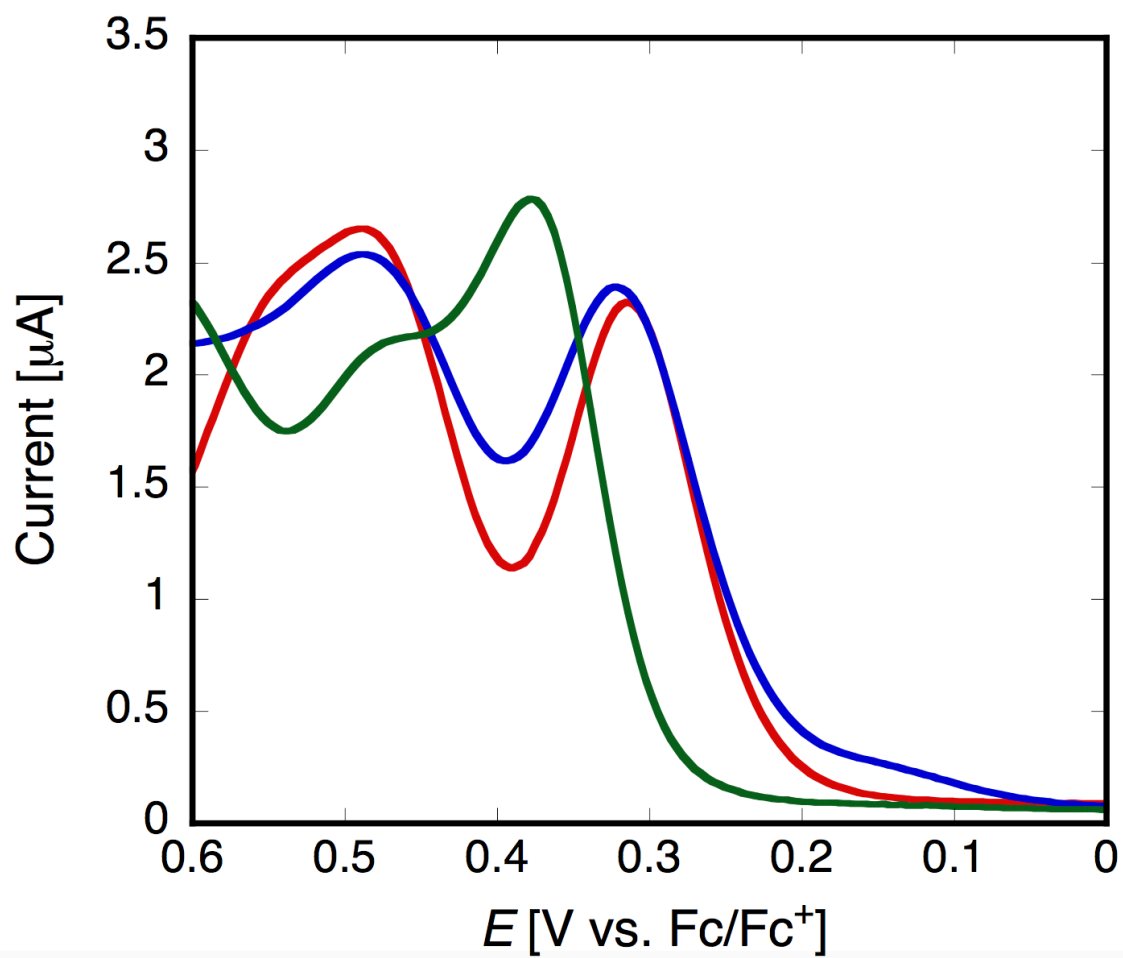


Figure S13. Differential pulse voltammetry (DPV) of the oxidation range for **2a** (red line), **2b** (blue line), and **2c** (green line) in THF.

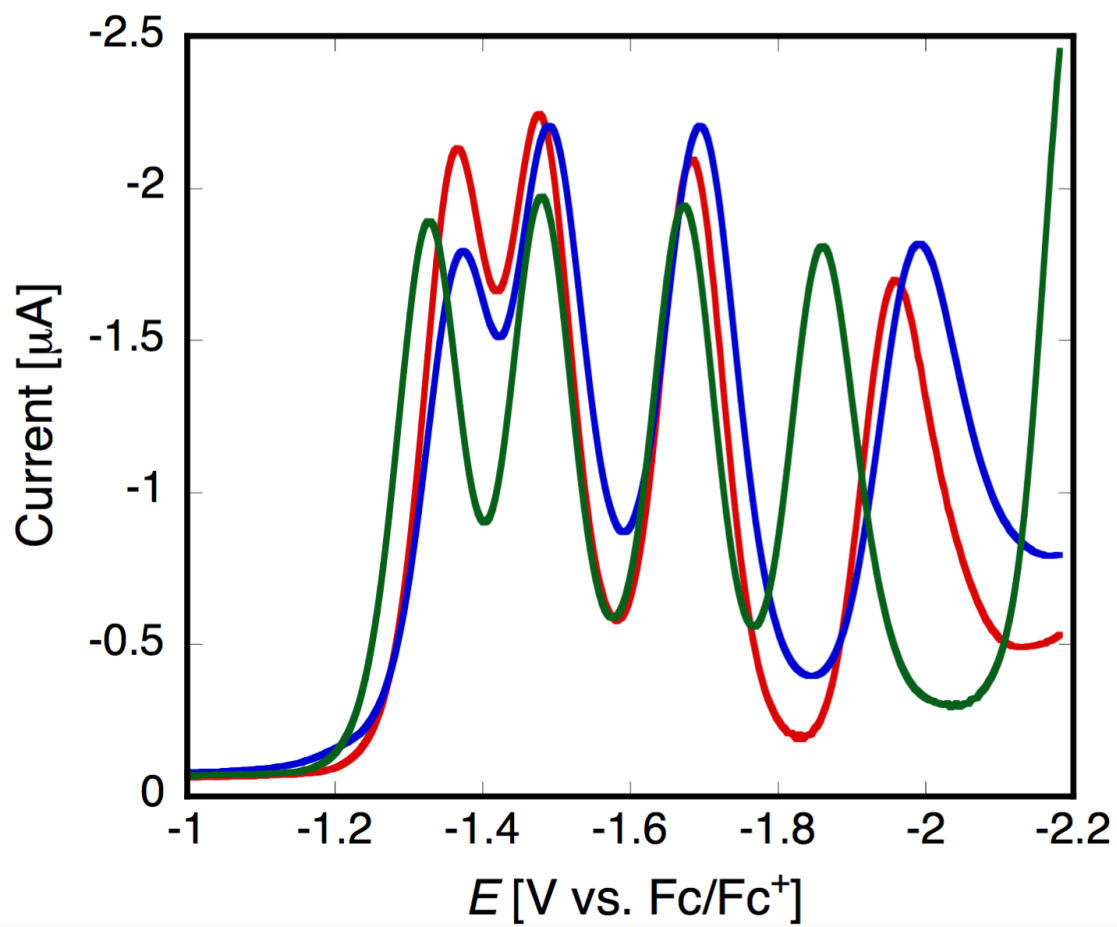


Figure S14. DPV of the reduction range for **2a** (red line), **2b** (blue line), and **2c** (green line) in THF.

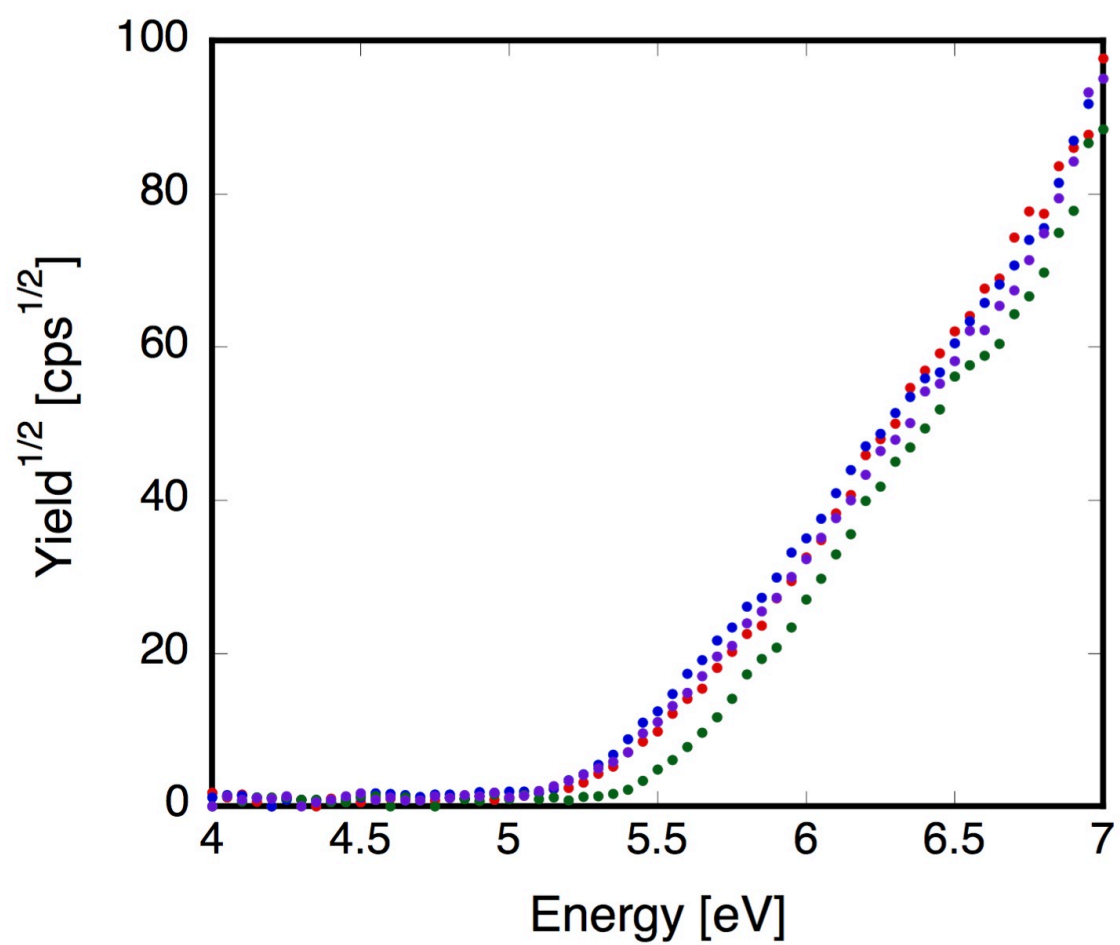


Figure S15. Photoelectron yield spectroscopies for **2a** (red line), **2b** (blue line), **2c** (green line), and **2d** (purple line) in thin films, which were fabricated by spin-coating on the ITO plates.

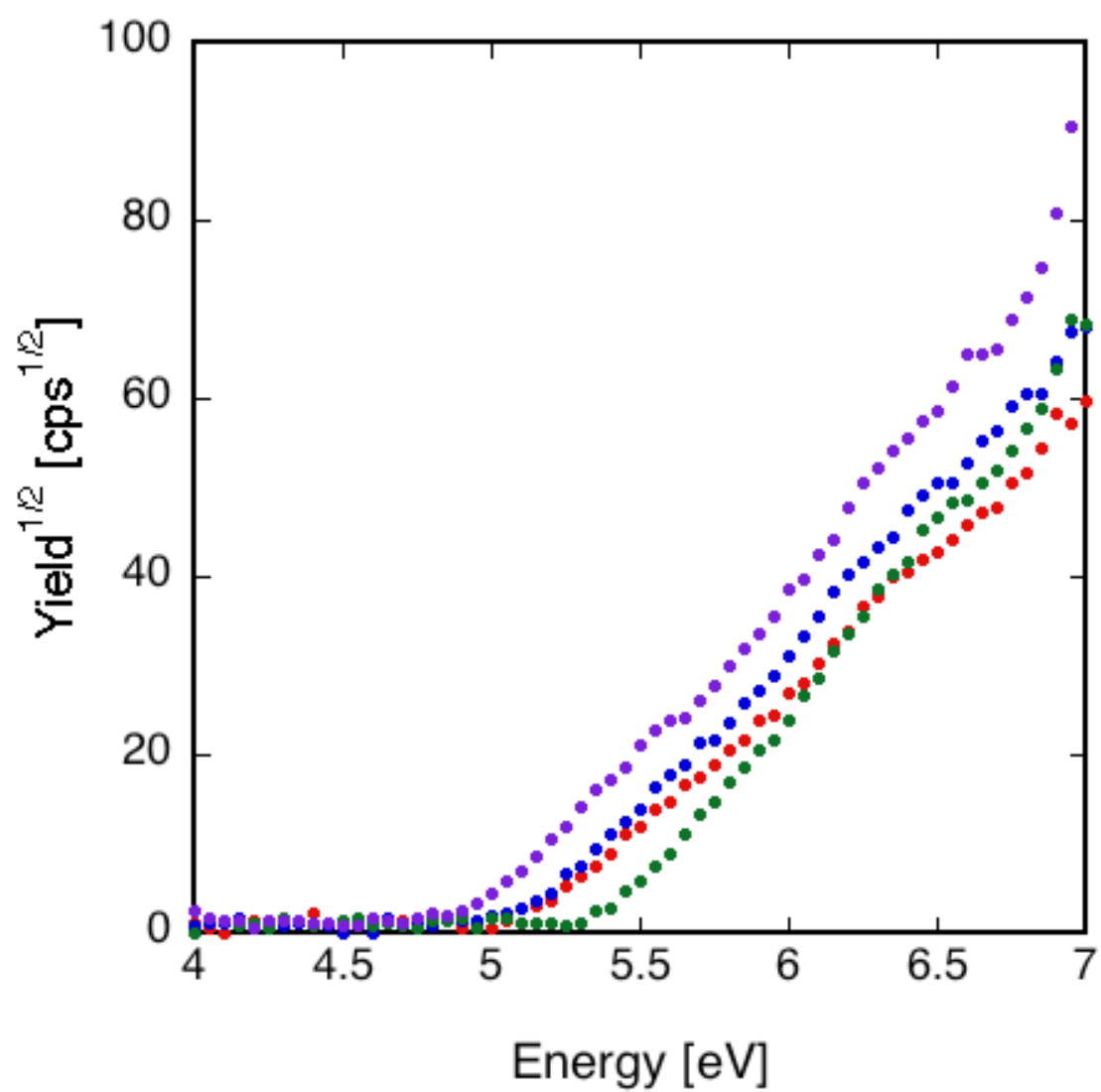


Figure S16. Photoelectron yield spectroscopies of solid samples of **2a** (red line), **2b** (blue line), **2c** (green line), and **2d** (purple line), which were prepared by crushing samples onto sample holders.

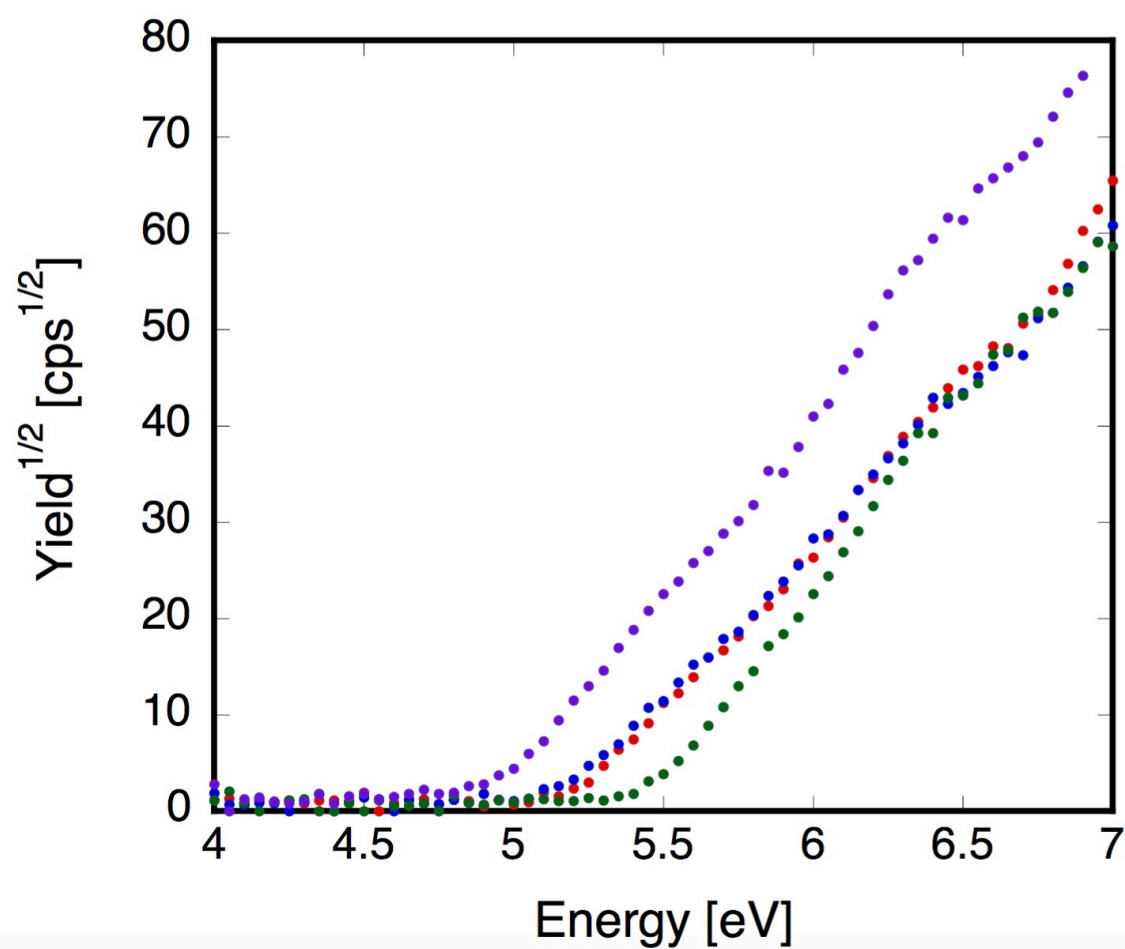


Figure S17. Photoelectron yield spectroscopies of pyridine complexes **2a**·py (red line), **2b**·py (blue line), **2c**·py (green line), and **2d**·py (purple line) as solid state.

