Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

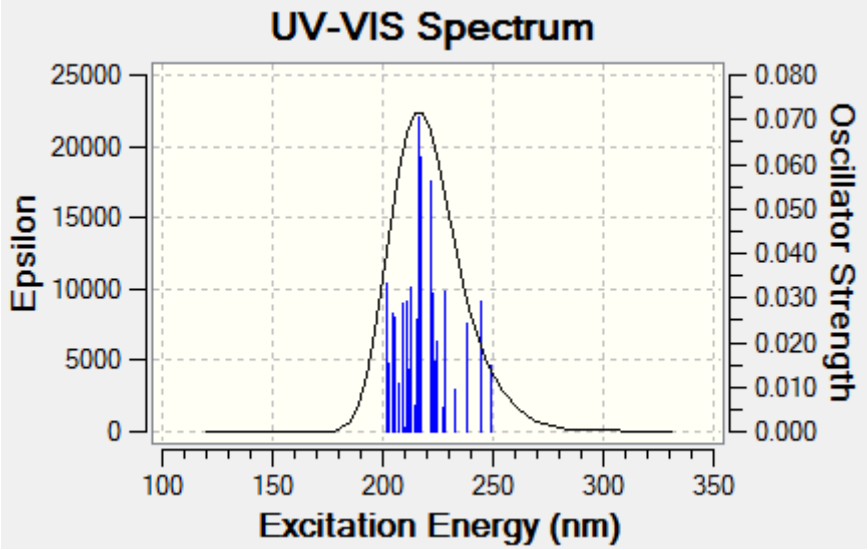

Figure S1. Theoretical UV-Vis absorption spectra of **1**.

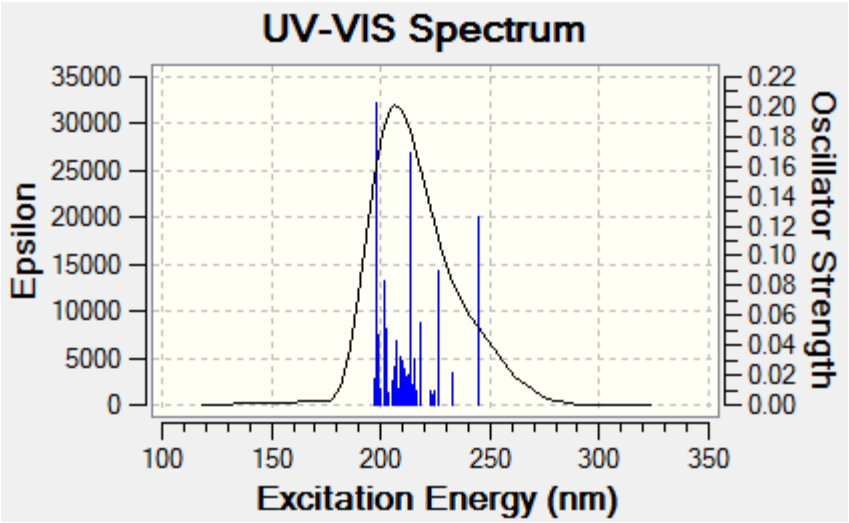

Figure S2. Theoretical UV-Vis absorption spectra of **2**.

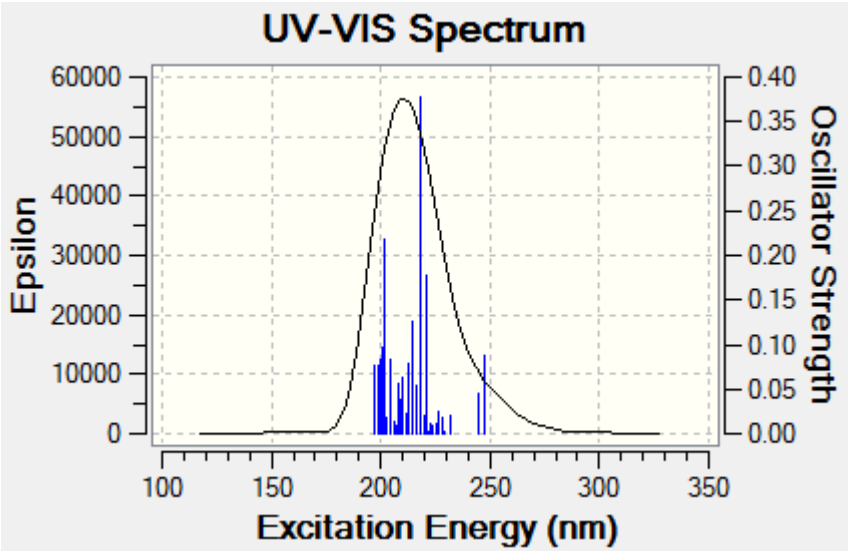

Figure S3. Theoretical UV-Vis absorption spectra of **3**.