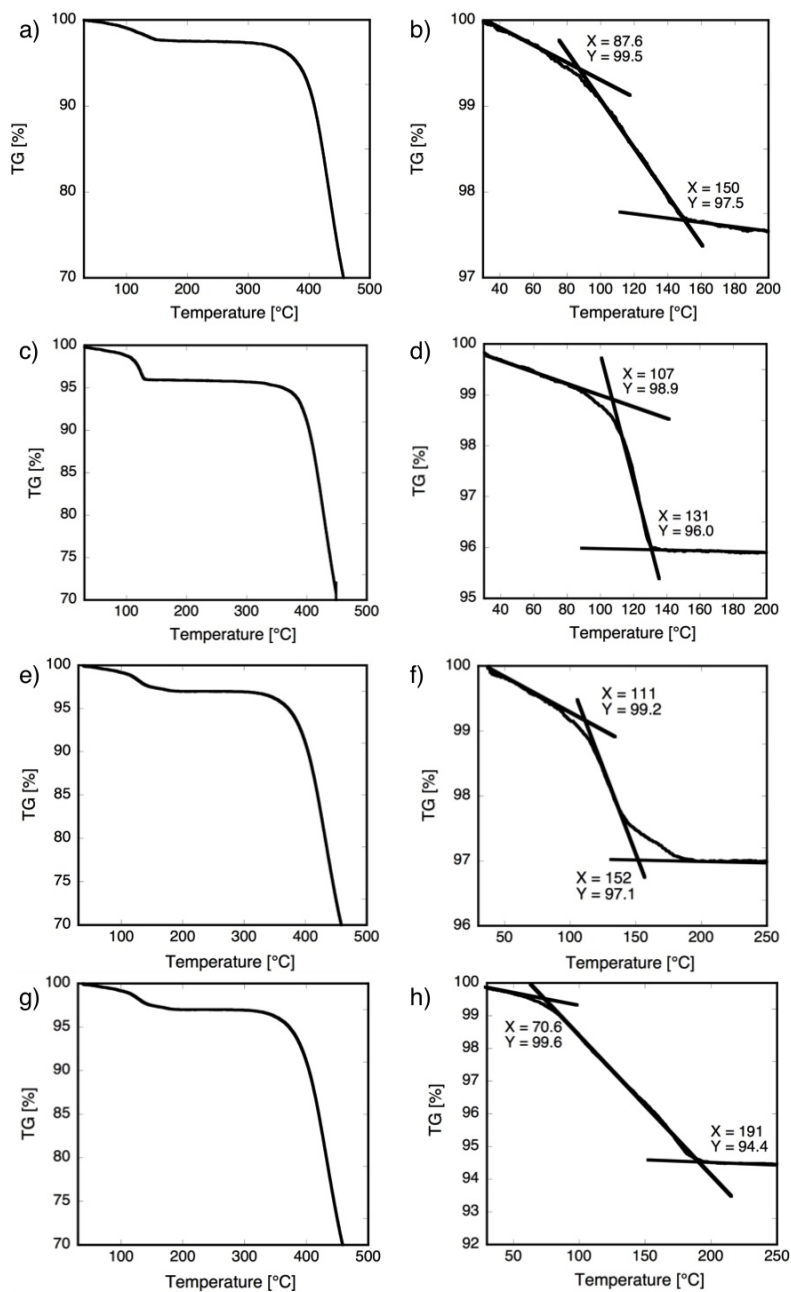


Figure S18. Thermogravimetry analyses of **2a**·py (a, b), **2b**·py (c, d), **2c**·py (e, f), and **2d**·py (g, h). The starting temperature to remove a coordinated pyridine was 87.6, 107, 111, and 70.6 °C, respectively.

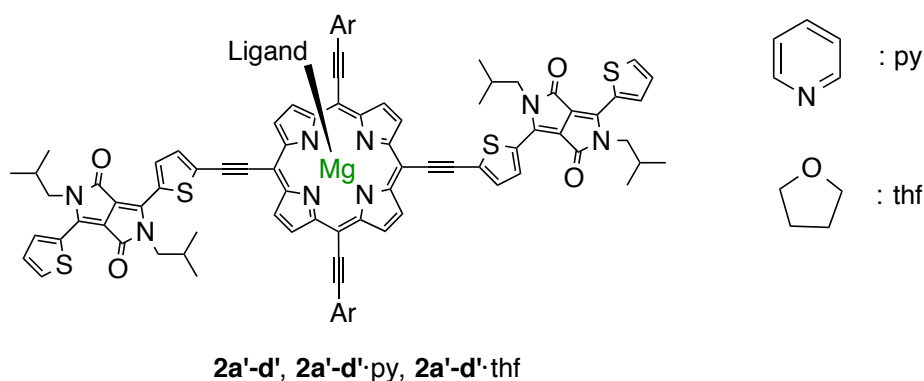


Figure S19. Chemical structures of calculated Mg-TEP-DPP₂Ar₂ (with coordinated ligands) and free ligands.

Table S1. Calculated energies and the numbers of imaginary frequency for the optimized structures. Calculations were carried out by using Gaussian09 package at the B3LYP/6-31G(d) level.

	Ar	Ligand	Number of imaginary frequencies	free energy / Hartree	HOMO / Hartree	LUMO / Hartree
2a'	Ph	(none)	0	-5770.093572	-0.17307	-0.11275
2b'	4-Me-C ₆ H ₄	(none)	0	-5848.681606	-0.17165	-0.11173
2c'	4-CF ₃ -C ₆ H ₄	(none)	0	-6444.16958	-0.17803	-0.11742
2d'	4-Me ₂ N-C ₆ H ₄	(none)	0	-6037.899345	-0.16291	-0.10701
2a'·py	Ph	py	0	-6018.325859	-0.16827	-0.10856
2b'·py	4-Me-C ₆ H ₄	py	0	-6096.913598	-0.16684	-0.10745
2c'·py	4-CF ₃ -C ₆ H ₄	py	0	-6692.402321	-0.17374	-0.11297
2d'·py	4-Me ₂ N-C ₆ H ₄	py	0	-6286.130985	-0.15818	-0.10332
2a'·thf	Ph	thf	0	-6002.462322	-0.1688	-0.10887
2b'·thf	4-Me-C ₆ H ₄	thf	0	-6081.049567	-0.16739	-0.10816
2c'·thf	4-CF ₃ -C ₆ H ₄	thf	0	-6676.5383	-0.17423	-0.1133
2d'·thf	4-Me ₂ N-C ₆ H ₄	thf	0	-6270.266479	-0.15867	-0.1037
py	—	—	0	-248.223331	-0.25259	-0.02246
thf	—	—	0	-232.360714	-0.2374	0.08753

Table S2. Cartesian coordinates for the optimized structures

1. 2a' (Ar = Ph, no ligand)				C	3.422667	-3.438611	-0.665521
Symbol	X	Y	Z	C	4.333616	-4.236477	-0.829488
C	-2.848608	1.534961	2.885765	C	-4.660771	3.862266	0.768485
C	-2.166789	0.678281	3.700375	C	5.380173	-5.146735	-0.999946
C	-1.212669	-0.014830	2.874296	C	0.958277	0.836991	-8.230817
N	-1.320867	0.418357	1.575108	C	0.987195	1.141963	-9.588229
C	-2.312988	1.365226	1.559892	C	0.048383	2.021476	-10.13386
C	-1.981995	2.217161	-3.127731	C	-0.923477	2.597090	-9.311245
C	-2.714401	2.650031	-2.060703	C	-0.960275	2.298629	-7.952588
C	-2.246520	1.921203	-0.910112	C	-1.397686	-1.329363	8.139284
N	-1.244744	1.060233	-1.279022	C	-1.434297	-1.642201	9.494717
C	-1.064696	1.224752	-2.630981	C	-0.498206	-2.524409	10.040682
C	-2.751867	2.077149	0.409855	C	0.478669	-3.094806	9.220369
C	2.455554	-1.978510	-2.964013	C	0.523173	-2.788464	7.863700
C	1.763000	-1.133271	-3.781496	C	-12.98081	13.260723	0.336151
C	0.804654	-0.444624	-2.956551	C	-12.41212	12.841180	-0.837889
N	0.918297	-0.871990	-1.655894	C	-11.48957	11.782537	-0.658926
C	1.920147	-1.808506	-1.638067	C	-11.34320	11.386500	0.665061
C	-0.115384	0.529723	-3.425600	S	-12.39083	12.367636	1.691629
C	1.581230	-2.668929	3.047419	C	-10.48267	10.309466	1.096111
C	2.324165	-3.090611	1.983202	C	-9.725749	9.480739	0.259013
C	1.856187	-2.361832	0.832582	C	-9.035043	8.518760	1.041150
N	0.844735	-1.511147	1.198935	C	-9.372110	8.742584	2.427871
C	0.658977	-1.681759	2.549367	N	-10.25829	9.869139	2.401326
C	-0.296517	-0.993363	3.342306	C	-9.379693	9.263270	-1.128868
C	2.369042	-2.509786	-0.485384	N	-8.479108	8.146771	-1.098159
C	-0.081127	0.838762	-4.813085	C	-8.260563	7.705238	0.208011
C	-0.338133	-1.310228	4.727821	O	-9.697493	9.821970	-2.177329
C	-0.051945	1.103291	-6.002171	O	-9.063744	8.179354	3.477455
C	-0.374294	-1.582034	5.915072	C	-10.75208	10.368224	3.685588
C	-0.018013	1.412070	-7.390970	C	-7.975635	7.611021	-2.360551
C	-0.416244	-1.899078	7.301787	C	-7.379774	6.649976	0.630644
C	-3.780386	3.032379	0.596588	C	-7.253263	6.213879	1.949681
Mg	-0.200912	-0.226435	-0.040295	C	-6.301550	5.198456	2.125793

C	-5.659162	4.822725	0.951634	H	7.204951	-10.56740	1.611177
S	-6.266751	5.758947	-0.402874	H	5.486869	-7.204190	3.770952
C	-9.719327	11.191381	4.485611	C	12.458184	-8.412144	-4.004022
C	-9.217575	12.431378	3.735419	C	13.540302	-8.016314	-2.991892
C	-10.32646	11.566482	5.845063	C	13.070498	-8.784578	-5.361996
H	-8.780783	12.169913	2.765409	H	13.109873	-7.749239	-2.020552
H	-10.65378	10.678648	6.399018	H	12.296808	-9.031253	-6.098771
C	-8.700885	6.347531	-2.872401	H	-3.641191	2.219478	3.152174
C	-10.20142	6.587951	-3.085599	H	-2.291705	0.525930	4.762710
C	-8.019488	5.875793	-4.165089	H	-2.049923	2.537148	-4.157479
H	-10.70165	6.869039	-2.153094	H	-3.499113	3.392998	-2.049163
H	-6.955200	5.663060	-4.006926	H	3.255180	-2.655540	-3.228506
C	6.002752	-5.548435	-2.176164	H	1.884738	-0.984309	-4.844679
C	7.031751	-6.481611	-1.981151	H	1.645861	-2.992422	4.076284
C	7.233815	-6.832633	-0.646112	H	3.115040	-3.827056	1.973322
S	6.099212	-5.959308	0.379351	H	1.687518	0.154366	-7.805393
C	8.252368	-7.741727	-0.194286	H	1.745191	0.691882	-10.22345
C	9.233217	-8.344530	-0.988701	H	0.074098	2.257052	-11.19414
C	10.090913	-9.127972	-0.173333	H	-1.655815	3.281582	-9.730552
C	9.632881	-9.019547	1.194580	H	-1.715350	2.744539	-7.312443
N	8.486234	-8.160676	1.116851	H	-2.124786	-0.644616	7.713603
C	9.693878	-8.449232	-2.353887	H	-2.196150	-1.196124	10.128150
N	10.843161	-9.302638	-2.277289	H	-0.529888	-2.766077	11.099421
C	11.079555	-9.721709	-0.967228	H	1.208970	-3.781303	9.639952
O	9.294019	-7.987746	-3.422200	H	1.282201	-3.230259	7.225380
O	10.032898	-9.486060	2.259834	H	-12.64528	13.275352	-1.803732
C	7.729880	-7.882287	2.335406	H	-10.94205	11.304470	-1.465164
C	11.564088	-9.574782	-3.521499	H	-11.66794	10.938582	3.526841
C	12.114857	-10.61434	-0.500708	H	-11.01971	9.483277	4.271074
C	12.303483	-10.95718	0.832721	H	-8.112075	8.421660	-3.082515
C	13.363159	-11.87238	1.040867	H	-6.898972	7.433159	-2.274596
C	13.989322	-12.24063	-0.121102	H	-7.841196	6.647061	2.753100
S	13.294450	-11.46591	-1.499498	H	-8.866218	10.525554	4.663803
C	6.449042	-8.724975	2.519864	H	-10.02691	13.149893	3.557709
C	6.745176	-10.23035	2.545886	H	-8.442443	12.941626	4.318892
C	5.739257	-8.271072	3.803667	H	-9.594107	12.095470	6.464939

H	-11.19496	12.227207	5.722526	C	3.565678	0.098025	-3.570351
H	-8.585493	5.555658	-2.119960	C	3.149319	0.116935	-2.191975
H	-10.37575	7.391535	-3.810194	N	4.248955	0.109575	-1.372411
H	-10.68382	5.677660	-3.460096	C	5.349905	0.086672	-2.193924
H	-8.490615	4.961437	-4.542053	C	1.797004	0.140139	-1.752742
H	-8.096736	6.638246	-4.950935	C	8.517459	0.094149	1.373611
H	7.636534	-6.900941	-2.779511	C	8.516017	0.076668	0.009029
H	8.424499	-8.100201	3.152081	C	7.138201	0.085820	-0.408442
H	7.500581	-6.813185	2.382267	N	6.318422	0.108081	0.693810
H	12.141567	-10.49377	-3.414999	C	7.139823	0.113309	1.792136
H	10.797606	-9.761095	-4.279955	C	6.701714	0.074440	-1.759567
H	11.678336	-10.55381	1.623161	C	3.569513	0.178951	4.963700
H	13.650006	-12.24408	2.018250	C	4.934193	0.166461	4.962921
H	5.779650	-8.522633	1.672948	C	5.350509	0.148602	3.584536
H	7.430192	-10.48522	3.362544	N	4.250789	0.150189	2.765026
H	5.818494	-10.79914	2.684823	C	3.149801	0.169246	3.586571
H	4.808950	-8.830151	3.952414	C	1.797948	0.179782	3.152189
H	6.373013	-8.439682	4.683873	C	6.702831	0.133078	3.145225
H	11.792698	-7.553207	-4.153419	C	7.705962	0.049312	-2.765330
H	14.257745	-8.829966	-2.830074	C	0.793645	0.200214	4.158001
H	14.100423	-7.146516	-3.354262	C	8.567085	0.027082	-3.627475
H	13.660211	-7.952876	-5.763239	C	-0.067532	0.218098	5.020194
H	13.739252	-9.650953	-5.271985	C	9.572202	-0.000343	-4.633302
H	14.821358	-12.91980	-0.252659	C	-1.072716	0.240607	6.026075
H	5.707511	-5.166753	-3.146549	C	0.795761	0.149775	-2.753934
H	-6.074425	4.740727	3.081509	Mg	4.249850	0.130479	0.696298
H	-13.71092	14.044510	0.489403	C	7.705093	0.139413	4.145421
				C	8.578069	0.147312	5.000549
2. 2b' (Ar = C ₆ H ₄ -Me-4, no ligand)				C	-0.073463	0.161174	-3.612837
Symbol	X	Y	Z	C	9.567452	0.160690	5.987240
C	-0.017663	0.176749	0.018754	C	10.939358	-0.012987	-4.289663
C	-0.016311	0.187051	1.383426	C	11.916162	-0.037114	-5.278459
C	1.361477	0.173317	1.800991	C	11.576891	-0.052294	-6.639176
N	2.181285	0.154359	0.698710	C	10.216009	-0.035119	-6.977663
C	1.359962	0.156298	-0.399703	C	9.227785	-0.010976	-6.000264
C	4.930262	0.078727	-3.571049	C	-2.439909	0.249475	5.682477

C	-3.416768	0.268940	6.671325	C	10.949268	0.170124	5.834320
C	-3.077526	0.283024	8.032058	C	11.652395	0.187886	7.047844
C	-1.716587	0.269593	8.370500	C	10.834050	0.187550	8.177728
C	-0.728312	0.250131	7.393053	S	9.141957	0.169994	7.689818
C	-7.159650	0.671142	-13.97294	C	11.322369	0.234508	9.529360
C	-5.798632	0.605723	-14.11866	C	12.658121	0.372045	9.921336
C	-5.109808	0.583231	-12.88216	C	12.735084	0.428797	11.337287
C	-5.947518	0.636682	-11.77478	C	11.392310	0.321618	11.864961
S	-7.627037	0.713275	-12.31064	N	10.564013	0.191378	10.700854
C	-5.484113	0.592656	-10.40736	C	13.998622	0.484164	9.394727
C	-4.156615	0.420140	-9.997616	N	14.827360	0.618661	10.556675
C	-4.096802	0.388753	-8.580010	C	14.071225	0.574662	11.729001
C	-5.439670	0.545511	-8.071094	O	14.467381	0.472072	8.257026
N	-6.251772	0.678817	-9.244885	O	10.927877	0.332947	13.003685
C	-2.811289	0.268782	-10.50766	C	9.125840	0.003707	10.876132
N	-1.999573	0.139845	-9.331904	C	16.263815	0.799831	10.341622
C	-2.769473	0.224749	-8.170150	C	14.551440	0.632483	13.090082
O	-2.334106	0.246413	-11.64096	C	13.725552	0.621733	14.207548
O	-5.920989	0.567408	-6.938809	C	14.429035	0.650046	15.435648
C	-7.685468	0.900423	-9.049986	C	15.789486	0.677577	15.273537
C	-0.565126	-0.090044	-9.486925	S	16.238438	0.675920	13.605652
C	-2.297056	0.192135	-6.812427	C	8.635272	-1.456253	10.762046
C	-3.126625	0.236130	-5.691601	C	9.311979	-2.376306	11.786923
C	-2.436580	0.225730	-4.470370	C	7.107300	-1.477330	10.913837
C	-1.053986	0.178519	-4.608290	H	10.396775	-2.412475	11.642906
S	-0.611158	0.141744	-6.306066	H	6.616331	-0.854616	10.156131
C	-8.051788	2.340039	-8.628847	C	16.661624	2.221801	9.890197
C	-7.639110	3.397555	-9.659898	C	16.289208	3.307894	10.906856
C	-9.556556	2.406208	-8.330286	C	18.163703	2.243795	9.572330
H	-6.567316	3.352702	-9.881605	H	15.219610	3.294596	11.143026
H	-9.846868	1.679704	-7.562159	H	18.425684	1.496847	8.813692
C	-0.116737	-1.560262	-9.339207	H	-0.868779	0.182084	-0.647082
C	-0.801627	-2.480505	-10.35843	H	-0.865319	0.202690	2.051510
C	1.412377	-1.627096	-9.464228	H	5.597029	0.061445	-4.421060
H	-1.889548	-2.481289	-10.23527	H	2.899341	0.099495	-4.421207
H	1.908035	-1.002731	-8.710947	H	9.368676	0.093785	2.039302

[illegible]