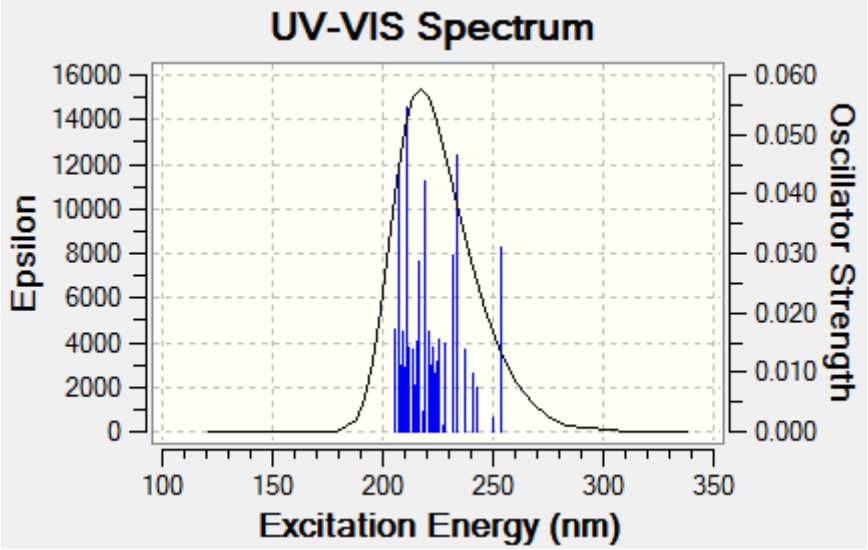

Figure S4. Theoretical UV-Vis absorption spectra of **4**.

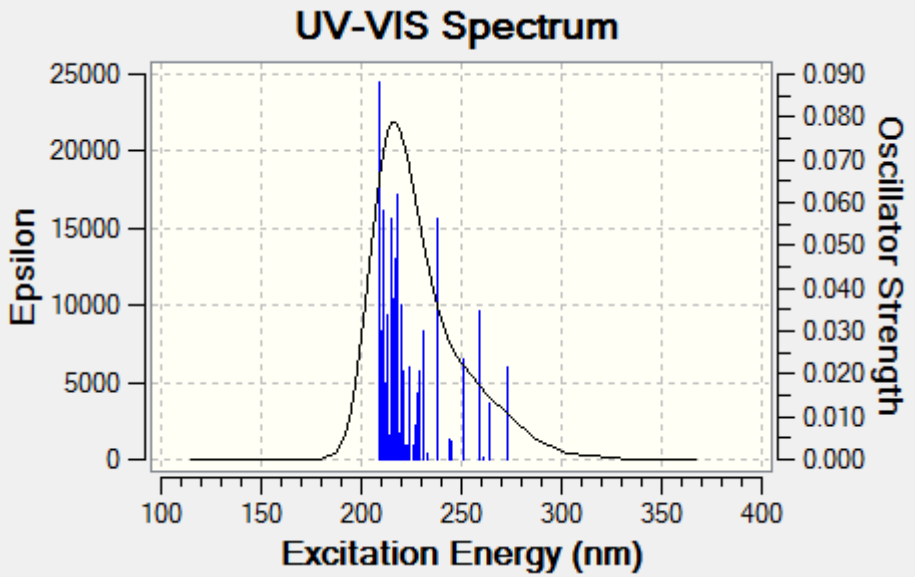

Figure S5. Theoretical UV-Vis absorption spectra of **5**.