C	8.539503	-0.012285	-0.005709	C	-4.981992	0.242512	-12.96134
C	7.161269	-0.015542	-0.423450	C	-5.826470	0.381866	-11.86635
N	6.341139	-0.015306	0.678108	S	-7.493645	0.533319	-12.42436
C	7.162178	-0.011571	1.776868	C	-5.378565	0.363001	-10.49356
C	6.723638	-0.017529	-1.773922	C	-4.063009	0.147717	-10.06438
C	3.590723	-0.015738	4.946234	C	-4.017710	0.163034	-8.646249
C	4.955194	-0.012699	4.946226	C	-5.357966	0.393238	-8.157137
C	5.372510	-0.012425	3.567841	N	-6.152550	0.521509	-9.343129
N	4.273205	-0.014889	2.747517	C	-2.720425	-0.076995	-10.55453
C	3.172100	-0.016708	3.568222	N	-1.925313	-0.194817	-9.366058
C	1.821314	-0.018492	3.131264	C	-2.702452	-0.038532	-8.216894
C	6.725218	-0.009768	3.130010	O	-2.234768	-0.164404	-11.68089
C	7.728753	-0.013504	-2.779613	O	-5.847754	0.469705	-7.031300
C	0.816195	-0.024621	4.136929	C	-7.580033	0.797531	-9.171101
C	8.590080	-0.007297	-3.641349	C	-0.505748	-0.515733	-9.496200
C	-0.045135	-0.032811	4.998651	C	-2.244076	-0.038478	-6.853346
C	9.595254	0.005243	-4.646876	C	-3.081956	0.060638	-5.742481
C	-1.050314	-0.047633	6.004134	C	-2.402042	0.075875	-4.515314
C	0.819363	-0.014285	-2.774921	C	-1.019982	-0.004388	-4.639895
Mg	4.272436	-0.016405	0.678729	S	-0.564293	-0.106501	-6.331629
C	7.727362	-0.003508	4.130428	C	-7.901160	2.259862	-8.793698
C	8.601513	0.003543	4.984178	C	-7.437790	3.274850	-9.845766
C	-0.046675	-0.010541	-3.636904	C	-9.406631	2.386214	-8.518777
C	9.594228	0.015351	5.967805	H	-6.365047	3.187986	-10.04979
C	10.961970	0.010023	-4.297888	H	-9.732980	1.689862	-7.737301
C	11.942215	0.025725	-5.282213	C	-0.148449	-2.000671	-9.271239
C	11.580637	0.035326	-6.632991	C	-0.876020	-2.927579	-10.25414
C	10.229706	0.027429	-6.994061	C	1.375128	-2.165591	-9.370592
C	9.245756	0.011728	-6.013457	H	-1.963491	-2.852039	-10.15210
C	-2.417010	-0.055177	5.655095	H	1.899119	-1.535558	-8.641538
C	-3.397256	-0.073170	6.639373	C	10.975138	0.024962	5.808630
C	-3.035719	-0.082355	7.990169	C	11.683577	0.039730	7.019129
C	-1.684825	-0.071655	8.351294	C	10.869744	0.037253	8.152170
C	-0.700869	-0.053656	7.370731	S	9.175924	0.021186	7.672062
C	-7.012832	0.405654	-14.07812	C	11.363699	0.080626	9.502447
C	-5.656161	0.259150	-14.20571	C	12.701268	0.214638	9.888210

C	12.785147	0.268508	11.303556	H	9.951502	0.026755	-8.042741
C	11.444762	0.163456	11.837620	H	8.197545	0.002619	-6.294209
N	10.610590	0.037090	10.676974	H	-2.698165	-0.044973	4.607005
C	14.040235	0.323887	9.355493	H	-4.446022	-0.073235	6.361500
N	14.874818	0.453640	10.513491	C	-4.097435	-0.167648	9.052275
C	14.124082	0.409611	11.688993	H	-1.406669	-0.070516	9.399985
O	14.502767	0.312514	8.215588	H	0.347308	-0.042213	7.651530
O	10.985686	0.173831	12.978367	H	-5.152233	0.165195	-15.16117
C	9.172649	-0.146510	10.858825	H	-3.908871	0.124812	-12.84756
C	16.311220	0.629911	10.291949	H	-8.119377	0.497648	-10.07024
C	14.610745	0.463428	13.047582	H	-7.917402	0.146299	-8.358968
C	13.789511	0.452135	14.168719	H	-0.248071	-0.232551	-10.52113
C	14.498342	0.476465	15.393590	H	0.074178	0.128244	-8.827798
C	15.858205	0.501468	15.225158	H	-4.160526	0.130807	-5.845504
S	16.300026	0.502380	13.555687	H	-7.365988	2.461324	-7.857741
C	8.677065	-1.604900	10.746003	H	-7.973182	3.144155	-10.79396
C	9.356700	-2.528094	11.766109	H	-7.624889	4.297021	-9.496942
C	7.149917	-1.621247	10.906595	H	-9.656290	3.400303	-8.187630
H	10.440466	-2.568009	11.615477	H	-9.995254	2.179482	-9.422407
H	6.656510	-0.995801	10.152657	H	-0.452878	-2.275925	-8.252394
C	16.712309	2.051252	9.841554	H	-0.622438	-2.682241	-11.29177
C	16.349373	3.136784	10.862256	H	-0.596741	-3.971579	-10.07085
C	18.212881	2.067725	9.516270	H	1.666447	-3.205031	-9.183979
H	15.280989	3.127363	11.104163	H	1.735987	-1.893915	-10.37099
H	18.468051	1.321553	8.754579	H	12.766579	0.060596	7.094027
H	-0.846196	-0.015475	-0.667828	H	8.968418	0.225096	11.867346
H	-0.844677	-0.017301	2.029841	H	8.634544	0.501931	10.160163
H	5.620935	-0.020051	-4.439041	H	16.857193	0.334758	11.188690
H	2.924197	-0.018650	-4.439960	H	16.582568	-0.075664	9.500815
H	9.391137	-0.006943	2.024714	H	12.707581	0.418048	14.087630
H	9.389462	-0.011871	-0.672711	H	14.016215	0.474966	16.364773
H	2.924191	-0.016716	5.796563	H	8.916509	-1.973377	9.739353
H	5.621216	-0.010878	5.797300	H	9.177076	-2.186132	12.791627
H	11.243148	-0.000531	-3.249809	H	8.970064	-3.549483	11.672028
H	12.990989	0.023681	-5.004384	H	6.759289	-2.639555	10.804177
C	12.642443	0.118051	-7.695219	H	6.855238	-1.249711	11.896457

H	16.160596	2.248178	8.914195	C	4.952573	0.162969	4.952989
H	16.907873	3.011530	11.797752	C	5.368109	0.145235	3.574995
H	16.588023	4.129497	10.463383	N	4.267823	0.146932	2.755904
H	18.516444	3.049536	9.136408	C	3.167054	0.166075	3.578147
H	18.816117	1.858190	10.409575	C	1.813338	0.176839	3.145740
H	16.630924	0.522855	15.982352	C	6.720284	0.130067	3.134541
H	11.445190	0.021488	4.832135	C	7.724857	0.050610	-2.776613
H	-2.893459	0.145630	-3.551894	C	0.810763	0.198204	4.150019
H	-7.762320	0.450055	-14.85734	C	8.586978	0.030510	-3.639823
F	-5.249030	0.422128	8.661513	C	-0.051367	0.217657	5.013233
F	-4.398360	-1.452919	9.354041	C	9.589220	0.007851	-4.642696
F	-3.706604	0.422992	10.203434	C	-1.053599	0.242023	6.016083
F	12.945516	1.402552	-7.997979	C	0.814260	0.144648	-2.761995
F	13.793055	-0.473421	-7.304100	Mg	4.267829	0.127536	0.686687
F	12.250508	-0.472817	-8.845904	C	7.722354	0.136141	4.134450
4. 2d' (Ar = C ₆ H ₄ -NMe ₂ -4, no ligand)				C	8.595266	0.143684	4.989990
Symbol	X	Y	Z	C	-0.055617	0.155112	-3.620592
C	0.000483	0.172484	0.009722	C	9.583843	0.156621	5.976913
C	0.001743	0.183307	1.374886	C	10.959972	-0.006830	-4.310617
C	1.378532	0.169876	1.792772	C	11.942988	-0.030081	-5.286454
N	2.198782	0.150630	0.690524	C	11.609190	-0.034209	-6.663587
C	1.377623	0.152127	-0.408270	C	10.231915	-0.028559	-6.996778
C	4.948325	0.077059	-3.580761	C	9.256526	-0.005311	-6.013298
C	3.583222	0.095130	-3.579634	C	-2.424395	0.252462	5.684064
C	3.167650	0.113475	-2.201646	C	-3.407410	0.276075	6.659903
N	4.267866	0.106839	-1.382510	C	-3.073467	0.296899	8.036842
C	5.368611	0.085042	-2.204733	C	-1.696371	0.276546	8.370173
C	1.815486	0.135839	-1.761262	C	-0.720965	0.252923	7.386709
C	8.535273	0.093067	1.363447	C	-7.158433	0.643862	-13.97241
C	8.533943	0.076409	-0.001647	C	-5.797323	0.587543	-14.12000
C	7.157120	0.084827	-0.419443	C	-5.106309	0.568410	-12.88447
N	6.336883	0.105929	0.682789	C	-5.942381	0.615308	-11.77576
C	7.158112	0.111122	1.781504	S	-7.623253	0.681233	-12.30899
C	6.722305	0.073784	-1.772356	C	-5.476985	0.572850	-10.40869
C	3.587397	0.175651	4.954180	C	-4.148630	0.406414	-10.00036
				C	-4.086983	0.374476	-8.582616

C	-5.429379	0.524694	-8.072015	O	14.483715	0.465936	8.251813
N	-6.243588	0.654658	-9.244958	O	10.939237	0.319885	12.995014
C	-2.803171	0.261522	-10.51198	C	9.139227	-0.005357	10.865284
N	-1.989496	0.135234	-9.337596	C	16.277100	0.790009	10.338890
C	-2.758031	0.216085	-8.174300	C	14.562481	0.617925	13.085998
O	-2.327317	0.242629	-11.64604	C	13.736033	0.607143	14.202851
O	-5.910154	0.544449	-6.939100	C	14.438825	0.632696	15.431603
C	-7.677574	0.870766	-9.048072	C	15.799360	0.658134	15.270796
C	-0.553929	-0.085473	-9.494578	S	16.249246	0.657738	13.602876
C	-2.283263	0.184067	-6.818090	C	8.647918	-1.464923	10.749332
C	-3.111250	0.225947	-5.695758	C	9.322577	-2.386242	11.774415
C	-2.419916	0.216051	-4.475535	C	7.119713	-1.485303	10.898723
C	-1.036993	0.171355	-4.614640	H	10.407585	-2.422583	11.632115
S	-0.596223	0.136372	-6.313204	H	6.630363	-0.862045	10.140465
C	-8.048659	2.308996	-8.626282	C	16.674809	2.212897	9.890197
C	-7.642184	3.367900	-9.658365	C	16.301566	3.296935	10.908725
C	-9.552989	2.369613	-8.324461	C	18.176990	2.236112	9.572974
H	-6.570762	3.326675	-9.882465	H	15.231890	3.282507	11.144356
H	-9.838817	1.642245	-7.555448	H	18.439499	1.490668	8.813017
C	-0.096076	-1.553199	-9.350560	H	-0.850661	0.177531	-0.656163
C	-0.777171	-2.475682	-10.37030	H	-0.847074	0.199144	2.043271
C	1.433169	-1.610009	-9.478626	H	5.615209	0.060600	-4.430747
H	-1.864743	-2.484046	-10.24437	H	2.916614	0.096212	-4.430351
H	1.926178	-0.984607	-8.724517	H	9.386507	0.092912	2.029206
C	10.966176	0.168130	5.825595	H	9.382751	0.060295	-0.670036
C	11.668125	0.184787	7.039564	H	2.920506	0.190660	5.804188
C	10.849198	0.181398	8.169272	H	5.619318	0.165613	5.803616
S	9.157091	0.162414	7.679411	H	11.250678	-0.002928	-3.264210
C	11.336842	0.226475	9.520509	H	12.980365	-0.045959	-4.974639
C	12.672621	0.363152	9.914197	N	12.585807	-0.039087	-7.640618
C	12.748148	0.417620	11.330553	H	9.919657	-0.043181	-8.034044
C	11.404735	0.309927	11.856563	H	8.209984	-0.000159	-6.303519
N	10.577620	0.181548	10.691737	H	-2.715234	0.238511	4.637780
C	14.013099	0.475809	9.389123	H	-4.444923	0.277588	6.348153
N	14.840772	0.608086	10.552323	N	-4.049696	0.339947	9.013477
C	14.083504	0.562474	11.724106	H	-1.384179	0.278483	9.407556

H	0.325468	0.239420	7.677058
H	-5.301238	0.559999	-15.08382
H	-4.026669	0.512479	-12.78689
H	-8.218018	0.575747	-9.948234
H	-7.978730	0.185498	-8.249830
H	-0.325325	0.265158	-10.50545
H	-0.011195	0.560419	-8.797343
H	-4.192388	0.271251	-5.785994
H	-7.505886	2.506402	-7.693827
H	-8.188705	3.241142	-10.60076
H	-7.861184	4.373063	-9.279754
H	-9.836640	3.364818	-7.964393
H	-10.14811	2.161611	-9.223601
H	-0.364509	-1.900019	-8.343637
H	-0.565116	-2.156749	-11.39711
H	-0.420453	-3.505255	-10.24997
H	1.795569	-2.635898	-9.350725
H	1.758175	-1.263247	-10.46807
H	12.750737	0.207804	7.119921
H	8.928074	0.365679	11.872617
H	8.603704	0.641321	10.163160
H	16.819707	0.497807	11.238694
H	16.555910	0.085710	9.549140
H	12.654601	0.572103	14.116002
H	13.951343	0.631790	16.400192
H	8.895402	-1.832698	9.744491
H	9.134114	-2.045025	12.798661
H	8.939905	-3.408900	11.677163
H	6.732569	-2.504759	10.794105
H	6.816724	-1.113728	11.886162
H	16.127088	2.406950	8.959913
H	16.855058	3.173789	11.847523
H	16.538148	4.290825	10.511368
H	18.478396	3.219115	9.194276
H	18.776375	2.029537	10.469617
H	16.568232	0.680698	16.031818

H	11.440801	0.165184	4.851345
H	-2.902619	0.241594	-3.505589
H	-7.919780	0.669414	-14.74086
C	13.984114	-0.168707	-7.266711
C	12.211221	-0.167278	-9.038859
C	-5.450674	0.232443	8.642488
C	-3.678093	0.232921	10.414313
H	14.300154	0.655923	-6.615157
H	14.193048	-1.114540	-6.744090
H	14.599944	-0.134356	-8.166903
H	11.687653	-1.112478	-9.248312
H	11.560296	0.658193	-9.354014
H	13.111192	-0.133288	-9.655032
H	-3.180833	-0.721415	10.645530
H	-3.004562	1.047070	10.710573
H	-4.576483	0.305988	11.029429
H	-5.747421	1.046321	7.968852
H	-5.681841	-0.722088	8.145594
H	-6.065425	0.305607	9.541121

5. 2a'·py (Ar = Ph, ligand = py)

Symbol	X	Y	Z
C	0.052563	0.323676	-0.044861
C	0.051204	0.344445	1.319807
C	1.430328	0.304093	1.739129
N	2.249910	0.250238	0.640320
C	1.433179	0.270525	-0.458636
C	5.007321	0.377003	-3.630388
C	3.644507	0.338940	-3.631553
C	3.229697	0.286402	-2.249658
N	4.325433	0.288554	-1.431307
C	5.423667	0.347385	-2.248533
C	1.875825	0.258452	-1.811909
C	8.584736	0.582288	1.322212
C	8.586261	0.557940	-0.042405
C	7.211993	0.425821	-0.459014

N	6.395921	0.359841	0.641775	S	-7.721438	0.225730	-12.23454
C	7.209000	0.464430	1.738718	C	-5.541047	0.276704	-10.37188
C	6.774724	0.393740	-1.811208	C	-4.198583	0.192509	-9.984774
C	3.631140	0.473885	4.908338	C	-4.111327	0.183730	-8.568100
C	4.993830	0.514905	4.909422	C	-5.451600	0.264398	-8.036236
C	5.412427	0.440630	3.529610	N	-6.291504	0.330774	-9.196214
N	4.319194	0.352680	2.712703	C	-2.856139	0.113402	-10.51806
C	3.218595	0.375758	3.528604	N	-2.017061	0.046619	-9.356351
C	1.867465	0.334691	3.091294	C	-2.769178	0.101963	-8.181129
C	6.766222	0.476680	3.091683	O	-2.398984	0.105702	-11.65980
C	7.780033	0.437049	-2.816244	O	-5.913580	0.273533	-6.895416
C	0.860516	0.348848	4.095528	C	-7.731846	0.470384	-8.976434
C	8.642687	0.468566	-3.676526	C	-0.573965	-0.092459	-9.535848
C	-0.003084	0.353215	4.955424	C	-2.271738	0.111213	-6.832484
C	9.649257	0.506083	-4.681705	C	-3.083662	0.131052	-5.697979
C	-1.010576	0.357645	5.960373	C	-2.374165	0.165800	-4.488801
C	0.875000	0.238223	-2.813286	C	-0.992867	0.178510	-4.648728
Mg	4.332088	-0.042021	0.646282	S	-0.576617	0.143090	-6.353514
C	7.762976	0.559679	4.093903	C	-8.174081	1.892616	-8.569444
C	8.627563	0.628911	4.955224	C	-7.854392	2.953975	-9.629264
C	0.000430	0.210802	-3.666859	C	-9.671589	1.873585	-8.230599
C	9.598583	0.712140	5.956255	H	-6.789286	2.965953	-9.884975
C	11.015103	0.535785	-4.330659	H	-9.896303	1.147938	-7.439998
C	11.995779	0.572615	-5.317295	C	-0.029694	-1.530523	-9.390781
C	11.638102	0.580517	-6.668070	C	-0.678556	-2.499062	-10.38860
C	10.288158	0.551356	-7.027797	C	1.497084	-1.499275	-9.552675
C	9.300283	0.514445	-6.048382	H	-1.760524	-2.570066	-10.23674
C	-2.376643	0.351449	5.609015	H	1.969545	-0.841298	-8.813256
C	-3.358149	0.355301	6.595510	C	10.980246	0.803731	5.829057
C	-3.001088	0.365142	7.946436	C	11.657804	0.876357	7.055102
C	-1.650925	0.371354	8.306471	C	10.819983	0.837835	8.170101
C	-0.662223	0.367749	7.327202	S	9.141398	0.712943	7.650921
C	-7.283716	0.195666	-13.90533	C	11.278057	0.928720	9.529605
C	-5.924467	0.222511	-14.07675	C	12.595331	1.149151	9.946172
C	-5.212590	0.262742	-12.85367	C	12.639896	1.225648	11.362795
C	-6.031017	0.272208	-11.73086	C	11.295197	1.045788	11.865187