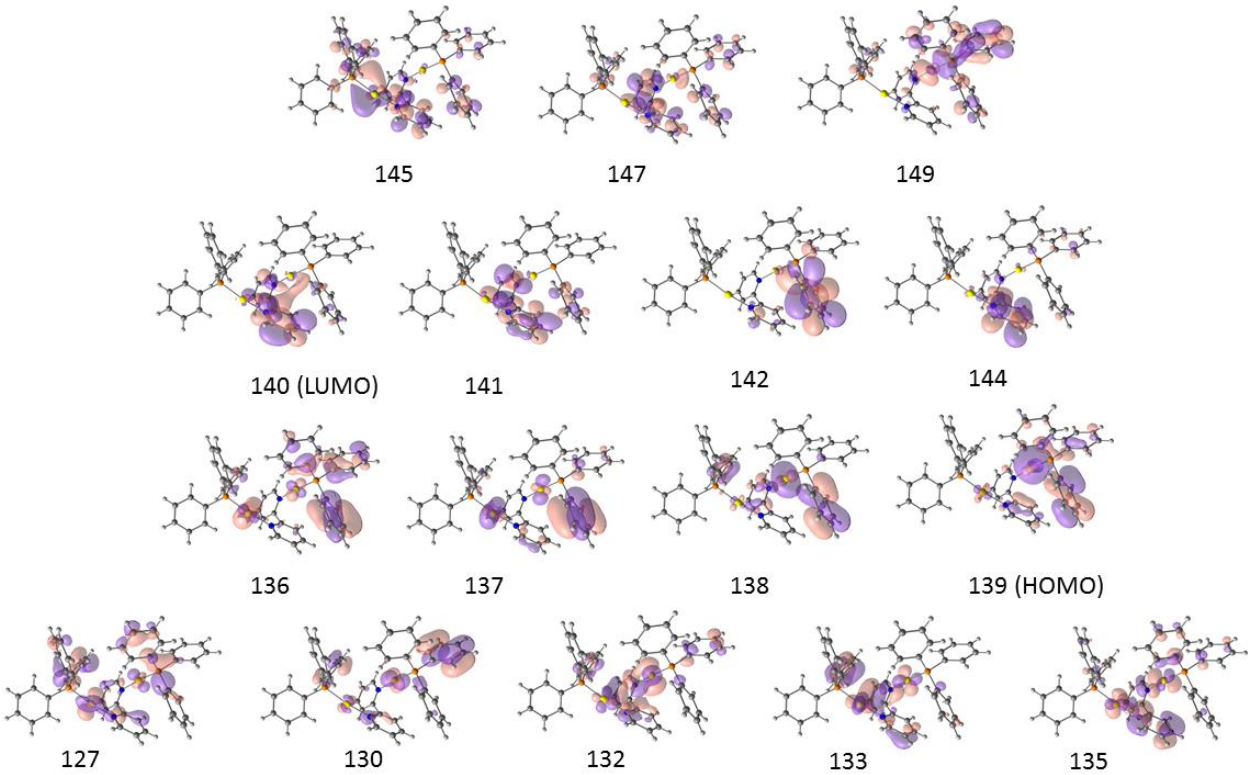

Figure S6. Plots of molecular orbitals involving in main contributing transitions in **1**.

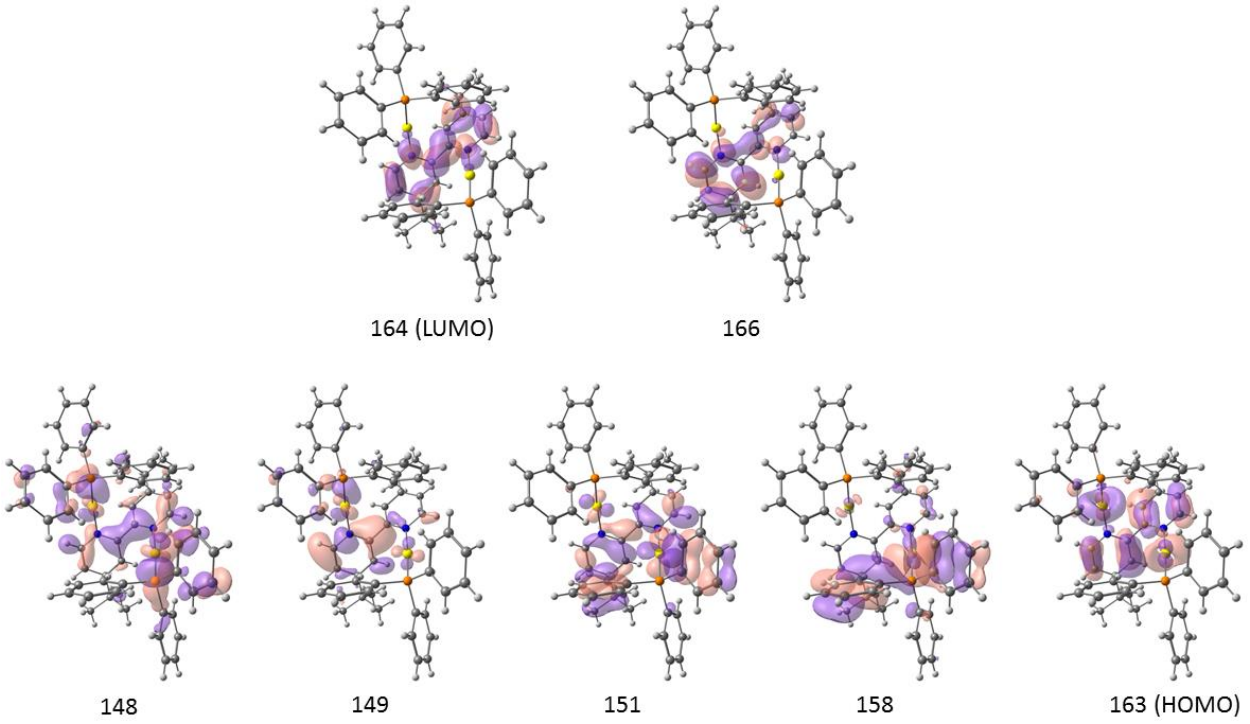

Figure S7. Plots of molecular orbitals involving in main contributing transitions in **2**.