N	10.499904	0.854324	10.686937	H	-2.653312	0.344593	4.559136
C	13.937386	1.331750	9.444792	H	-4.406471	0.351193	6.309475
N	14.733283	1.525595	10.621321	H	-3.770177	0.368510	8.713804
C	13.957125	1.450870	11.779167	H	-1.367223	0.379580	9.355401
O	14.429473	1.334062	8.316668	H	0.387066	0.372834	7.606073
O	10.807779	1.042106	12.994419	H	-5.444319	0.213482	-15.04893
C	9.073048	0.578196	10.835952	H	-4.130065	0.274762	-12.77494
C	16.161153	1.785968	10.433319	H	-8.271292	0.131474	-9.861611
C	14.405537	1.549630	13.148926	H	-7.980114	-0.217361	-8.162348
C	13.558585	1.509500	14.249666	H	-0.381894	0.262906	-10.55259
C	14.234404	1.586658	15.491260	H	-0.057962	0.588461	-8.851787
C	15.594783	1.680670	15.356313	H	-4.167016	0.126949	-5.771498
S	16.077421	1.683156	13.697647	H	-7.620604	2.136775	-7.654554
C	8.679928	-0.911059	10.727298	H	-8.420792	2.782726	-10.55274
C	9.378048	-1.773711	11.787081	H	-8.115893	3.952295	-9.259631
C	7.152069	-1.030033	10.827512	H	-10.00346	2.858519	-7.883771
H	10.467536	-1.734501	11.686796	H	-10.27509	1.612475	-9.110086
H	6.648434	-0.449623	10.044956	H	-0.256297	-1.883351	-8.375660
C	16.488024	3.223814	9.975327	H	-0.509948	-2.175738	-11.42201
C	16.030129	4.296397	10.971072	H	-0.259256	-3.505055	-10.27058
C	17.993840	3.328681	9.693368	H	1.922207	-2.501301	-9.428312
H	14.956828	4.226842	11.178548	H	1.778579	-1.139856	-10.55088
H	18.317025	2.589051	8.951317	H	12.735486	0.964920	7.154400
H	-0.796578	0.357230	-0.712605	H	8.818845	0.946140	11.834457
H	-0.798480	0.398241	1.985307	H	8.511284	1.181393	10.115950
H	5.674510	0.431953	-4.478610	H	16.700427	1.535176	11.347452
H	2.977905	0.357096	-4.482199	H	16.494979	1.089298	9.658293
H	9.429860	0.686307	1.987851	H	12.482437	1.416392	14.142462
H	9.432108	0.638659	-0.710064	H	13.728411	1.572424	16.450190
H	2.961057	0.518546	5.754886	H	8.983373	-1.274993	9.736417
H	5.657156	0.599488	5.758554	H	9.126368	-1.438258	12.799610
H	11.292224	0.530014	-3.280889	H	9.072224	-2.821672	11.687009
H	13.043916	0.595861	-5.031492	H	6.836161	-2.074026	10.724856
H	12.406525	0.609784	-7.435557	H	6.791874	-0.668051	11.799161
H	10.003956	0.558085	-8.076601	H	15.952807	3.375873	9.030046
H	8.251150	0.492673	-6.327030	H	16.564271	4.212406	11.925249

H	16.223666	5.297534	10.568737	C	7.153054	-0.271864	1.762190
H	18.247830	4.322019	9.307042	C	6.711863	-0.322559	-1.785471
H	18.581724	3.169321	10.607095	C	3.589672	-0.135490	4.947764
H	16.346084	1.752524	16.131702	C	4.952577	-0.191534	4.942849
H	11.472214	0.818574	4.863522	C	5.365347	-0.152707	3.560455
H	-2.842949	0.182213	-3.511836	N	4.268463	-0.067450	2.747517
H	-8.058227	0.163790	-14.66028	C	3.171053	-0.061719	3.569055
N	4.383523	-2.279570	0.678364	C	1.818175	-0.007506	3.134631
C	5.552159	-2.945277	0.679623	C	6.716091	-0.222405	3.116224
C	3.245262	-2.995676	0.695453	C	7.711261	-0.425972	-2.791784
C	3.229702	-4.387658	0.714774	C	0.814484	0.013402	4.141777
C	5.628660	-4.335224	0.698265	C	8.568565	-0.506419	-3.654528
C	4.444748	-5.071358	0.716268	C	-0.045511	0.037658	5.005252
H	2.324415	-2.420812	0.693084	C	9.569142	-0.601759	-4.660827
H	2.282595	-4.917134	0.728224	C	-1.049254	0.063372	6.012585
H	6.447244	-2.331086	0.664679	C	0.816392	0.003706	-2.768400
H	6.598056	-4.822887	0.698346	Mg	4.286629	0.249786	0.669823
H	4.468629	-6.157414	0.731036	C	7.717873	-0.274311	4.115621
6. 2b' ·py (Ar = C ₆ H ₄ -Me-4, ligand = py)				C	8.590662	-0.313293	4.970541
Symbol	X	Y	Z	C	-0.051459	0.034468	-3.628711
C	-0.001860	0.008022	0.001908	C	9.579617	-0.352102	5.956515
C	-0.001746	0.008458	1.365884	C	10.935957	-0.657842	-4.319695
C	1.379698	0.008858	1.782125	C	11.908549	-0.747354	-5.308993
N	2.198200	0.013936	0.682466	C	11.565620	-0.787502	-6.668249
C	1.380063	0.006941	-0.413915	C	10.205510	-0.727047	-7.004624
C	4.934503	-0.307095	-3.596957	C	9.221507	-0.637255	-6.026642
C	3.573277	-0.219767	-3.592504	C	-2.416957	0.087180	5.671427
C	3.168335	-0.107273	-2.211847	C	-3.392346	0.114869	6.661703
N	4.268994	-0.119144	-1.399618	C	-3.051589	0.117425	8.022042
C	5.360062	-0.246658	-2.219822	C	-1.690184	0.098320	8.358249
C	1.818070	-0.023660	-1.768083	C	-0.703445	0.070395	7.379357
C	8.527337	-0.423195	1.348214	C	-7.053733	0.651138	-14.04129
C	8.525744	-0.455063	-0.015379	C	-5.695899	0.525800	-14.17627
C	7.151304	-0.321336	-0.433294	C	-5.016238	0.494352	-12.93475
N	6.338878	-0.206415	0.664820	C	-5.857562	0.600970	-11.83413
				S	-7.529040	0.739951	-12.38283

C	-5.404810	0.560032	-10.46280	C	14.031765	-0.470392	9.354339
C	-4.087787	0.343731	-10.04121	N	14.880534	-0.385410	10.506750
C	-4.038195	0.332157	-8.622650	C	14.139427	-0.172654	11.670301
C	-5.376626	0.547881	-8.125305	O	14.481832	-0.673851	8.226876
N	-6.175788	0.693536	-9.306645	O	11.018996	0.309254	12.930265
C	-2.746031	0.132300	-10.53939	C	9.168062	0.112516	10.828999
N	-1.947349	-0.008979	-9.356454	C	16.323899	-0.489980	10.287704
C	-2.720593	0.123352	-8.201009	C	14.633076	-0.079679	13.024856
O	-2.263245	0.071699	-11.66902	C	13.834611	0.195313	14.128080
O	-5.864423	0.604804	-6.996678	C	14.540135	0.195207	15.355605
C	-7.602889	0.962303	-9.125034	C	15.873655	-0.083096	15.207750
C	-0.525697	-0.315100	-9.497586	S	16.295407	-0.346183	13.553148
C	-2.257290	0.094161	-6.840686	C	8.406264	-1.229888	10.878957
C	-3.090594	0.182276	-5.725100	C	8.889109	-2.130004	12.024154
C	-2.408004	0.166635	-4.499809	C	6.901888	-0.942324	10.990346
C	-1.026626	0.071650	-4.628300	H	9.949356	-2.382309	11.920770
S	-0.576308	-0.004043	-6.323238	H	6.541828	-0.337348	10.149371
C	-7.927225	2.417487	-8.723472	C	16.970458	0.788762	9.712563
C	-7.472368	3.449645	-9.762413	C	16.824569	2.007015	10.632600
C	-9.431697	2.534785	-8.439381	C	18.444890	0.503296	9.392648
H	-6.400296	3.369306	-9.972334	H	15.775652	2.212761	10.872098
H	-9.751821	1.825739	-7.666771	H	18.550464	-0.338183	8.697759
C	-0.155872	-1.802758	-9.314268	H	-0.852438	-0.004752	-0.664745
C	-0.876019	-2.708406	-10.32209	H	-0.851249	-0.003467	2.033696
C	1.369000	-1.952328	-9.418267	H	5.593878	-0.415166	-4.446242
H	-1.964006	-2.643897	-10.21846	H	2.901831	-0.242767	-4.439177
H	1.887888	-1.338273	-8.672196	H	9.373054	-0.506609	2.015895
C	10.946679	-0.562026	5.812366	H	9.368800	-0.570152	-0.681536
C	11.654194	-0.535885	7.022968	H	2.923568	-0.155876	5.798454
C	10.854868	-0.306745	8.143494	H	5.619062	-0.267779	5.790378
S	9.174696	-0.117079	7.648200	H	11.223535	-0.626547	-3.273098
C	11.356308	-0.211138	9.487162	H	12.956860	-0.786120	-5.021544
C	12.699019	-0.277497	9.875672	C	12.626137	-0.918611	-7.734848
C	12.797498	-0.098116	11.280380	H	9.913147	-0.749963	-8.052042
C	11.462671	0.094714	11.803425	H	8.174109	-0.590423	-6.309153
N	10.613802	0.000134	10.651012	H	-2.702824	0.086638	4.623897

H	-4.441112	0.135676	6.374076	H	18.918811	1.377688	8.932858
C	-4.117368	0.113863	9.091479	H	19.009538	0.262085	10.303137
H	-1.398970	0.106263	9.406220	H	16.638046	-0.146983	15.970932
H	0.344986	0.057314	7.661641	H	11.406376	-0.732636	4.845895
H	-5.194323	0.457170	-15.13519	H	-2.896112	0.222993	-3.533856
H	-3.941342	0.387984	-12.82708	H	-7.806982	0.700399	-14.81655
H	-8.145255	0.675408	-10.02665	H	13.568791	-0.456661	-7.422681
H	-7.935151	0.297669	-8.321659	H	12.839113	-1.973524	-7.955234
H	-0.271372	-0.001905	-10.51463	H	12.312156	-0.449008	-8.673080
H	0.049581	0.314385	-8.811671	H	-5.029207	0.615888	8.751067
H	-4.168781	0.264783	-5.823879	H	-4.396116	-0.911368	9.370671
H	-7.387956	2.606210	-7.787213	H	-3.773539	0.615100	10.002520
H	-8.011350	3.330382	-10.71011	N	4.405608	2.479173	0.649093
H	-7.661640	4.466077	-9.398079	C	3.644898	3.217031	1.476102
H	-9.683397	3.543025	-8.092064	C	5.240560	3.119033	-0.187703
H	-10.02403	2.339273	-9.343143	C	5.348068	4.506423	-0.230850
H	-0.457249	-2.108899	-8.303476	C	3.687785	4.608347	1.499799
H	-0.624299	-2.433329	-11.35270	C	4.556244	5.266016	0.629591
H	-0.588688	-3.754788	-10.16666	H	5.837047	2.488027	-0.839488
H	1.668818	-2.994066	-9.259964	H	6.038453	4.973937	-0.925293
H	1.727548	-1.650582	-10.41093	H	2.983969	2.664060	2.136658
H	12.727919	-0.674785	7.106605	H	3.052383	5.157167	2.187213
H	9.041539	0.633533	11.782833	H	4.614988	6.350817	0.622033
H	8.758873	0.761399	10.048374	7. 2c' ·py (Ar = C ₆ H ₄ -CF ₃ -4, ligand = py)			
H	16.813877	-0.790705	11.214338	Symbol	X	Y	Z
H	16.461073	-1.303549	9.568967	C	0.040415	0.299345	-0.029530
H	12.768706	0.377442	14.034079	C	0.039634	0.310090	1.335045
H	14.073800	0.394192	16.314115	C	1.419535	0.271250	1.753205
H	8.580391	-1.759035	9.932391	N	2.238610	0.228126	0.654267
H	8.758759	-1.640282	12.995856	C	1.421121	0.253556	-0.444295
H	8.323056	-3.068711	12.034197	C	4.992641	0.399196	-3.615679
H	6.328121	-1.875522	11.000645	C	3.630247	0.354423	-3.616757
H	6.672330	-0.400748	11.917112	C	3.216171	0.288278	-2.235102
H	16.451216	0.999882	8.769878	N	4.312324	0.288326	-1.416938
H	17.363936	1.863333	11.576767	C	5.409378	0.359851	-2.233824
H	17.233893	2.901504	10.148768				

C	1.862596	0.252308	-1.797723	C	-7.269996	0.274325	-13.90860
C	8.572160	0.583699	1.337712	C	-5.909975	0.286283	-14.07641
C	8.573080	0.569873	-0.026819	C	-5.201296	0.315392	-12.85136
C	7.198952	0.433009	-0.443523	C	-6.022966	0.331140	-11.73079
N	6.384045	0.353418	0.656539	S	-7.712335	0.305201	-12.23931
C	7.197223	0.454801	1.753994	C	-5.536395	0.327159	-10.37085
C	6.759802	0.410300	-1.795217	C	-4.195166	0.230865	-9.981031
C	3.621386	0.428011	4.924200	C	-4.111415	0.217198	-8.564411
C	4.983675	0.475183	4.925188	C	-5.452820	0.306685	-8.035490
C	5.402178	0.411798	3.544686	N	-6.289270	0.383647	-9.197066
N	4.308965	0.324485	2.727320	C	-2.852099	0.143942	-10.51144
C	3.209095	0.337315	3.543490	N	-2.016286	0.068438	-9.347648
C	1.858519	0.293215	3.104909	C	-2.771153	0.125445	-8.174537
C	6.755583	0.456377	3.107188	O	-2.392136	0.135671	-11.65193
C	7.764073	0.471163	-2.800078	O	-5.916765	0.315078	-6.895776
C	0.852117	0.291992	4.109468	C	-7.729325	0.533301	-8.980455
C	8.625991	0.519659	-3.660295	C	-0.573814	-0.080975	-9.524102
C	-0.011119	0.279846	4.969653	C	-2.277430	0.128338	-6.823929
C	9.630717	0.580474	-4.664043	C	-3.092174	0.146990	-5.691610
C	-1.017107	0.258226	5.973737	C	-2.385200	0.176028	-4.480590
C	0.861533	0.236208	-2.799260	C	-1.003830	0.185462	-4.637686
Mg	4.321958	-0.060014	0.658355	S	-0.583726	0.153902	-6.341489
C	7.752829	0.537983	4.109336	C	-8.162021	1.957280	-8.569362
C	8.618840	0.606405	4.969055	C	-7.830044	3.020558	-9.623474
C	-0.012238	0.212670	-3.653525	C	-9.660930	1.948209	-8.236302
C	9.593825	0.689274	5.966633	H	-6.763790	3.025931	-9.874654
C	10.996921	0.619704	-4.314127	H	-9.894281	1.220819	-7.449832
C	11.976931	0.680446	-5.296825	C	-0.040267	-1.523105	-9.379644
C	11.616531	0.701752	-6.647900	C	-0.694507	-2.485793	-10.37962
C	10.266456	0.661068	-7.010197	C	1.486958	-1.502782	-9.539045
C	9.282751	0.600231	-6.031125	H	-1.777139	-2.549620	-10.22925
C	-2.383782	0.241140	5.623921	H	1.962975	-0.848682	-8.798415
C	-3.364894	0.214350	6.607056	C	10.975107	0.772941	5.832689
C	-3.005073	0.205647	7.958410	C	11.658509	0.847885	7.055444
C	-1.654507	0.226350	8.320605	C	10.825094	0.819516	8.173882
C	-0.669724	0.253345	7.341120	S	9.143918	0.701034	7.663063

C	11.289572	0.914277	9.531493	H	13.025133	0.704605	-5.017664
C	12.610143	1.127232	9.940438	C	12.676444	0.831322	-7.706743
C	12.662163	1.210891	11.356160	H	9.988855	0.670391	-8.059028
C	11.318717	1.043867	11.866108	H	8.235398	0.565960	-6.313184
N	10.516294	0.851808	10.692479	H	-2.663955	0.251555	4.575536
C	13.951685	1.296825	9.431744	H	-4.413356	0.207319	6.327924
N	14.754657	1.490643	10.603218	C	-4.067046	0.109526	9.018692
C	13.983490	1.428040	11.764866	H	-1.377302	0.228363	9.369585
O	14.437712	1.289516	8.301307	H	0.378065	0.272526	7.623001
O	10.836599	1.050315	12.997468	H	-5.427353	0.274275	-15.04730
C	9.087454	0.590987	10.849909	H	-4.118908	0.315598	-12.76966
C	16.183674	1.739866	10.407070	H	-8.268642	0.201576	-9.868397
C	14.439195	1.530367	13.131680	H	-7.984908	-0.155798	-8.169803
C	13.596812	1.502573	14.236492	H	-0.377153	0.274214	-10.54002
C	14.278814	1.580916	15.474448	H	-0.054287	0.595651	-8.838377
C	15.639323	1.663537	15.332512	H	-4.175334	0.146849	-5.767718
S	16.114519	1.653687	13.671987	H	-7.610344	2.193644	-7.651318
C	8.678272	-0.894866	10.753534	H	-8.393763	2.857401	-10.55002
C	9.375393	-1.757949	11.813651	H	-8.085778	4.019190	-9.250764
C	7.150049	-0.996778	10.866409	H	-9.986428	2.934102	-7.886271
H	10.464304	-1.733539	11.702723	H	-10.26310	1.695777	-9.119194
H	6.646389	-0.415592	10.084383	H	-0.271087	-1.875500	-8.365270
C	16.518735	3.173222	9.941086	H	-0.522269	-2.162262	-11.41234
C	16.073437	4.253662	10.934076	H	-0.282279	-3.494777	-10.26246
C	18.023940	3.265558	9.651556	H	1.904469	-2.507988	-9.414720
H	15.000647	4.193146	11.147098	H	1.772760	-1.144801	-10.53649
H	18.338102	2.520405	8.911180	H	12.737094	0.930658	7.149632
H	-0.809056	0.335023	-0.696681	H	8.841786	0.968097	11.847111
H	-0.810398	0.356535	2.000622	H	8.528405	1.195304	10.128645
H	5.658561	0.464871	-4.464102	H	16.725391	1.489033	11.319717
H	2.963265	0.376789	-4.466939	H	16.508531	1.037146	9.633731
H	9.416935	0.687779	2.003694	H	12.519464	1.417433	14.134809
H	9.418566	0.661002	-0.693550	H	13.777319	1.575673	16.435793
H	2.952023	0.464269	5.771693	H	8.970402	-1.268396	9.762772
H	5.646955	0.557007	5.774581	H	9.137679	-1.411226	12.825710
H	11.277619	0.600012	-3.266014	H	9.055324	-2.802644	11.724880

H	6.822215	-2.037913	10.772818	C	4.929192	-0.154026	-3.584144
H	6.801648	-0.624915	11.838564	C	3.566274	-0.078103	-3.580051
H	15.980242	3.325103	8.997612	C	3.160165	0.032341	-2.200824
H	16.611599	4.170273	11.886019	N	4.261214	0.031139	-1.388090
H	16.272383	5.251426	10.526119	C	5.354520	-0.089803	-2.208392
H	18.283424	4.255292	9.259754	C	1.809115	0.106411	-1.756040
H	18.614957	3.105752	10.563154	C	8.520054	-0.268920	1.360916
H	16.394707	1.733407	16.104125	C	8.519014	-0.288351	-0.003012
H	11.463100	0.780194	4.865039	C	7.143956	-0.164379	-0.420365
H	-2.856372	0.190986	-3.504735	N	6.329783	-0.069155	0.678197
H	-8.042634	0.252911	-14.66586	C	7.144341	-0.134243	1.775140
F	-5.222529	0.692854	8.629205	C	6.707978	-0.157396	-1.774129
F	-4.360593	-1.179096	9.315777	C	3.577645	-0.023608	4.959133
F	-3.681939	0.697972	10.172998	C	4.941559	-0.079625	4.954827
F	12.949381	2.128125	-7.985185	C	5.355409	-0.028370	3.574407
F	13.841218	0.260473	-7.325758	N	4.258763	0.065204	2.761120
F	12.300585	0.253026	-8.869403	C	3.159471	0.061990	3.582268
N	4.380373	-2.296045	0.677295	C	1.805526	0.117450	3.147786
C	3.244253	-3.015990	0.683697	C	6.706636	-0.094181	3.129299
C	5.551047	-2.958450	0.682499	C	7.707585	-0.241831	-2.779147
C	5.631711	-4.348167	0.694480	C	0.802844	0.137121	4.153111
C	3.232875	-4.408029	0.695692	C	8.566363	-0.304879	-3.643670
C	4.449992	-5.088046	0.701248	C	-0.057690	0.159093	5.017896
H	6.444528	-2.341772	0.676599	C	9.565704	-0.377090	-4.647792
H	6.602544	-4.832902	0.698344	C	-1.059031	0.183553	6.022339
H	2.321497	-2.444244	0.678815	C	0.808008	0.130485	-2.756204
H	2.287386	-4.940496	0.700460	Mg	4.276481	0.385858	0.683877
H	4.477137	-6.174045	0.710614	C	7.707520	-0.149078	4.128618
8. 2d' ·py (Ar = C ₆ H ₄ -NMe ₂ -4, ligand = py)				C	8.579241	-0.190000	4.985001
Symbol	X	Y	Z	C	-0.059409	0.158632	-3.617501
C	-0.011156	0.136531	0.013423	C	9.566252	-0.230129	5.972061
C	-0.010870	0.137502	1.377504	C	10.936039	-0.427066	-4.317964
C	1.370055	0.135068	1.793881	C	11.916102	-0.498437	-5.294900
N	2.188722	0.136572	0.694516	C	11.579978	-0.518208	-6.670977
C	1.370703	0.132820	-0.401839	C	10.203076	-0.477947	-7.001828
				C	9.230534	-0.406344	-6.017389

C	-2.430085	0.202628	5.692375	H	1.900430	-1.141073	-8.671065
C	-3.412124	0.223535	6.669727	C	10.934793	-0.434879	5.830188
C	-3.077150	0.233603	8.046160	C	11.639739	-0.410842	7.041966
C	-1.700105	0.204140	8.377447	C	10.837894	-0.188676	8.162460
C	-0.725505	0.183153	7.392621	S	9.157540	-0.002839	7.664233
C	-7.063893	0.778562	-14.03014	C	11.336967	-0.096624	9.506450
C	-5.704552	0.672435	-14.16539	C	12.679441	-0.161404	9.897690
C	-5.024666	0.640263	-12.92383	C	12.774657	0.013824	11.303326
C	-5.867333	0.726974	-11.82266	C	11.438285	0.202214	11.824137
S	-7.540476	0.847831	-12.37083	N	10.591970	0.109306	10.670075
C	-5.414801	0.680987	-10.45119	C	14.013131	-0.349686	9.378467
C	-4.096105	0.475959	-10.03008	N	14.859404	-0.266703	10.533083
C	-4.047239	0.454329	-8.611440	C	14.115572	-0.059015	11.696031
C	-5.387676	0.651803	-8.113379	O	14.466672	-0.548167	8.251171
N	-6.187776	0.797374	-9.294302	O	10.992043	0.412666	12.950884
C	-2.751721	0.283215	-10.52885	C	9.145806	0.219088	10.845396
N	-1.952274	0.141472	-9.346834	C	16.303242	-0.366041	10.316442
C	-2.727230	0.256764	-8.190308	C	14.606351	0.030703	13.052076
O	-2.267630	0.237403	-11.65878	C	13.805988	0.302430	14.154560
O	-5.877326	0.695923	-6.984633	C	14.509332	0.299049	15.383508
C	-7.617051	1.052051	-9.111496	C	15.843125	0.021473	15.237676
C	-0.526507	-0.143492	-9.489357	S	16.267785	-0.237063	13.582818
C	-2.263885	0.222004	-6.830939	C	8.385931	-1.124557	10.890490
C	-3.098261	0.295300	-5.714713	C	8.867263	-2.026558	12.034833
C	-2.416587	0.276546	-4.489345	C	6.880802	-0.839767	10.998565
C	-1.033886	0.193862	-4.617039	H	9.928314	-2.276379	11.933842
S	-0.582007	0.133800	-6.312494	H	6.522018	-0.233690	10.157877
C	-7.954410	2.501636	-8.700416	C	16.946978	0.916870	9.747351
C	-7.508693	3.544338	-9.732742	C	16.795197	2.131191	10.671596
C	-9.459823	2.603835	-8.415588	C	18.422965	0.637448	9.429335
H	-6.436056	3.474291	-9.943358	H	15.745026	2.332735	10.909039
H	-9.773568	1.887051	-7.647500	H	18.532590	-0.201263	8.731708
C	-0.135947	-1.627544	-9.319908	H	-0.861722	0.126699	-0.653369
C	-0.842503	-2.533429	-10.33711	H	-0.860006	0.128765	2.045856
C	1.390939	-1.754829	-9.423788	H	5.589730	-0.258463	-4.433043
H	-1.931328	-2.485869	-10.23316	H	2.895430	-0.108574	-4.427063

H	9.366433	-0.348741	2.028281	H	12.740191	0.484294	14.058999
H	9.363063	-0.387953	-0.670437	H	14.041021	0.495371	16.341640
H	2.910649	-0.052717	5.808927	H	8.563281	-1.651172	9.943165
H	5.607031	-0.164554	5.802417	H	8.733234	-1.539514	13.007407
H	11.228916	-0.412928	-3.272231	H	8.303088	-2.966469	12.040921
H	12.953010	-0.541021	-4.983934	H	6.308577	-1.773973	11.005248
N	12.555018	-0.569397	-7.650144	H	6.647886	-0.300568	11.925934
H	9.888008	-0.504363	-8.038043	H	16.428860	1.129698	8.804446
H	8.184006	-0.376478	-6.306301	H	17.332389	1.985418	11.616705
H	-2.722224	0.195790	4.646366	H	17.203107	3.028795	10.192296
H	-4.449836	0.230147	6.358638	H	18.895029	1.514981	8.973563
N	-4.053244	0.276062	9.025130	H	18.986613	0.394789	10.340085
H	-1.386429	0.195333	9.414372	H	16.606162	-0.044183	16.002043
H	0.321103	0.161328	7.681973	H	11.396670	-0.600202	4.863852
H	-5.201762	0.618111	-15.12462	H	-2.905539	0.322021	-3.523263
H	-3.948520	0.547118	-12.81654	H	-7.817586	0.824001	-14.80518
H	-8.156827	0.766535	-10.01513	C	13.946699	-0.753937	-7.274703
H	-7.943582	0.379346	-8.312475	C	12.172664	-0.735877	-9.042197
H	-0.275409	0.182707	-10.50311	C	-5.452800	0.149159	8.654735
H	0.039066	0.487320	-8.796621	C	-3.680702	0.131988	10.422408
H	-4.177089	0.369276	-5.813604	H	14.295240	0.062318	-6.629547
H	-7.416716	2.688941	-7.762978	H	14.118245	-1.703393	-6.744526
H	-8.046799	3.426396	-10.68111	H	14.563628	-0.750077	-8.174919
H	-7.706485	4.556836	-9.361955	H	11.630528	-1.677218	-9.220883
H	-9.720581	3.607576	-8.061878	H	11.536223	0.091386	-9.380731
H	-10.05041	2.408727	-9.320604	H	13.070771	-0.737026	-9.662192
H	-0.433772	-1.947681	-8.312455	H	-3.201779	-0.836427	10.634602
H	-0.594809	-2.244183	-11.36483	H	-2.990826	0.926728	10.732341
H	-0.539833	-3.577031	-10.19215	H	-4.576069	0.212158	11.041261
H	1.704955	-2.793853	-9.275389	H	-5.757314	0.954598	7.974920
H	1.746202	-1.438331	-10.41307	H	-5.674946	-0.811689	8.165265
H	12.713782	-0.546564	7.127074	H	-6.068525	0.224485	9.552669
H	9.016420	0.737679	11.800193	N	4.390187	2.621042	0.668578
H	8.737254	0.868906	10.065263	C	3.958592	3.341334	1.718538
H	16.792686	-0.668761	11.242748	C	4.891254	3.279416	-0.391056
H	16.444303	-1.176247	9.594638	C	4.980919	4.667844	-0.442889

C	4.008771	4.732341	1.750496
C	4.530375	5.409044	0.648700
H	5.226534	2.661862	-1.218612
H	5.394951	5.150146	-1.322373
H	3.563805	2.772468	2.554756
H	3.645894	5.266250	2.622742
H	4.584809	6.494126	0.640936

9. **2a'**·thf (Ar = Ph, ligand = thf)

Symbol	X	Y	Z
C	0.008624	0.181210	-0.005222
C	0.008490	0.206193	1.358619
C	1.389526	0.202918	1.775650
N	2.208323	0.168310	0.676556
C	1.390380	0.162440	-0.420701
C	4.951935	0.348028	-3.605502
C	3.589429	0.284856	-3.601104
C	3.180780	0.215383	-2.218689
N	4.280524	0.230820	-1.404955
C	5.374840	0.317928	-2.226287
C	1.829112	0.163047	-1.775053
C	8.540654	0.563939	1.339263
C	8.540496	0.550211	-0.024742
C	7.164907	0.420313	-0.439955
N	6.350344	0.351270	0.660493
C	7.164483	0.442843	1.756538
C	6.726514	0.386456	-1.791504
C	3.596191	0.413853	4.939564
C	4.959127	0.466898	4.935151
C	5.373663	0.395632	3.554467
N	4.277408	0.296510	2.742098
C	3.178956	0.310164	3.562135
C	1.827179	0.248589	3.127089
C	6.725573	0.442113	3.110810
C	7.728699	0.443810	-2.798961
C	0.822265	0.252621	4.133445

C	8.588101	0.484727	-3.662111
C	-0.038590	0.250192	4.996110
C	9.592014	0.532162	-4.669569
C	-1.044029	0.248414	6.003162
C	0.826308	0.138951	-2.774585
Mg	4.293341	-0.067541	0.673903
C	7.726175	0.516447	4.110023
C	8.596759	0.571450	4.966289
C	-0.046296	0.117437	-3.630281
C	9.580885	0.633888	5.955971
C	10.958420	0.568707	-4.321363
C	11.936652	0.614045	-5.310057
C	11.575902	0.624000	-6.660001
C	10.225360	0.588366	-7.016883
C	9.239893	0.542771	-6.035403
C	-2.410662	0.232010	5.654342
C	-3.390275	0.230628	6.642712
C	-3.030705	0.245207	7.992930
C	-1.679954	0.261472	8.350428
C	-0.693112	0.263194	7.369273
C	-7.243791	0.411766	-13.92346
C	-5.882894	0.395389	-14.08283
C	-5.181239	0.391005	-12.85326
C	-6.009024	0.409195	-11.73740
S	-7.695471	0.428772	-12.25625
C	-5.530984	0.375253	-10.37461
C	-4.194611	0.247180	-9.978183
C	-4.119965	0.212131	-8.561217
C	-5.462193	0.319215	-8.038880
N	-6.289821	0.429240	-9.204321
C	-2.849749	0.145968	-10.50157
N	-2.022476	0.042138	-9.334162
C	-2.783466	0.095012	-8.164521
O	-2.383056	0.144747	-11.63951
O	-5.933461	0.319061	-6.901927
C	-7.727818	0.603349	-8.994319

C	-0.581939	-0.130791	-9.503902	S	16.202672	1.341672	13.603886
C	-2.297069	0.074514	-6.811932	C	8.653112	-0.940809	10.748382
C	-3.117262	0.083957	-5.683347	C	9.334883	-1.833982	11.793478
C	-2.416501	0.094938	-4.468442	C	7.124267	-0.985597	10.886097
C	-1.034104	0.099810	-4.618142	H	10.421546	-1.853370	11.661141
S	-0.605501	0.084984	-6.320249	H	6.630157	-0.383468	10.113942
C	-8.135872	2.028946	-8.563858	C	16.609867	2.896637	9.886476
C	-7.771811	3.102408	-9.596819	C	16.208340	3.976546	10.898571
C	-9.637885	2.044941	-8.245401	C	18.112938	2.950388	9.577095
H	-6.702629	3.091876	-9.834927	H	15.137509	3.942080	11.126701
H	-9.893902	1.308323	-7.474709	H	18.395432	2.207030	8.822284
C	-0.074446	-1.583068	-9.368160	H	-0.841779	0.188605	-0.672127
C	-0.739111	-2.525696	-10.38032	H	-0.841204	0.238102	2.025503
C	1.453868	-1.588504	-9.517697	H	5.614079	0.421814	-4.456291
H	-1.823643	-2.571740	-10.23723	H	2.919490	0.296987	-4.449216
H	1.936391	-0.949241	-8.768421	H	9.386725	0.660337	2.004759
C	10.962241	0.697336	5.809683	H	9.385543	0.633192	-0.693134
C	11.658385	0.748665	7.026179	H	2.929254	0.453618	5.788891
C	10.835790	0.722446	8.152839	H	5.624673	0.558398	5.781876
S	9.147612	0.636156	7.656871	H	11.237881	0.561204	-3.272236
C	11.316345	0.792036	9.505836	H	12.985267	0.642261	-5.026510
C	12.646844	0.963757	9.903366	H	12.342437	0.659850	-7.429086
C	12.715543	1.030463	11.319468	H	9.938823	0.596752	-8.065034
C	11.373052	0.896591	11.841406	H	8.190280	0.515986	-6.311837
N	10.553739	0.738702	10.674551	H	-2.689236	0.221740	4.605007
C	13.987245	1.099214	9.382813	H	-4.439073	0.218778	6.358693
N	14.807433	1.255610	10.548168	H	-3.798342	0.244536	8.761749
C	14.046406	1.203563	11.717126	H	-1.394366	0.273524	9.398804
O	14.462171	1.091957	8.247374	H	0.356642	0.276360	7.646175
O	10.902625	0.906907	12.977768	H	-5.394512	0.386349	-15.05091
C	9.118085	0.528816	10.844449	H	-4.099637	0.366063	-12.76510
C	16.240455	1.467503	10.339336	H	-8.267566	0.295952	-9.890745
C	14.518770	1.276899	13.080364	H	-8.002115	-0.093000	-8.196014
C	13.687650	1.264014	14.193774	H	-0.373802	0.229147	-10.51587
C	14.384755	1.307728	15.425183	H	-0.054389	0.531119	-8.810006
C	15.745570	1.348998	15.269731	H	-4.199981	0.092491	-5.765061

H	-7.588786	2.239186	-7.636740
H	-8.326814	2.964174	-10.53262
H	-8.013710	4.099658	-9.211331
H	-9.946509	3.030826	-7.880312
H	-10.23646	1.821147	-9.138423
H	-0.317825	-1.939629	-8.358216
H	-0.554589	-2.196524	-11.40917
H	-0.345373	-3.542758	-10.26930
H	1.852518	-2.602045	-9.399191
H	1.752598	-1.227382	-10.51023
H	12.739211	0.810793	7.110390
H	8.895182	0.911044	11.845055
H	8.574912	1.155258	10.129966
H	16.785418	1.190725	11.242556
H	16.537147	0.765813	9.553832
H	12.607178	1.213820	14.102714
H	13.893267	1.308154	16.391727
H	8.915257	-1.320277	9.751577
H	9.131442	-1.480217	12.810523
H	8.970943	-2.864632	11.709113
H	6.755890	-2.013366	10.795683
H	6.806703	-0.603314	11.864773
H	16.063179	3.075359	8.952477
H	16.757537	3.867283	11.841585
H	16.428217	4.973532	10.499465
H	18.395253	3.937740	9.195104
H	18.711734	2.761088	10.477923
H	16.510812	1.387097	16.033796
H	11.440713	0.705692	4.837322
H	-2.892439	0.101671	-3.494830
H	-8.012034	0.418586	-14.68543
O	4.396244	-2.182252	0.711331
C	3.477047	-3.041644	1.439438
C	5.369542	-2.975882	-0.019754
C	4.092783	-4.438751	1.365341
C	4.823863	-4.402485	0.013703

H	5.459725	-2.554507	-1.023251
H	2.500602	-2.994902	0.945041
H	3.382051	-2.649206	2.454432
H	6.335122	-2.893057	0.491515
H	4.117487	-4.562161	-0.809017
H	3.336528	-5.226573	1.426484
H	4.807024	-4.587385	2.183300
H	5.617690	-5.150465	-0.068484

10. **2b'**·thf (Ar = C₆H₄-Me-4, ligand = thf)

Symbol	X	Y	Z
C	0.009453	-0.015407	-0.007787
C	0.009500	-0.020757	1.356410
C	1.390475	-0.023962	1.773801
N	2.209240	-0.013137	0.673999
C	1.391133	-0.015311	-0.422998
C	4.964138	-0.235782	-3.590231
C	3.601524	-0.173391	-3.594477
C	3.185229	-0.097990	-2.214706
N	4.280394	-0.110551	-1.394534
C	5.379412	-0.198455	-2.208998
C	1.831892	-0.033693	-1.776535
C	8.539533	-0.444996	1.363835
C	8.539819	-0.428808	-0.000236
C	7.165079	-0.292865	-0.416288
N	6.350451	-0.222126	0.684194
C	7.163874	-0.318566	1.780256
C	6.729428	-0.261854	-1.768884
C	3.584134	-0.233133	4.946531
C	4.946324	-0.305227	4.950584
C	5.369070	-0.248036	3.571977
N	4.278574	-0.137473	2.752641
C	3.175589	-0.131284	3.566521
C	1.825976	-0.058126	3.126482
C	6.722472	-0.311285	3.133897
C	7.734554	-0.320952	-2.773067