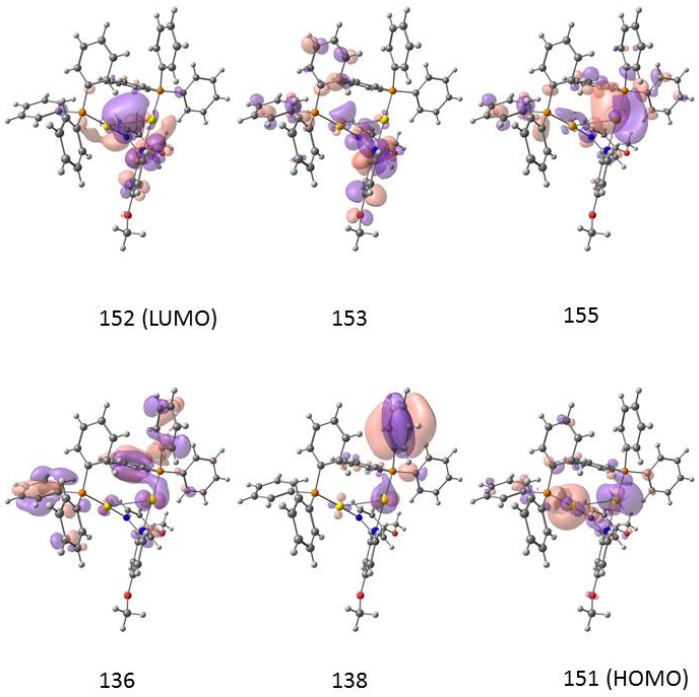

Figure S8. Plots of molecular orbitals involving in main contributing transitions in **3**.

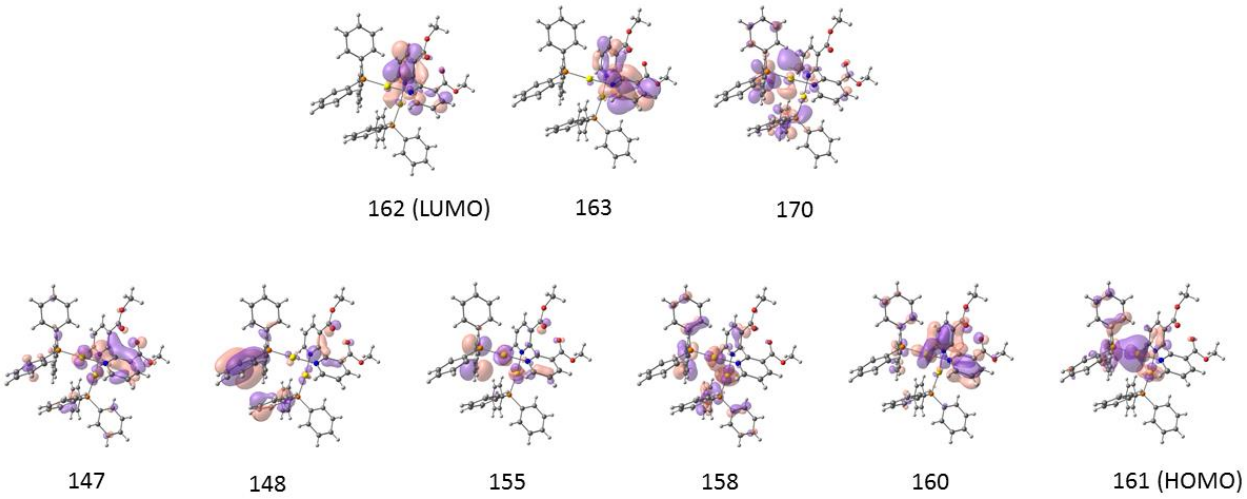

Figure S9. Plots of molecular orbitals involving in main contributing transitions in **4**.