C	0.818772	-0.043678	4.130218	C	-7.573451	0.966491	-9.150864
C	8.596594	-0.363312	-3.633770	C	-0.477179	-0.203042	-9.519958
C	-0.044320	-0.027582	4.990761	C	-2.225232	0.125762	-6.862587
C	9.602527	-0.412735	-4.637993	C	-3.063757	0.183732	-5.748970
C	-1.051333	-0.011839	5.995000	C	-2.385729	0.153291	-4.521404
C	0.833589	-0.002424	-2.780035	C	-1.002925	0.076237	-4.646084
Mg	4.295747	0.207394	0.680946	S	-0.545267	0.036550	-6.340270
C	7.720317	-0.387382	4.135476	C	-7.916109	2.410786	-8.725883
C	8.591683	-0.440432	4.991186	C	-7.469190	3.465440	-9.745483
C	-0.031210	0.032848	-3.643288	C	-9.422980	2.505810	-8.446198
C	9.580965	-0.493424	5.976164	H	-6.395516	3.400873	-9.952682
C	10.969062	-0.447518	-4.292901	H	-9.738042	1.779963	-7.687240
C	11.946781	-0.491726	-5.280183	C	-0.080611	-1.687290	-9.366470
C	11.609480	-0.506084	-6.641381	C	-0.779598	-2.584076	-10.39690
C	10.249571	-0.467034	-6.981602	C	1.447194	-1.806394	-9.466717
C	9.260488	-0.422466	-6.005631	H	-1.868973	-2.543243	-10.29580
C	-2.418039	0.009961	5.649783	H	1.951527	-1.199574	-8.704906
C	-3.396581	0.026804	6.637180	C	10.962412	-0.530457	5.821380
C	-3.060031	0.020212	7.998555	C	11.666880	-0.570145	7.033452
C	-1.699623	0.003416	8.338865	C	10.850650	-0.571293	8.164920
C	-0.709798	-0.013770	7.362861	S	9.157964	-0.515014	7.679697
C	-7.003440	0.747006	-14.06968	C	11.342170	-0.575218	9.515684
C	-5.643265	0.646349	-14.20183	C	12.681695	-0.482633	9.908752
C	-4.967564	0.602890	-12.95854	C	12.761982	-0.466498	11.325801
C	-5.814406	0.675389	-11.85935	C	11.417509	-0.554937	11.852826
S	-7.486009	0.797196	-12.41174	N	10.584643	-0.631380	10.687282
C	-5.365851	0.615951	-10.48736	C	14.023039	-0.386066	9.382571
C	-4.047351	0.410275	-10.06489	N	14.856401	-0.301563	10.546107
C	-4.002609	0.373155	-8.646664	C	14.101293	-0.360726	11.718693
C	-5.345722	0.561275	-8.150490	O	14.490120	-0.378259	8.243830
N	-6.142661	0.717479	-9.331904	O	10.955041	-0.564664	12.992434
C	-2.701041	0.226902	-10.56188	C	9.143249	-0.794970	10.859761
N	-1.904692	0.074284	-9.378719	C	16.296333	-0.149659	10.332443
C	-2.683788	0.174485	-8.224025	C	14.584736	-0.349994	13.080016
O	-2.213309	0.195175	-11.69054	C	13.761099	-0.376531	14.198773
O	-5.838035	0.591405	-7.022818	C	14.467431	-0.394457	15.425563

C	15.827793	-0.386716	15.261200	H	-4.142460	0.255444	-5.850572
S	16.273225	-0.350753	13.592581	H	-7.382797	2.589848	-7.784310
C	8.622922	-2.240325	10.701411	H	-8.003347	3.355951	-10.69705
C	9.285762	-3.206156	11.692665	H	-7.671397	4.473382	-9.364908
C	7.095522	-2.235905	10.859915	H	-9.687823	3.504947	-8.082729
H	10.369006	-3.258649	11.542083	H	-10.00921	2.319037	-9.355760
H	6.614058	-1.578484	10.125816	H	-0.380522	-2.020914	-8.363960
C	16.726433	1.273147	9.914397	H	-0.530122	-2.281015	-11.42016
C	16.386422	2.341989	10.960279	H	-0.472159	-3.627828	-10.26381
C	18.226705	1.267092	9.587580	H	1.765347	-2.845737	-9.330085
H	15.319086	2.344881	11.206826	H	1.804329	-1.476212	-10.45077
H	18.465741	0.535153	8.807052	H	12.749752	-0.587653	7.111199
H	-0.841021	-0.024854	-0.674707	H	8.942239	-0.450140	11.878419
H	-0.840283	-0.035170	2.023759	H	8.618568	-0.117150	10.179164
H	5.631332	-0.311843	-4.436836	H	16.834225	-0.475132	11.223599
H	2.936567	-0.188737	-4.446485	H	16.556119	-0.842292	9.526068
H	9.384931	-0.546087	2.029529	H	12.678985	-0.390997	14.114538
H	9.384735	-0.514216	-0.668454	H	13.982618	-0.413003	16.395301
H	2.911971	-0.258474	5.792253	H	8.857251	-2.580879	9.683882
H	5.606006	-0.401079	5.801469	H	9.110062	-2.893957	12.728373
H	11.252269	-0.435180	-3.244718	H	8.883051	-4.217772	11.565873
H	12.994704	-0.514565	-4.989613	H	6.687707	-3.243519	10.723915
C	12.676346	-0.587723	-7.706589	H	6.805523	-1.891627	11.861034
H	9.961431	-0.470608	-8.030430	H	16.177716	1.501790	8.992660
H	8.213312	-0.391241	-6.291089	H	16.946582	2.186653	11.890315
H	-2.700672	0.016343	4.601396	H	16.640262	3.339210	10.582353
H	-4.444524	0.046206	6.346469	H	18.550405	2.251710	9.232165
C	-4.129102	0.004712	9.064588	H	18.826141	1.022642	10.474592
H	-1.411695	0.004689	9.387770	H	16.598961	-0.396598	16.020171
H	0.337799	-0.024959	7.648288	H	11.434858	-0.527236	4.846053
H	-5.137312	0.603771	-15.15995	H	-2.878213	0.186049	-3.556578
H	-3.891483	0.511831	-12.84874	H	-7.754652	0.798325	-14.84678
H	-8.109279	0.688903	-10.05925	H	13.606279	-0.109612	-7.380864
H	-7.900638	0.284312	-8.360225	H	12.916080	-1.631995	-7.949081
H	-0.224409	0.135728	-10.52913	H	12.353853	-0.105540	-8.635491
H	0.083504	0.422642	-8.818543	H	-5.041538	0.506417	8.725305

H	-4.405324	-1.023614	9.334795	C	4.954216	0.405702	4.948910
H	-3.789767	0.499862	9.980625	C	5.368057	0.347011	3.567325
O	4.409639	2.322781	0.693814	N	4.271360	0.252755	2.754578
C	3.495755	3.204446	-0.014188	C	3.173944	0.257511	3.575180
C	5.388989	3.093261	1.440867	C	1.822498	0.197336	3.139069
C	4.115304	4.597493	0.099056	C	6.719515	0.400061	3.123846
C	4.847225	4.521533	1.448552	C	7.715225	0.468967	-2.785128
H	5.482618	2.644473	2.432038	C	0.818399	0.188794	4.145898
H	2.517648	3.147074	0.475628	C	8.573895	0.525646	-3.648100
H	3.403085	2.840214	-1.039917	C	-0.042059	0.173378	5.008814
H	6.352000	3.021927	0.922891	C	9.576178	0.593898	-4.653882
H	4.141929	4.659458	2.276109	C	-1.046205	0.151024	6.014796
H	3.360987	5.388599	0.060571	C	0.815126	0.137830	-2.761978
H	4.829471	4.767407	-0.714809	Mg	4.285943	-0.095253	0.683150
H	5.643097	5.264839	1.551087	C	7.721117	0.468081	4.122803
11. 2c' ·thf (Ar = C ₆ H ₄ -CF ₃ -4, ligand = thf)				C	8.593470	0.517982	4.977347
Symbol	X	Y	Z	C	-0.057424	0.121505	-3.617612
C	-0.000118	0.155018	0.008544	C	9.581617	0.575241	5.963711
C	0.000745	0.167952	1.372348	C	10.942935	0.636081	-4.306511
C	1.382538	0.163113	1.788086	C	11.920776	0.702053	-5.291029
N	2.200388	0.139494	0.688692	C	11.557573	0.726002	-6.641304
C	1.381456	0.142076	-0.408121	C	10.206898	0.682975	-7.001036
C	4.939280	0.369320	-3.592738	C	9.225332	0.616769	-6.020146
C	3.577215	0.301297	-3.588105	C	-2.413339	0.128257	5.667093
C	3.169788	0.215741	-2.206103	C	-3.392807	0.102470	6.651871
N	4.270213	0.225984	-1.392848	C	-3.030849	0.100274	8.002689
C	5.363043	0.325823	-2.213788	C	-1.679831	0.126326	8.362741
C	1.818596	0.155637	-1.762680	C	-0.696643	0.152415	7.381589
C	8.532259	0.544681	1.352169	C	-7.244256	0.480859	-13.91427
C	8.530954	0.545327	-0.011686	C	-5.883278	0.455167	-14.07263
C	7.155059	0.414905	-0.426881	C	-5.183018	0.442707	-12.84251
N	6.341879	0.331036	0.672898	C	-6.011983	0.464012	-11.72739
C	7.156775	0.414430	1.769316	S	-7.697691	0.497044	-12.24779
C	6.714267	0.394658	-1.777865	C	-5.535181	0.423297	-10.36461
C	3.591582	0.350124	4.953644	C	-4.199413	0.286410	-9.967912
				C	-4.125936	0.246765	-8.551237

C	-5.468424	0.359819	-8.029461	O	14.474310	1.003663	8.231675
N	-6.294533	0.478218	-9.194924	O	10.936652	0.847955	12.979076
C	-2.854836	0.179517	-10.49082	C	9.139300	0.479764	10.854812
N	-2.028904	0.068173	-9.322896	C	16.266051	1.369585	10.314303
C	-2.790704	0.121538	-8.154072	C	14.555884	1.194802	13.063341
O	-2.387279	0.178624	-11.62829	C	13.729597	1.187783	14.180594
O	-5.939768	0.358298	-6.892853	C	14.432458	1.229255	15.408619
C	-7.731983	0.659458	-8.985556	C	15.792817	1.262971	15.246587
C	-0.589316	-0.113269	-9.492170	S	16.242428	1.251203	13.578994
C	-2.305891	0.094967	-6.800464	C	8.663141	-0.986622	10.763522
C	-3.127128	0.102533	-5.672800	C	9.344936	-1.883324	11.805579
C	-2.427048	0.107600	-4.457271	C	7.134918	-1.019735	10.911087
C	-1.044843	0.109657	-4.606344	H	10.430484	-1.911529	11.665833
S	-0.615026	0.099654	-6.308068	H	6.640342	-0.414827	10.141347
C	-8.132881	2.085921	-8.551313	C	16.643524	2.795470	9.857940
C	-7.760766	3.160760	-9.579973	C	16.254999	3.879605	10.870628
C	-9.635473	2.109024	-8.235950	C	18.145393	2.837680	9.541003
H	-6.691024	3.145827	-9.815391	H	15.185159	3.853327	11.104565
H	-9.897254	1.371033	-7.468533	H	18.418615	2.091583	8.785502
C	-0.090772	-1.568817	-9.358486	H	-0.850955	0.167043	-0.657671
C	-0.760446	-2.505715	-10.37267	H	-0.849000	0.192855	2.039427
C	1.437587	-1.583384	-9.507079	H	5.599854	0.454773	-4.443624
H	-1.845322	-2.545661	-10.23034	H	2.906614	0.320385	-4.435503
H	1.923570	-0.947957	-8.756720	H	9.378474	0.637357	2.017923
C	10.962368	0.630708	5.810943	H	9.375609	0.638702	-0.679157
C	11.664320	0.678813	7.024339	H	2.925733	0.381598	5.804149
C	10.846322	0.658243	8.154294	H	5.620169	0.491115	5.795903
S	9.155805	0.581245	7.666350	H	11.225782	0.614093	-3.259030
C	11.333119	0.726124	9.505698	H	12.969472	0.728036	-5.013929
C	12.666280	0.889837	9.896491	C	12.615163	0.860484	-7.701951
C	12.742291	0.957884	11.311919	H	9.927171	0.694503	-8.049278
C	11.401603	0.833269	11.840643	H	8.177504	0.580573	-6.300235
N	10.575615	0.679135	10.677690	H	-2.695146	0.133979	4.619120
C	14.005555	1.015730	9.369343	H	-4.441676	0.091361	6.374420
N	14.832327	1.168160	10.530319	C	-4.091212	0.005764	9.064814
C	14.076585	1.122695	11.702740	H	-1.401035	0.133412	9.411269

H	0.351506	0.176194	7.661815	H	11.436723	0.635505	4.836530
H	-5.394166	0.445018	-15.04029	H	-2.903841	0.112223	-3.484049
H	-4.101683	0.410069	-12.75344	H	-8.011640	0.494909	-14.67702
H	-8.272277	0.357458	-9.883453	F	-5.247617	0.587312	8.675505
H	-8.010671	-0.037997	-8.189768	F	-4.383275	-1.282378	9.365168
H	-0.378671	0.247059	-10.50348	F	-3.704894	0.597230	10.217135
H	-0.058012	0.544558	-8.797187	F	12.884810	2.158527	-7.977565
H	-4.209732	0.114435	-5.755318	F	13.781744	0.291018	-7.324643
H	-7.586694	2.290325	-7.622334	F	12.238101	0.284328	-8.865260
H	-8.314080	3.028333	-10.51758	O	4.392492	-2.208786	0.699747
H	-7.998707	4.157927	-9.191909	C	5.368662	-2.993715	-0.037510
H	-9.939281	3.095247	-7.867846	C	3.475886	-3.077712	1.420731
H	-10.23340	1.891935	-9.131028	C	4.824933	-4.421153	-0.019674
H	-0.336988	-1.925675	-8.349284	C	4.093832	-4.472949	1.331403
H	-0.573258	-2.175903	-11.40081	H	3.382032	-2.696137	2.439998
H	-0.372800	-3.525254	-10.26319	H	6.333067	-2.914851	0.476611
H	1.829837	-2.599522	-9.389633	H	5.460016	-2.561851	-1.036430
H	1.739240	-1.222944	-10.49893	H	2.498717	-3.027335	0.928227
H	12.745843	0.734533	7.103714	H	4.808132	-4.629561	2.147775
H	8.924099	0.865110	11.855894	H	5.619789	-5.167086	-0.109616
H	8.597127	1.109219	10.142147	H	4.119024	-4.572916	-0.844251
H	16.813218	1.089712	11.215215	H	3.338730	-5.262435	1.383822
H	16.553828	0.664717	9.528359				
H	12.648437	1.143551	14.094665	12. 2d' ·thf (Ar = C ₆ H ₄ -NMe ₂ -4, ligand = thf)			
H	13.945592	1.233530	16.377453	Symbol	X	Y	Z
H	8.916305	-1.369411	9.765614	C	-0.028140	0.184568	0.028438
H	9.151229	-1.526181	12.823315	C	-0.026846	0.200835	1.392907
H	8.972325	-2.911186	11.725560	C	1.353810	0.186270	1.808784
H	6.758205	-2.044804	10.824658	N	2.171590	0.166485	0.708108
H	6.826681	-0.633628	11.891201	C	1.352647	0.159687	-0.388059
H	16.093568	2.977188	8.926421	C	4.905931	-0.190193	-3.570742
H	16.808458	3.767895	11.810838	C	3.544484	-0.096554	-3.566541
H	16.479938	4.874350	10.468836	C	3.140223	0.019349	-2.186696
H	18.433047	3.822542	9.156660	N	4.241476	0.002374	-1.374467
H	18.747253	2.644819	10.439002	C	5.332306	-0.130628	-2.194886
H	16.561732	1.297747	16.007134	C	1.790602	0.114661	-1.742186

C	8.499301	-0.313815	1.372875	C	-5.686552	0.713600	-14.16953
C	8.497030	-0.348111	0.008743	C	-5.010834	0.678328	-12.92581
C	7.123935	-0.210432	-0.409428	C	-5.855594	0.780854	-11.82759
N	6.312146	-0.090993	0.689371	S	-7.525410	0.920747	-12.38135
C	7.126503	-0.155643	1.786916	C	-5.407617	0.735416	-10.45463
C	6.685117	-0.211949	-1.762708	C	-4.092655	0.516477	-10.02882
C	3.564386	0.047835	4.972738	C	-4.048092	0.500670	-8.609973
C	4.927062	-0.026837	4.968130	C	-5.387502	0.716528	-8.116682
C	5.339382	-0.010987	3.585946	N	-6.182424	0.866343	-9.300528
N	4.242518	0.078600	2.772496	C	-2.749356	0.304826	-10.52282
C	3.145452	0.110384	3.594651	N	-1.955069	0.158690	-9.337843
C	1.791971	0.178940	3.162308	C	-2.731887	0.288710	-8.184152
C	6.689372	-0.096847	3.141021	O	-2.262713	0.247494	-11.65110
C	7.682416	-0.317823	-2.767902	O	-5.879718	0.771442	-6.989549
C	0.791078	0.226911	4.168381	C	-7.609452	1.137025	-9.123121
C	8.540409	-0.400388	-3.631575	C	-0.532993	-0.146848	-9.474987
C	-0.068958	0.272815	5.032733	C	-2.272862	0.254562	-6.823217
C	9.538187	-0.495405	-4.635293	C	-3.109230	0.343527	-5.709665
C	-1.069035	0.325566	6.037297	C	-2.431013	0.322470	-4.482337
C	0.789539	0.145257	-2.742381	C	-1.049156	0.222127	-4.605942
Mg	4.261741	0.361394	0.693485	S	-0.593626	0.148163	-6.299873
C	7.691371	-0.148651	4.139418	C	-7.932698	2.591715	-8.718814
C	8.567149	-0.183529	4.991952	C	-7.472282	3.625714	-9.753454
C	-0.077195	0.179852	-3.604121	C	-9.437947	2.711149	-8.439808
C	9.561963	-0.216929	5.971400	H	-6.399599	3.543917	-9.959552
C	10.907983	-0.559218	-4.305591	H	-9.762206	2.000441	-7.670436
C	11.886494	-0.653109	-5.282142	C	-0.163815	-1.635301	-9.296730
C	11.549255	-0.683078	-6.657793	C	-0.879275	-2.536460	-10.31188
C	10.172755	-0.628579	-6.988438	C	1.361522	-1.784305	-9.394392
C	9.201809	-0.534510	-6.004371	H	-1.967713	-2.472013	-10.21322
C	-2.439974	0.358876	5.707998	H	1.876796	-1.174203	-8.642635
C	-3.420787	0.407705	6.685563	C	10.942518	-0.269376	5.809142
C	-3.084487	0.433392	8.061491	C	11.654589	-0.282902	7.016932
C	-1.707677	0.389307	8.392247	C	10.846308	-0.247933	8.153892
C	-0.734330	0.340343	7.407226	S	9.150437	-0.189604	7.677966
C	-7.044818	0.837816	-14.03885	C	11.347401	-0.221606	9.500035