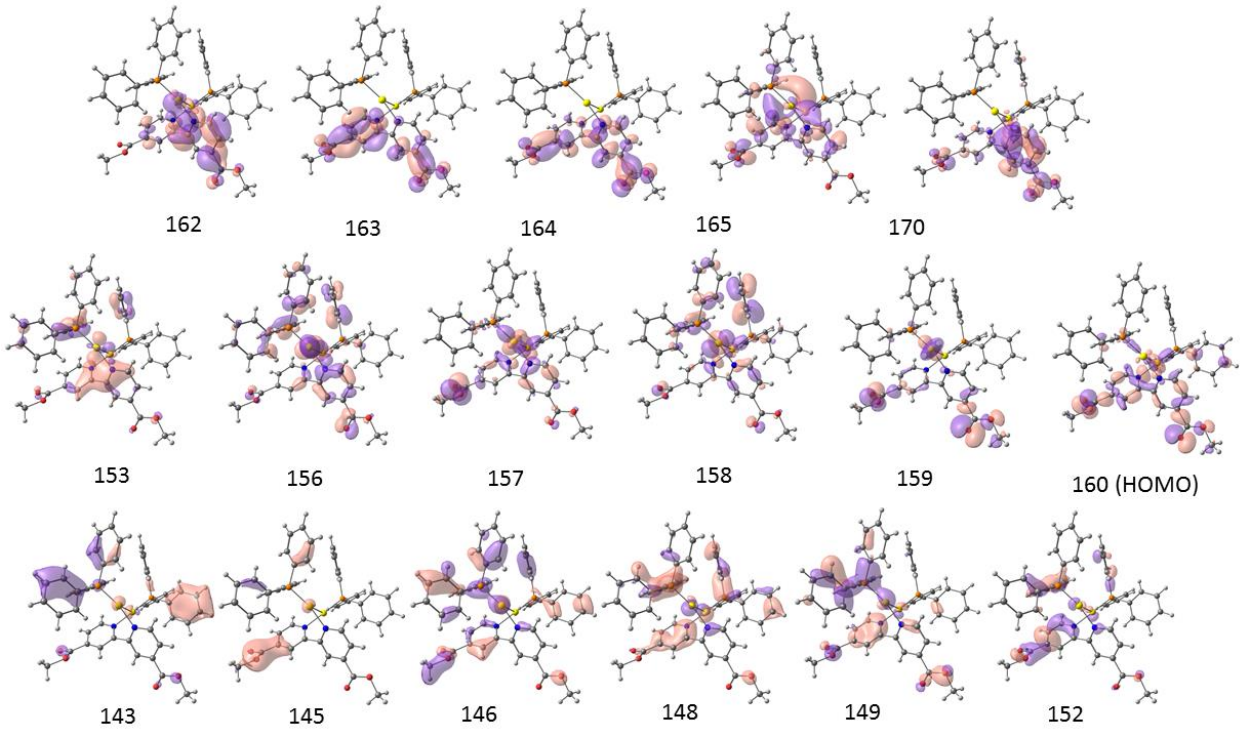

Figure S10. Plots of molecular orbitals involving in main contributing transitions in **5**.

Table S1. Cartesian atomic coordinates for model structures.

Atom	X	Y	Z
1			
Au	3.468532	1.099026	16.182974
Au	6.732465	4.156441	15.933158
P	6.590749	5.590138	14.220716
P	1.843309	1.398583	17.695307
N	6.677564	2.655476	17.365491
C	-1.614653	-1.631198	17.489226
H	-2.330848	-2.253154	17.438025
C	0.080996	-0.345980	16.390549
H	0.520694	-0.085034	15.588408
C	3.904027	8.067329	15.944678
H	3.690948	8.351857	16.825753
C	3.217745	8.601479	14.860935
H	2.506469	9.211761	15.010270
C	5.055174	0.646562	13.644924
H	4.195675	0.498099	13.267321
C	1.939756	4.096772	17.088155
H	2.807808	3.910480	16.751085
C	6.445942	1.366800	16.981488
N	5.146177	0.914751	14.944136
C	6.281050	0.346935	17.854029
H	6.077810	-0.530984	17.553226
C	7.390754	0.818263	13.365455
H	8.169615	0.800052	12.821450

C	2.577875	1.230569	19.321776
C	-0.215434	-0.162457	18.769237
H	0.022400	0.220995	19.605511
C	3.635023	-0.172361	20.970857
H	3.904488	-1.036031	21.258860
C	6.361658	1.154312	15.513741
C	-1.244437	-1.087545	18.703103
H	-1.696569	-1.350074	19.496710
C	10.444797	6.945297	14.054528
H	11.281312	6.726814	14.447065
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H	2.002186	6.069648	16.708418
C	-0.924237	-1.255098	16.341482
H	-1.162369	-1.642956	15.507341
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H	11.113747	8.506833	12.972918
C	4.919237	4.166670	12.520647
H	4.234926	4.367299	13.147853
C	1.145081	3.048429	17.608693
C	8.077486	6.547009	13.811325
C	4.621865	3.407132	11.411304
H	3.734820	3.093717	11.274769
C	6.752157	2.916988	18.668970
H	6.888296	3.814148	18.952705
C	9.162465	8.304881	12.597448

H	9.120565	9.018674	11.970242
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C	4.889706	7.128102	15.750543
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C	6.638146	1.919491	19.624712
H	6.710945	2.126573	20.548453
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H	7.173912	7.811587	12.503580
C	6.418418	0.629129	19.217241
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H	2.844482	-0.809053	19.215108
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H	-0.675000	2.675412	18.427901
C	6.173940	0.573985	12.819316
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C	6.926087	3.561957	10.715831
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2			
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Au	3.342279	14.326279	3.789282
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P	1.924799	12.614473	3.767410
N	4.997392	15.593256	4.019443
N	4.640198	15.138486	7.437319
C	3.777977	10.859800	2.720646

H	4.336727	11.209782	3.376790
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H	3.081891	17.144981	5.463777
C	9.494565	13.303462	8.329552
H	8.836703	13.926802	8.544179
C	4.394946	15.896228	6.348856
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C	5.166438	8.454311	10.022170
C	5.729085	8.127426	8.792183
H	6.130333	8.795168	8.249037
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C	4.859904	10.090407	11.727216

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C	7.537507	5.734352	4.731934
H	7.967096	5.475973	3.924405
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H	10.612956	4.957471	13.191015
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H	11.748663	6.821453	14.012696
C	10.674481	8.174154	12.971555
H	11.146386	8.932139	13.295859
C	6.519205	5.184530	12.968685

H	7.017169	5.965600	13.177596
C	7.029440	4.260996	12.058753
C	6.281060	3.116258	11.747309
H	6.624937	2.475244	11.135186
C	5.043506	2.919224	12.334316
H	4.527216	2.155100	12.105613
C	4.554622	3.831099	13.251424
H	3.713014	3.679243	13.666362
C	5.287827	4.969378	13.572914
H	4.947107	5.596330	14.200007
C	9.645716	3.140294	11.480358
C	10.701650	2.939623	10.603436
H	10.778606	3.470528	9.819373
C	11.633328	1.970175	10.874693
H	12.368049	1.849297	10.285605
C	11.520007	1.182908	11.972639
H	12.169810	0.511773	12.146287
C	10.462061	1.355818	12.836644
H	10.386950	0.793977	13.599408
C	9.506227	2.332148	12.615620
H	8.778044	2.449116	13.213879
C	9.615726	8.355166	12.080281
H	9.322630	9.228146	11.849454
N	7.393641	5.569219	7.118712
N	5.098654	5.827165	9.113673

O	5.294792	9.730598	10.398199
O	5.915272	7.174559	3.626811
P	5.237930	1.674291	7.912390
P	8.569620	4.552312	11.150687
Au	5.217601	3.821761	8.550348
Au	8.097598	4.950135	9.002156
4			
Au	1.780649	9.503966	16.587017
Au	1.958804	7.389886	13.930619
P	1.436486	8.303380	18.451862
P	3.948426	6.377636	13.793089
N	1.953768	10.521023	14.758170
O	-0.741484	12.309558	14.824349
O	0.273931	11.031409	10.374242
O	-1.253260	10.806367	12.002613
N	0.053625	8.204187	14.283282
O	-2.927201	11.785189	14.811415
C	0.953195	10.389057	13.852154
C	5.537491	5.733099	16.029352
H	5.524674	4.832932	15.727562
C	4.970082	8.053431	15.738341
H	4.562073	8.743850	15.227454
C	4.920439	6.729400	15.285656
C	2.822314	8.352758	19.609873
C	3.589434	9.508554	19.674542

H	3.352785	10.266704	19.155033
C	-1.147557	9.257294	18.540675
H	-1.092402	9.235445	17.592193
C	-0.195855	9.523848	14.276815
C	2.333794	5.864191	17.549080
H	3.176047	6.301165	17.488722
C	3.032146	11.256450	14.444956
H	3.714130	11.372248	15.095959
C	1.042399	10.970232	12.586792
C	4.843212	3.775455	13.324022
H	5.682927	4.166547	13.112769
C	3.177391	7.236289	20.370815
H	2.656023	6.443182	20.327702
C	3.764787	4.586042	13.673236
C	-1.416267	10.030738	14.699321
C	3.183617	11.846365	13.214084
H	3.962089	12.355440	13.017921
C	-1.631788	11.498971	14.774769
C	-0.125185	10.898132	11.640466
C	1.210019	6.565534	18.014698
C	-0.911530	7.354272	14.679921
H	-0.727840	6.423518	14.688543
C	2.185712	11.693424	12.256979
H	2.283717	12.075776	11.394722
C	4.691148	9.552252	20.497998

H	5.206002	10.347544	20.554044
C	4.298399	7.295281	21.187803
H	4.543897	6.539316	21.707313
C	5.617972	8.368052	16.934722
H	5.657294	9.270403	17.232200
C	5.056630	8.442338	21.248161
H	5.826199	8.477296	21.804317
C	-0.053545	8.848724	19.310239
C	3.467298	1.833106	13.561142
H	3.368407	0.889242	13.513718
C	2.530163	3.998312	13.938380
H	1.780531	4.544530	14.143166
C	-2.308122	9.694268	19.150722
H	-3.049794	9.963007	18.620434
C	4.697375	2.409912	13.283065
H	5.440248	1.859324	13.065345
C	2.389898	2.617474	13.901734
H	1.554606	2.217643	14.112987
C	-0.143897	8.898976	20.687694
H	0.591180	8.623682	21.222293
C	0.996479	3.897808	17.249446
H	0.920329	2.991087	16.975679
C	6.180998	6.063014	17.230045
H	6.607768	5.381335	17.736621
C	6.199179	7.367382	17.689196

H	6.612425	7.574944	18.519119
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C	-2.146648	7.786877	15.067936
H	-2.818446	7.162004	15.315835
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H	-3.257475	9.460487	15.382660
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H	3.412488	6.888895	11.047664
C	2.211396	4.535790	17.180465
H	2.974999	4.061673	16.874364
C	-0.011207	5.912258	18.118169
H	-0.770632	6.371081	18.456605
C	-1.322691	9.355613	21.299896
H	-1.385590	9.399311	22.248379
C	-2.389749	9.740150	20.515243
H	-3.190510	10.041663	20.926970
C	-0.116195	4.575118	17.719375
H	-0.952999	4.129404	17.771111
C	-0.797473	10.983341	9.387820
H	-0.452897	11.269559	8.516941
H	-1.523183	11.581996	9.665898
H	-1.137117	10.065696	9.320995
C	-3.258534	13.190060	14.979555
H	-2.938497	13.696950	14.203524
H	-2.829966	13.530900	15.792232

H	-4.231139	13.288379	15.057158
C	6.335806	7.052760	12.502722
H	6.751469	6.967550	13.354201
C	6.519904	7.476625	10.163851
H	7.045259	7.690742	9.402909
C	7.106592	7.356457	11.379633
H	8.044824	7.476625	11.468014
C	5.157105	7.290911	10.034512
H	4.759057	7.363012	9.174411
5			
Au	9.705586	9.247757	4.990704
Au	10.505596	11.997379	3.650453
P	8.159468	8.209085	3.754001
P	9.277692	13.704359	4.418562
N	11.668315	10.393841	2.910162
O	15.032915	11.671808	8.776851
C	12.650272	10.782292	7.761462
H	12.668640	11.039864	8.674848
C	7.896991	4.152163	3.335172
H	7.242331	3.513402	3.070893
C	7.513357	13.330317	4.424744
C	9.103795	3.740910	3.716909
H	9.291766	2.812096	3.778729
C	13.754672	10.466152	5.675048
H	14.537396	10.485630	5.135671
C	8.521498	6.429467	3.656635
C	6.268021	8.408079	5.729140