C	12.690612	-0.130034	9.882244	N	12.522845	-0.757378	-7.636704
C	12.780382	-0.078963	11.298067	H	9.856811	-0.661443	-8.024197
C	11.438660	-0.143696	11.835648	H	8.155575	-0.494198	-6.293037
N	10.597553	-0.242444	10.678075	H	-2.733127	0.340751	4.662399
C	14.028581	-0.058244	9.345140	H	-4.458570	0.424082	6.375083
N	14.870389	0.048303	10.500953	N	-4.058978	0.504204	9.040359
C	14.122744	0.025322	11.679826	H	-1.393222	0.391186	9.428963
O	14.488896	-0.083274	8.203540	H	0.312122	0.308183	7.696130
O	10.983909	-0.122045	12.978344	H	-5.181665	0.648461	-15.12699
C	9.156707	-0.395035	10.863809	H	-3.936291	0.571884	-12.81486
C	16.309877	0.181229	10.274323	H	-8.149386	0.853628	-10.02732
C	14.615472	0.066362	13.037477	H	-7.945661	0.471018	-8.322503
C	13.799639	0.074715	14.162051	H	-0.274681	0.170679	-10.48969
C	14.514360	0.081987	15.384265	H	0.039585	0.479455	-8.783957
C	15.873503	0.074595	15.210977	H	-4.186805	0.430239	-5.811851
S	16.307465	0.064783	13.538698	H	-7.396356	2.776865	-7.780176
C	8.628857	-1.841180	10.740581	H	-8.007905	3.509578	-10.70346
C	9.293941	-2.787733	11.748776	H	-7.661175	4.641614	-9.387363
C	7.102595	-1.826136	10.908908	H	-9.689051	3.718868	-8.090468
H	10.375933	-2.848387	11.592346	H	-10.02736	2.519360	-9.346297
H	6.619270	-1.184225	10.162453	H	-0.469717	-1.945976	-8.288731
C	16.750630	1.589094	9.818345	H	-0.622596	-2.256998	-11.34011
C	16.425877	2.687021	10.838665	H	-0.592951	-3.583603	-10.15953
C	18.249003	1.561376	9.484086	H	1.660690	-2.826856	-9.240133
H	15.359479	2.707546	11.088394	H	1.724654	-1.477278	-10.38381
H	18.477586	0.806520	8.722454	H	12.737810	-0.307251	7.088061
H	-0.879508	0.177045	-0.637412	H	8.964474	-0.027361	11.876131
H	-0.875679	0.209488	2.061673	H	8.630241	0.270155	10.172218
H	5.565134	-0.301415	-4.419796	H	16.850875	-0.127286	11.169688
H	2.873107	-0.116850	-4.413421	H	16.557898	-0.533285	9.483447
H	9.345108	-0.399723	2.040214	H	12.716906	0.066707	14.085334
H	9.339237	-0.467288	-0.657823	H	14.035948	0.091868	16.357341
H	2.898339	0.048421	5.823754	H	8.855070	-2.205013	9.729355
H	5.592926	-0.099494	5.816544	H	9.126427	-2.451658	12.778397
H	11.201668	-0.537911	-3.260196	H	8.886000	-3.800142	11.647281
H	12.922990	-0.705448	-4.971294	H	6.689257	-2.834797	10.799809

H	6.821045	-1.456528	11.903462
H	16.199003	1.799485	8.893980
H	16.987406	2.548182	11.770493
H	16.689369	3.671833	10.435530
H	18.579115	2.533205	9.100407
H	18.851200	1.335825	10.374269
H	16.649798	0.077664	15.964742
H	11.408136	-0.295860	4.830908
H	-2.922009	0.378566	-3.517840
H	-7.795561	0.889443	-14.81636
C	13.912647	-0.953200	-7.260066
C	12.137705	-0.931095	-9.027104
C	-5.460512	0.391292	8.672890
C	-3.687349	0.375033	10.439365
H	14.271375	-0.133063	-6.625439
H	14.073442	-1.897852	-6.718142
H	14.528780	-0.968011	-8.160700
H	11.581763	-1.865999	-9.196689
H	11.513369	-0.097810	-9.373416
H	13.035501	-0.951457	-9.647197
H	-3.223154	-0.597384	10.665528
H	-2.985158	1.163628	10.736952
H	-4.580794	0.478062	11.057618
H	-5.754107	1.190188	7.980713
H	-5.696719	-0.573913	8.198805
H	-6.074362	0.489500	9.569900
O	4.398358	2.476841	0.656011
C	3.715184	3.367023	1.579687
C	5.179626	3.236029	-0.304839
C	3.876419	4.764293	0.980741
C	5.228410	4.655727	0.257493
H	6.156427	2.756241	-0.395937
H	4.198462	3.280122	2.558994
H	2.678096	3.034428	1.663450
H	4.669457	3.194874	-1.273784

H	6.054243	4.757093	0.970996
H	3.856796	5.546007	1.745583
H	3.073745	4.969011	0.262974
H	5.360970	5.406651	-0.526772

13. py

Symbol	X	Y	Z
N	-0.000004	-0.000007	-0.000022
C	-0.000948	-0.000086	1.339054
C	1.192834	0.000123	-0.608462
C	2.411697	0.000180	0.072469
C	1.158894	-0.000041	2.116282
C	2.392858	0.000091	1.466783
H	1.172226	0.000188	-1.697393
H	3.347377	0.000289	-0.479138
H	-0.980681	-0.000195	1.814786
H	1.091918	-0.000112	3.200385
H	3.319517	0.000130	2.034794

14. thf

Symbol	X	Y	Z
O	0.002633	-0.059811	0.000145
C	-0.002010	-0.000446	1.430938
C	1.346418	-0.000895	-0.488210
C	1.426263	0.363854	1.857810
C	2.255704	-0.251298	0.720423
H	1.463143	-0.748625	-1.281297
H	-0.298607	-0.980878	1.834282
H	-0.747933	0.736367	1.752303
H	1.537328	0.991545	-0.926275
H	2.387392	-1.327756	0.883763
H	1.684910	-0.023854	2.848049
H	1.555354	1.452765	1.875671
H	3.246896	0.199123	0.608244

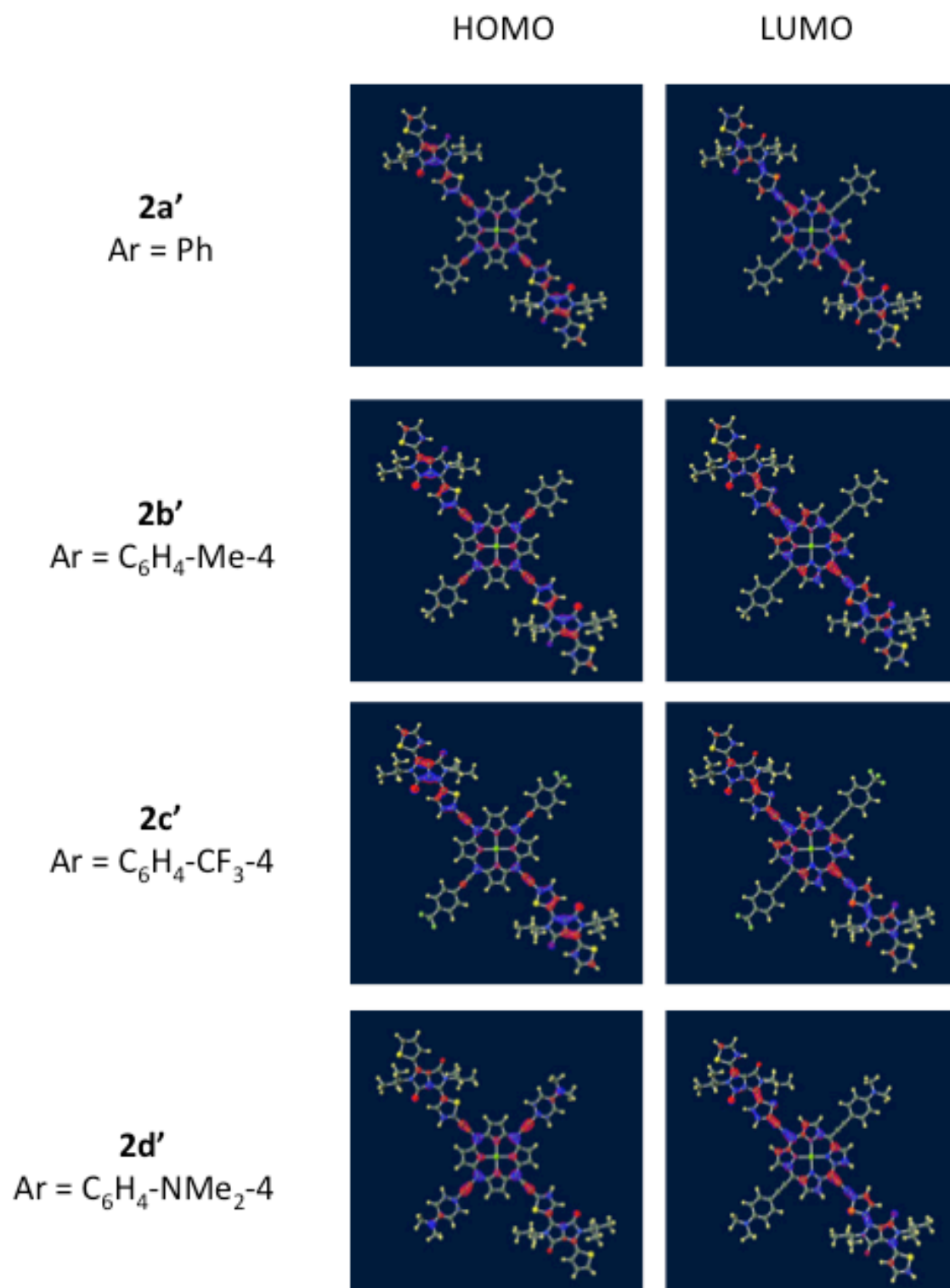


Figure S20. Spatial distribution of HOMOs and LUMOs for **2a'-d'**.

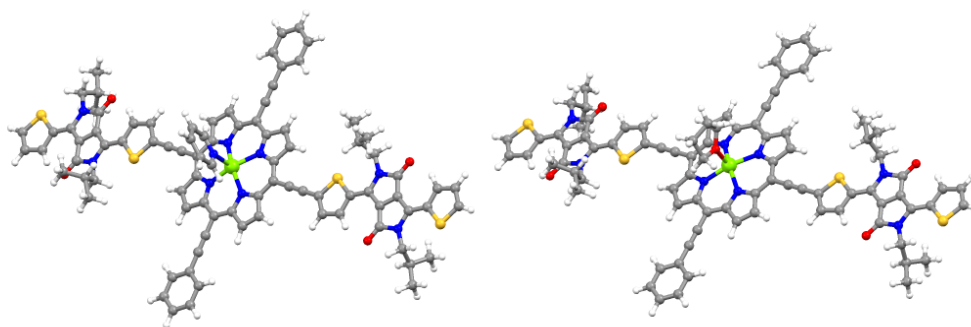


Figure S21. Optimized structures of pyridine- or THF-coordinated Mg-TEP-DPP₂Ph₂, **2a'·py** (left) and **2a'·thf** (right).

Table S3. Calculated HOMO, LUMO and energy band gap ($E_g = \text{LUMO} - \text{HOMO}$) values for Mg-TEP-DPP₂Ar₂ and them with coordination ligands.

Ar		HOMO levels [eV]	LUMO levels [eV]	E_g [eV]
Ph	2a'	−4.709	−3.068	1.641
	2a'·py	−4.579	−2.954	1.625
	2a'·thf	−4.593	−2.963	1.631
4-Me-C ₆ H ₄	2b'	−4.671	−3.040	1.631
	2b'·py	−4.540	−2.924	1.616
	2b'·thf	−4.555	−2.943	1.612
4-CF ₃ -C ₆ H ₄	2c'	−4.844	−3.195	1.649
	2c'·py	−4.728	−3.074	1.654
	2c'·thf	−4.741	−3.083	1.658
4-Me ₂ N-C ₆ H ₄	2d'	−4.433	−2.912	1.521
	2d'·py	−4.304	−2.811	1.493
	2d'·thf	−4.318	−2.822	1.496

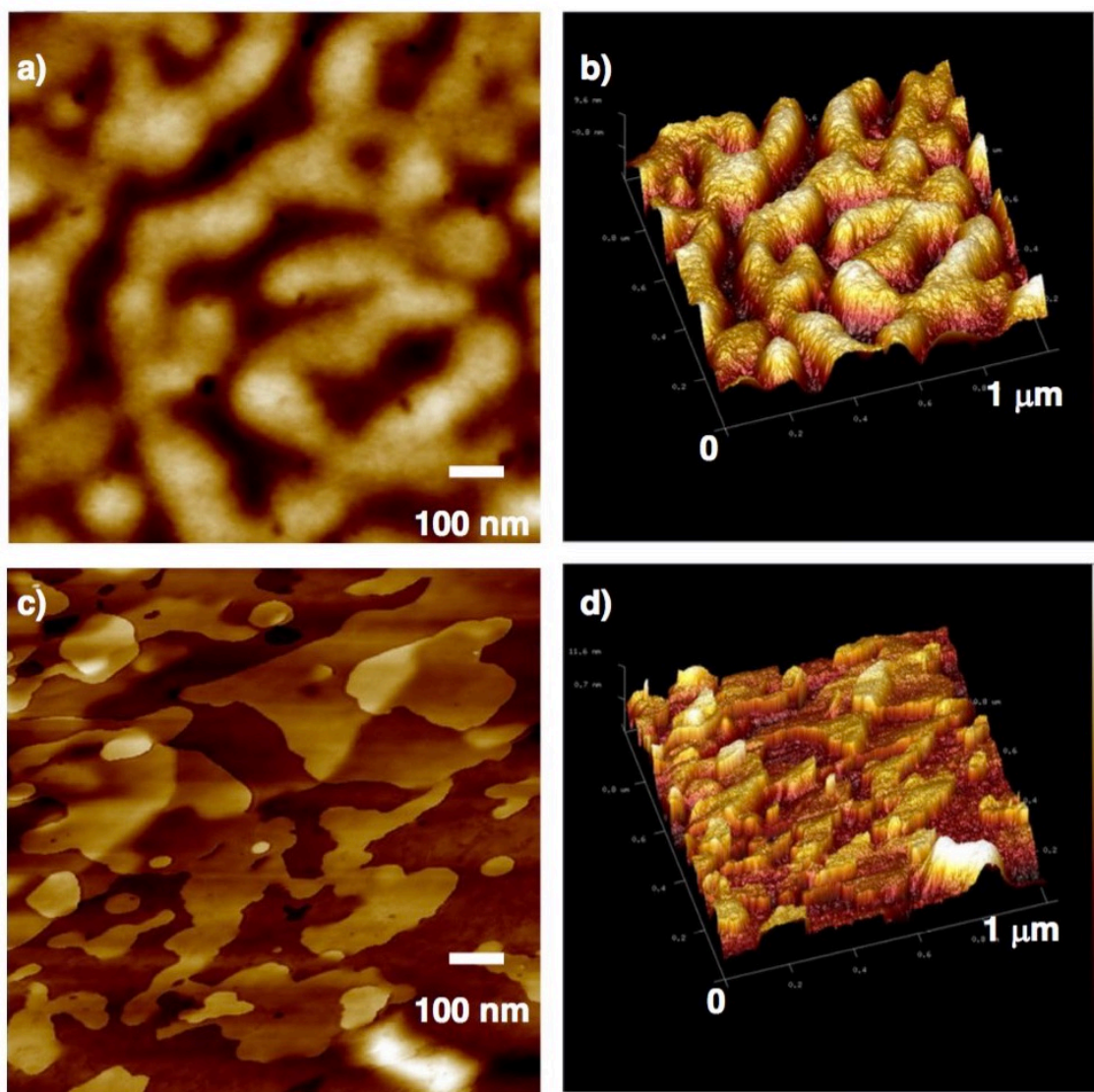


Figure S22. AFM images. 1 μm square AFM height (a, c) and 3D (b, d) images of thin films of **2c**:PC₆₁BM which was fabricated in PhCl with 1% pyridine solution (a, b) and **2d**:PC₆₁BM in the same condition (c, d). Root-mean-square roughness values (R_q) were 3.51 nm and 3.05 nm, respectively.

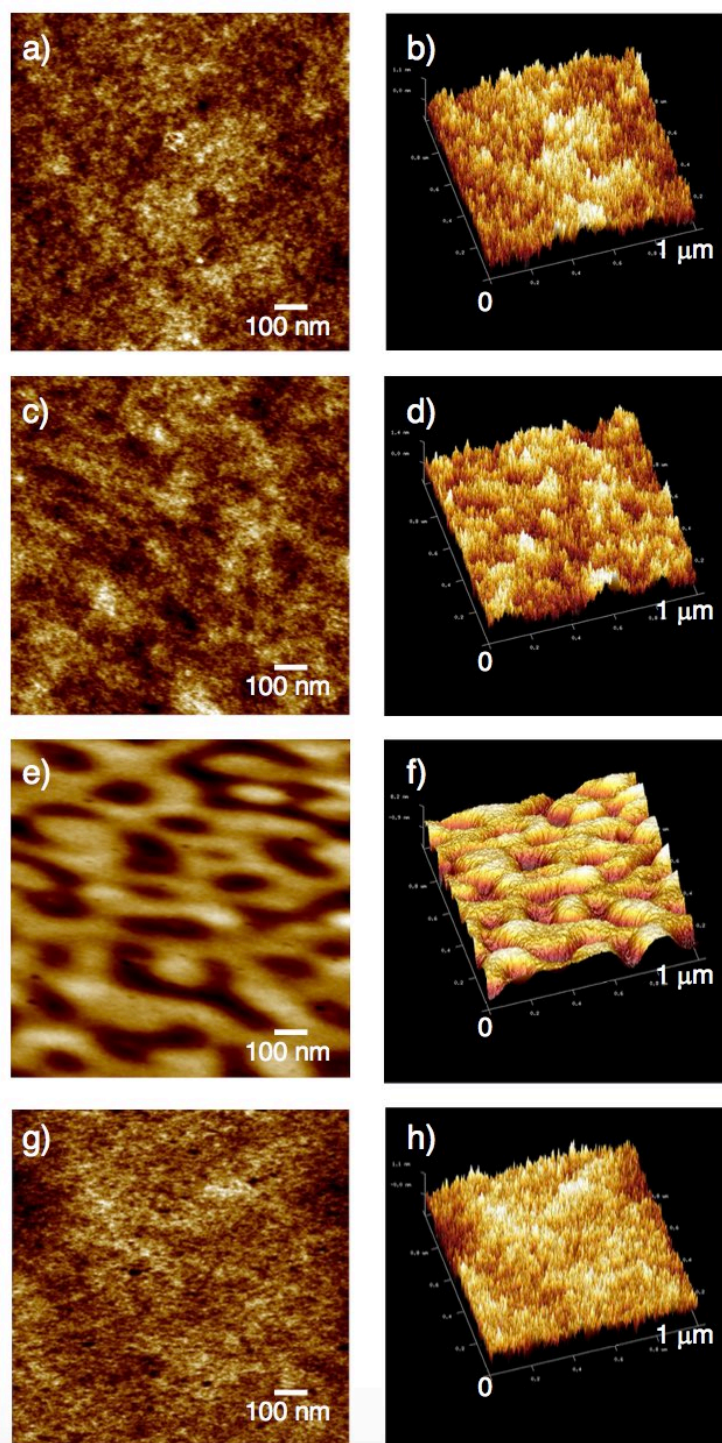


Figure S23. AFM images. 1 μm square AFM height (a, c, e, g) and 3D (b, d, f, h) images of thin films of **2a**:PC₆₁BM (a, b), **2b**:PC₆₁BM (c, d), **2c**:PC₆₁BM (e, f), and **2d**:PC₆₁BM (g, h). These films were spin-coated using PhCl with 1% pyridine and then annealed at 100 $^{\circ}\text{C}$ for 5 min. Root-mean-square roughness values (R_q) were 0.30 nm, 0.41 nm, 3.04, and 0.32 nm, respectively.