H	7.011947	8.447812	6.321063
N	11.439529	10.029188	5.886780
C	9.727985	14.146480	6.112422
C	9.490451	15.198439	3.440266
C	7.572072	5.509581	3.316626
H	6.700094	5.792297	3.070893
O	16.179713	11.123139	7.019626
C	8.175009	8.877673	2.061687
C	11.510513	10.385200	7.197358
H	10.723676	10.350452	7.727461
C	8.645819	8.710900	-0.293644
H	8.906919	8.189504	-1.043207
C	5.727913	11.930816	5.143398
H	5.429190	11.185064	5.650320
C	8.793689	14.641509	7.005717
H	7.885828	14.716851	6.736801
C	8.553053	8.125675	0.962842
H	8.752599	7.202810	1.069481
C	6.474100	8.342466	4.362925
C	12.487325	9.704387	3.701454
C	4.988695	8.417749	6.232970
H	4.856319	8.440554	7.172630
C	11.499619	10.022925	1.639767
H	10.894367	10.511619	1.094209
C	7.065440	12.286011	5.225309
H	7.658339	11.828677	5.811051
C	12.575064	10.094746	5.143398
C	11.039300	14.025786	6.504977

H	11.691376	13.685260	5.903781
C	9.035788	16.439539	3.869913
H	8.596384	16.518454	4.710660
C	13.821164	10.813640	6.994898
C	9.810461	6.004766	4.007462
H	10.483663	6.636940	4.230012
C	11.403491	14.413773	7.804736
H	12.310187	14.337838	8.082925
C	12.182698	8.944184	1.089572
H	12.072260	8.702816	0.177732
C	5.369054	8.302273	3.529904
H	5.488912	8.282750	2.587154
C	8.357666	10.058014	-0.454375
H	8.443910	10.462469	-1.309032
C	10.083900	15.129228	2.213145
H	10.384945	14.294283	1.874682
C	10.080505	4.657582	4.024462
H	10.956234	4.356861	4.248558
C	3.886189	8.394353	5.392223
H	3.001619	8.447096	5.732231
C	10.241628	16.289494	1.452763
H	10.681830	16.235057	0.615106
C	9.802913	17.486335	1.885501
H	9.919271	18.259617	1.347669
C	10.455174	14.901030	8.674848
H	10.709967	15.152744	9.555779
C	13.182801	8.623550	3.225442
H	13.771287	8.141306	3.794184

C	15.174524	11.246218	7.576003
C	7.850759	10.216263	1.910228
H	7.571622	10.734331	2.656701
C	9.155695	15.027011	8.282293
H	8.508654	15.376448	8.881944
C	9.212288	17.578290	3.060075
H	8.896910	18.422556	3.362991
C	6.598984	13.998439	3.608724
H	6.898014	14.708135	3.052347
C	13.014412	8.248987	1.908683
C	7.947748	10.803174	0.613560
H	7.725325	11.718997	0.493012
C	4.126613	8.283935	4.044553
H	3.390527	8.207189	3.452630
C	4.804559	12.602835	4.362925
H	3.889075	12.350017	4.361379
C	5.242711	13.632237	3.602543
H	4.627702	14.113684	3.060075
C	16.354305	11.985348	9.303864
H	17.041126	11.655215	8.677939
H	16.476407	11.558513	10.170885
H	16.448922	12.957262	9.395048
O	13.573862	6.622635	0.191641
C	13.520591	6.977754	1.247212
O	13.772747	6.055629	2.080233
C	14.219481	4.802492	1.452763
H	14.056971	4.853483	0.482194
H	13.714641	4.053092	1.823681

H	15.173938	4.677123	1.615039

Table S2. Calculated energies of HOMOs and LUMOs in model structures.

Complex	HOMO, eV	LUMO, eV	HOMO-LUMO gap, eV
1	-13.2	-5.5	7.8
2	-13.1	-5.2	7.9
3	-13.0	-4.9	8.1
4	-13.2	-5.3	7.9
5	-13.2	-5.9	7.3