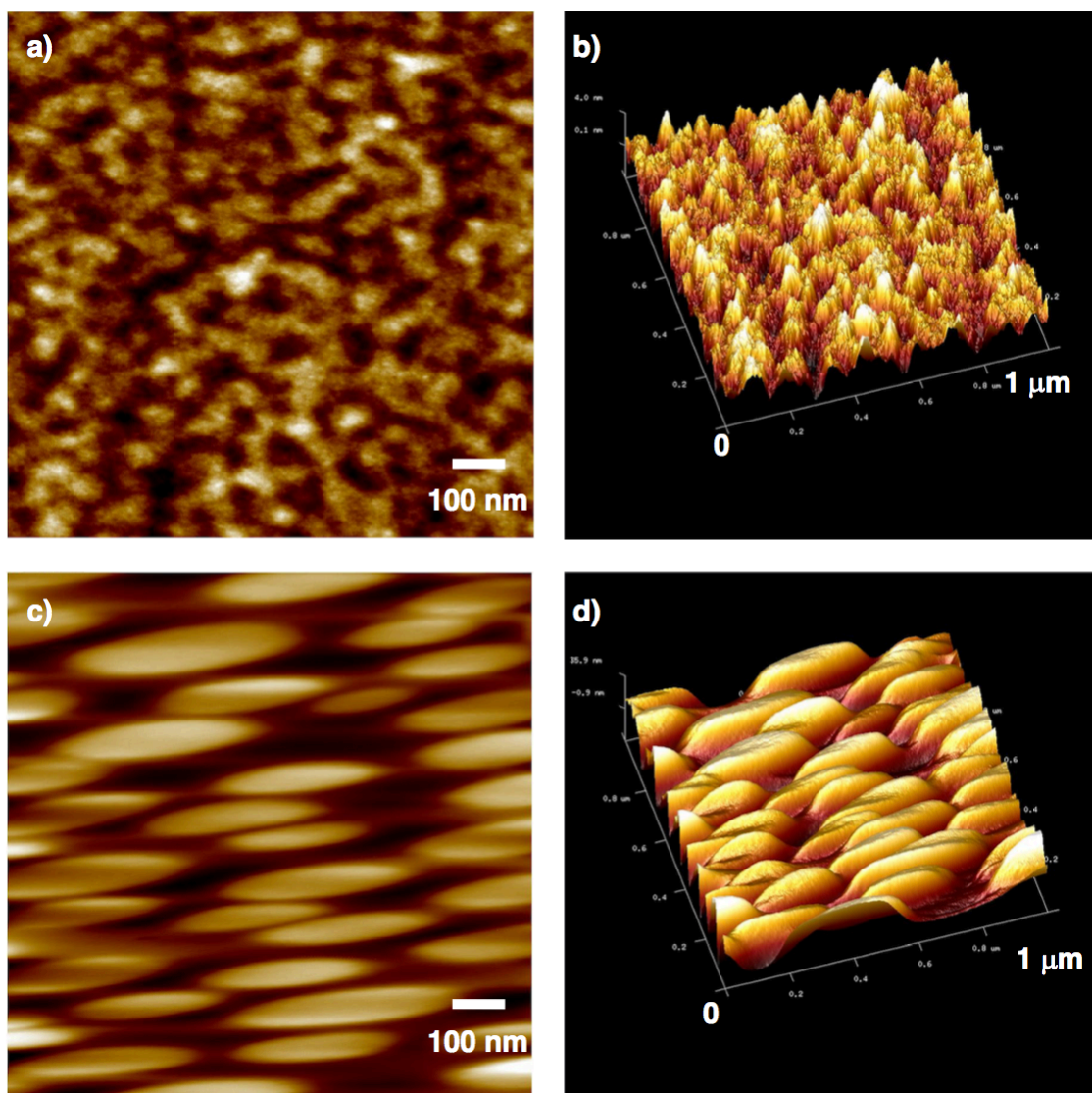


Figure S24. AFM images. 1 μm square AFM height (a, c) and 3D (b, d) images of thin films of **2a:PC₇₁BM** (a, b) and **2b:PC₇₁BM** (c, d). Root-mean-square roughness values (R_q) were 1.18 nm and 13.1 nm, respectively.

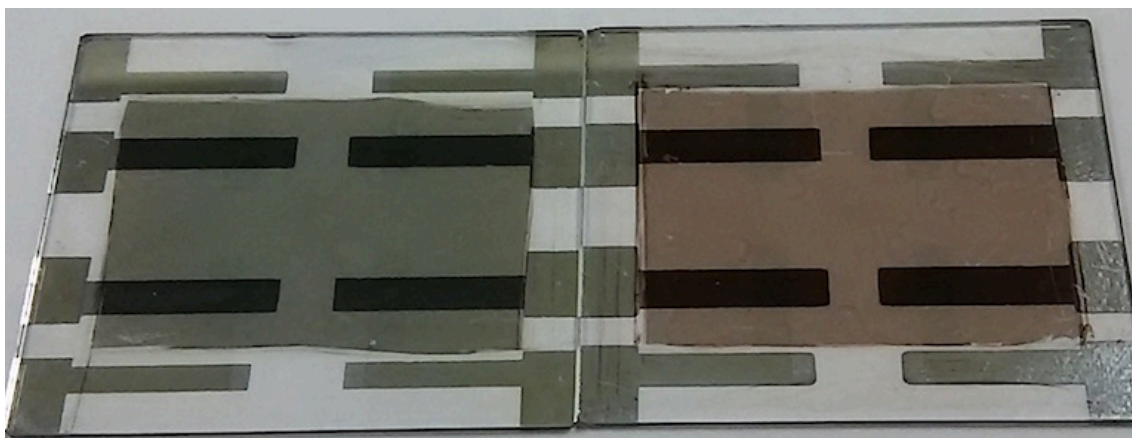


Figure S25. Appearance of the devices using **2a** with PC₆₁BM and PC₇₁BM. We observed color difference greater than we expected. Gray colored PC₆₁BM devices gave higher performance than reddish colored PC₇₁BM ones. We consider that the origin of the reddish color in the PC₇₁BM devices is unique aggregation behavior of the present porphyrin donor molecules in the presence of PC₇₁BM.

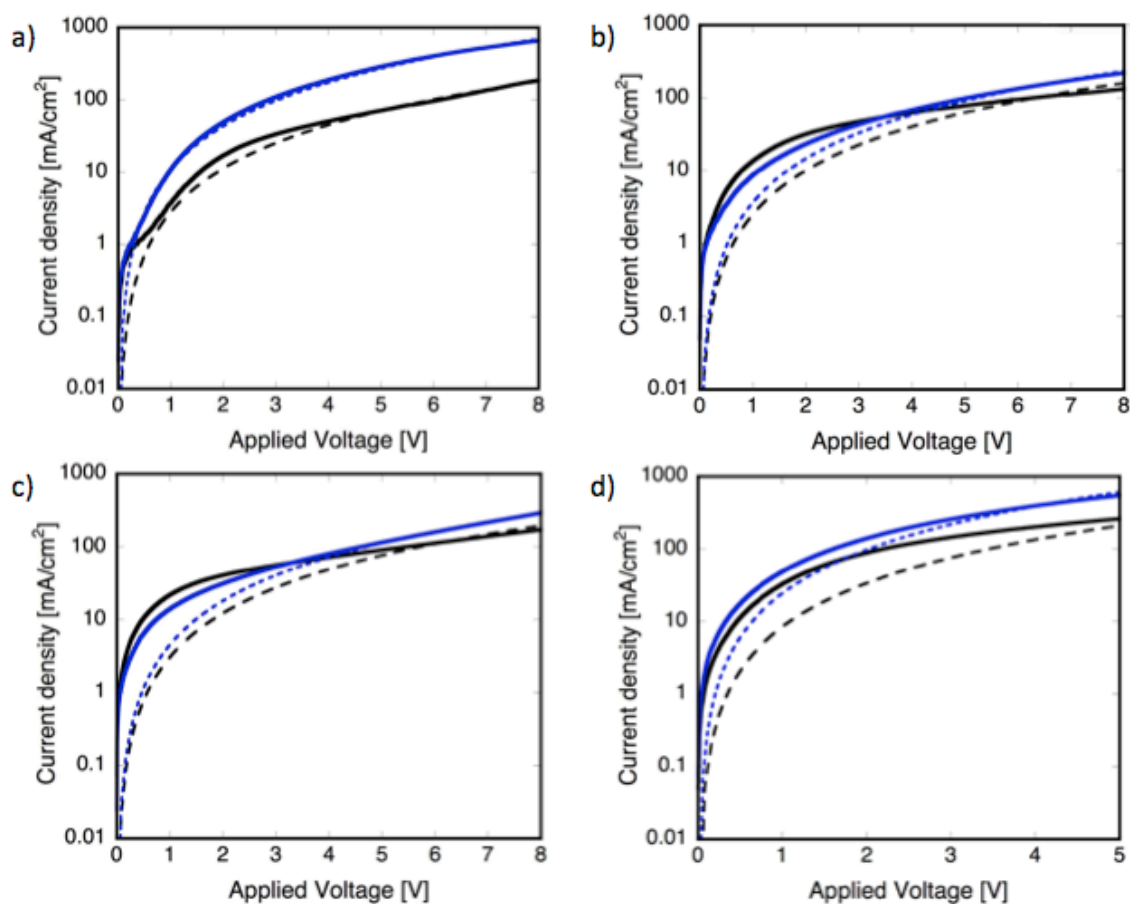


Figure S26. Hole mobilities of **2a**, **2b**, **2c**, and **2d** with PC₆₁BM and these thickness are 130 nm, 120 nm, 120 nm, 120 nm respectively. Device configuration is ITO/PEDOT:PSS/active layer/MoO₃/Al. The black line is no annealed film and the blue line is annealed at 100 °C for 5 min. after spin coat of the active layer. These mobilities are calculated to be a) 2.07×10^{-5} and 8.00×10^{-5} (**2a**: without annealing and annealing), b) 1.45×10^{-5} and 2.12×10^{-5} (**2b**: without annealing and annealing), c) 1.78×10^{-5} and 2.63×10^{-5} (**2c**: without annealing and annealing), and d) 4.88×10^{-5} and 1.4×10^{-4} (**2d**: without annealing and annealing).

Table S4. Photovoltaic performance for the thermal annealed devices. The device configuration is ITO/PEDOT:PSS/active layer/LiF/Al. The D:A ratio of the active layer was 1:1.5, concentration was 30 mg/mL for the donor and acceptor mixture, chlorobenzene was spin-coating solvent, and 1% pyridine was used as a solvent additive. These devices were thermal annealed at 100 °C for 5–10 min after the active layer spin-coating.

donor	V_{oc} [V]	J_{sc} [mA/cm ²]	FF	PCE [%]	R_s [$\Omega \cdot \text{cm}^2$]	R_{sh} [$\Omega \cdot \text{cm}^2$]
2a	0.71	10.48	0.48	3.55	2.29	2.09×10^2
2b	0.70	11.90	0.51	4.21	3.65	1.96×10^2
2b ^[a]	0.64	3.33	0.32	0.68	4.99	2.60×10^2
2c ^[b]	—	—	—	—	—	—
2d	0.41	4.08	0.45	0.75	1.72	3.27×10^2

^[a]The use of PC₇₁BM as acceptor. ^[b] Large grains were observed.

Table S5. Photovoltaic performance of the normal-type bulk heterojunction organic solar cells with other coordinating solvents.

donor	additive	V_{oc} [V]	J_{sc} [mA/cm ²]	FF	PCE [%]	R_s [$\Omega \cdot \text{cm}^2$]	R_{sh} [$\Omega \cdot \text{cm}^2$]
2b	5% THF	0.65	9.61	0.40	2.53	2.91	1.76×10^2
2b	5eq. DMAP	0.48	2.29	0.16	0.17	244	1.42×10^2
2a ^[a]	1% NEt ₃	0.53	1.39	0.33	0.24	2.32	7.17×10^2
2a ^[a]	1% PhCN	0.46	0.99	0.32	0.14	4.66	7.43×10^2

^[a] Donor and acceptor ratio was 1:1. D:A = 1:1.5 unless otherwise noted.

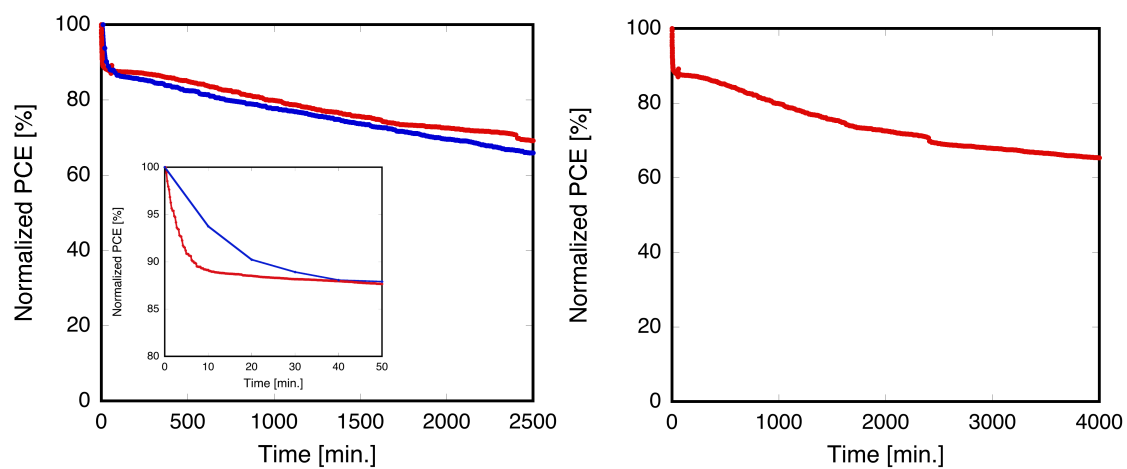


Figure S27. Stability tests of the **2b**:PCBM devices with use of pyridine (red line) and without pyridine (blue line). T_{80} numbers were 970 min. and 720 min. and T_{S80} numbers were 2400 min and 2000 min, respectively.

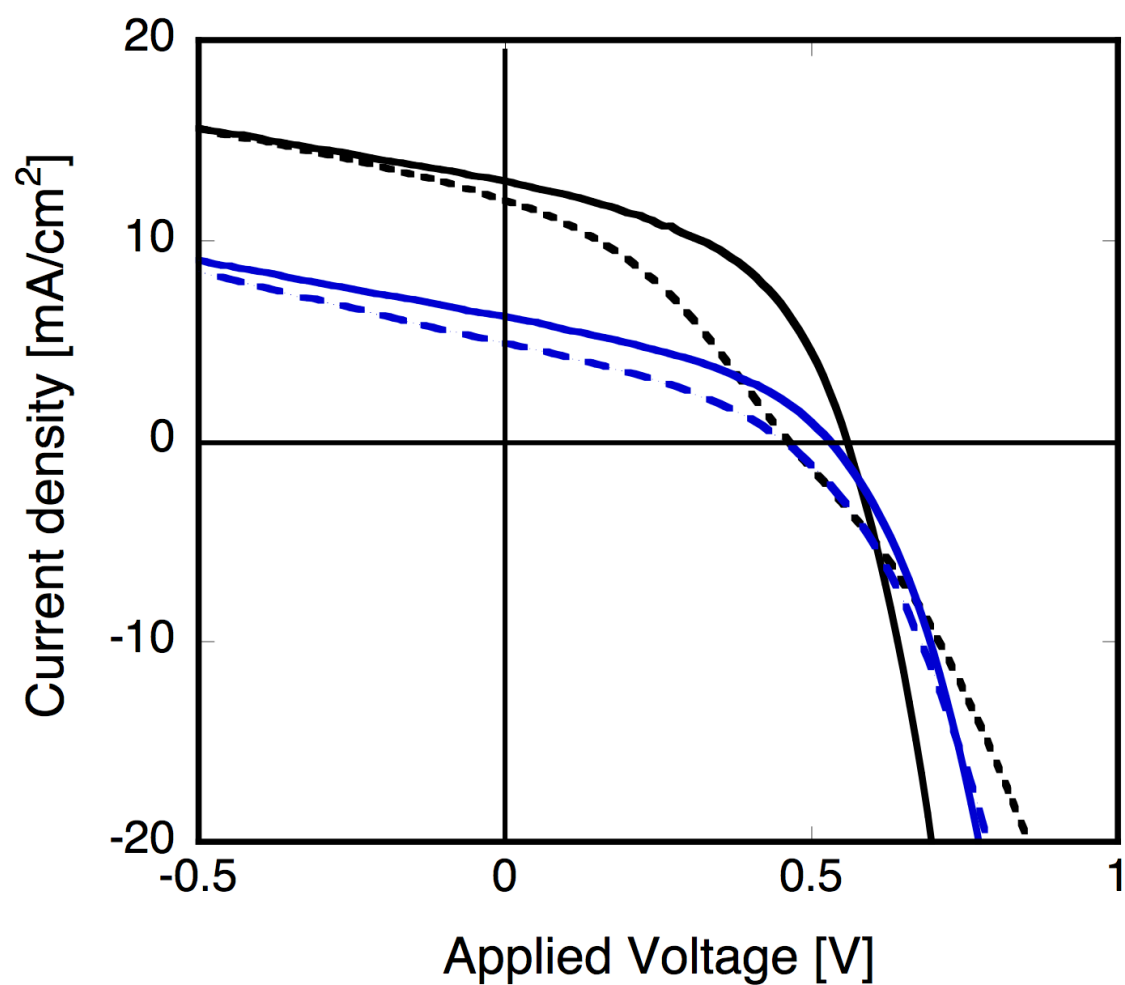


Figure S28. J - V curves of the inverted devices using active layers of **2b** with PC₆₁BM (black dashed line) or PC₇₁BM (blue dashed line). The device configuration is ITO/ZnO/active layer/MoO₃/Au. The D:A ratio of the active layer was 1:1, concentration was 10 mg/mL for the donor and acceptor mixture, chlorobenzene was spin-coating solvent, and 1% pyridine was used as a solvent additive. These devices were annealed after deposition of Au electrodes at 60 °C for 10 min (bold lines).

Table S6. Photovoltaic performance of inverted organic solar cells.

donor	anneal	V_{OC} [V]	J_{SC} [mA/cm ²]	FF	PCE [%]	R_s [$\Omega \cdot \text{cm}^2$]	R_{sh} [$\Omega \cdot \text{cm}^2$]
2b	—	0.46	11.99	0.36	1.97	11.7	97.7
2b	60 °C	0.56	12.96	0.47	3.39	2.63	1.49 x 10 ²
2b ^[a]	—	0.45	4.88	0.34	0.76	7.21	1.56 x 10 ²
2b ^[a]	60 °C	0.53	6.21	0.38	1.26	4.37	1.54 x 10 ²

^[a]The use of PC₇₁BM as acceptor.