Table S3. Experimental details

	1	**2**	**3**	**4**
Chemical formula	$C_{48}H_{38}Au_2F_6N_2O_6P_2S_2$	$C_{56}H_{54}Au_2F_6N_2O_6P_2S_2$	$C_{50.50}H_{43}Au_2ClF_6N_2O_8P_2S_2$	$C_{52}H_{42}Au_2F_6N_2O_{10}P_2S_2$
M_r	1372.79	1485.00	1475.31	1488.87
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/c$
a, b, c (Å)	10.5373(8), 10.6701(7), 21.6072(17)	13.399(3), 20.709(4), 20.441(4)	12.9143(6), 14.7849(7), 14.8938(6)	11.0607(5), 21.8487(10), 22.2046(11)
α, β, γ (°)	93.626(2), 98.353(2), 90.210(2)	90, 90.35 (3), 90	99.471(2), 100.075(1), 101.094(2)	90, 103.878 (2), 90
V (Å^3)	2398.6 (3)	5672 (2)	2689.2 (2)	5209.4 (4)
Z	2	4	2	4
μ (mm^{-1})	6.34	5.37	5.71	5.85
Crystal size (mm)	0.16 × 0.11 × 0.03	0.15 × 0.12 × 0.12	0.14 × 0.12 × 0.08	0.15 × 0.10 × 0.10
T_{min}, T_{max}	0.552, 0.745	0.542, 0.746	0.424, 0.746	0.620, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23514, 7904, 5712	65621, 17312, 13123	41670, 16266, 13216	68561, 13432, 11267
R_{int}	0.084	0.057	0.041	0.054
θ values (°)	θ_{max} = 24.5, θ_{min} = 1.9	θ_{max} = 30.5, θ_{min} = 2.0	θ_{max} = 30.5, θ_{min} = 2.2	θ_{max} = 28.7, θ_{min} = 1.9
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.583	0.715	0.715	0.676
Range of h, k, l	$-12 \le h \le 11$, $-12 \le k \le 12$, $-25 \le l \le 25$	$-17 \le h \le 19$, $-29 \le k \le 29$, $-29 \le l \le 27$	$-18 \le h \le 18$, $-21 \le k \le 21$, $-18 \le l \le 21$	$-14 \le h \le 14$, $-29 \le k \le 28$, $-29 \le l \le 29$
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.102, 1.01	0.043, 0.088, 1.05	0.033, 0.071, 1.04	0.033, 0.079, 1.06
No. of reflections, parameters, restraints	7904, 613, 6	17312, 691, 18	16266, 670, 60	13432, 678, 36
Weighting scheme	$w = 1/[\sigma^2(F_o^2)]$	$w = 1/[\sigma^2(F_o^2) + (0.026P)^2 + 15.2597P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0223P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.030P)^2 + 9.1876P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.19, -1.31	2.29, -1.66	1.07, -0.95	1.24, -1.22

	5
Chemical formula	$C_{52}H_{42}Au_2F_6N_2O_{10}P_2S_2$
M_r	1488.87
Crystal system, space group	Triclinic, $P\bar{1}$
a, *b*, *c* (Å)	13.7418 (10), 14.3338 (11), 15.9801 (13)
a, b, g (°)	75.497 (2), 82.103 (2), 67.250 (2)
V (Å^3)	2807.4 (4)
Z	2
μ (mm^{-1})	5.43
Crystal size (mm)	0.15 × 0.12 × 0.11
T_{min}, T_{max}	0.661, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	45120, 12919, 9744
R_{int}	0.056
θ values (°)	θ_{max} = 27.9, θ_{min} = 2.0
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.658
Range of *h*, *k*, *l*	$-18 \le h \le 17$, $-18 \le k \le 18$, $-21 \le l \le 21$
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.085, 0.195, 1.22
No. of reflections, parameters, restraints	12919, 677, 73
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + 95.3723P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	4.90, -6.54

Computer programs: *APEX2* (Bruker-AXS, 2004), *SAINT* (Bruker-AXS, 2004), *SHELXS2014* (Sheldrick, 2014), *SHELXL2014* (Sheldrick, 2014), ShelXle (Hübschle, 2011), CIFTAB-2014 (Sheldrick, 2014).

Table S4. Selected geometric parameters (Å)

1			
Au1—P1	2.240 (2)	Au1—N1	2.095 (7)
Au2—P2	2.238 (2)	Au2—N2	2.075 (7)
Au1—Au2	4.479 (1)		
N1—Au1—P1	173.0 (2)	N2—Au2—P2	171.8 (2)
2			
Au1—P1	2.2349 (13)	Au1—N1	2.089 (4)
Au2—P2	2.2224 (12)	Au2—N2	2.098 (4)
Au1—Au2	4.589 (1)		
N1—Au1—P1	171.66 (10)	N2—Au2—P2	165.90 (11)
3			
P1—Au1	2.2385 (8)	N1—Au2	2.104 (3)
P2—Au2	2.2351 (8)	N2—Au1	2.087 (3)
Au1—Au2	3.1262 (2)		
N2—Au1—P1	177.32 (7)	N1—Au2—P2	169.44 (7)
4			
Au1—P1	2.2445 (10)	Au1—N1	2.102 (3)
Au2—P2	2.2367 (11)	Au2—N2	2.102 (4)
Au1—Au2	3.400 (1)		
N1—Au1—P1	174.43 (9)	N2—Au2—P2	172.88 (10)
5			
Au1—P1	2.235 (3)	Au1—N1	2.104 (12)
Au2—P2	2.239 (4)	Au2—N2	2.113 (11)
Au1—Au2	3.1618 (8)		
N1—Au1—P1	168.2 (3)	N2—Au2—P2	179.5 (4)

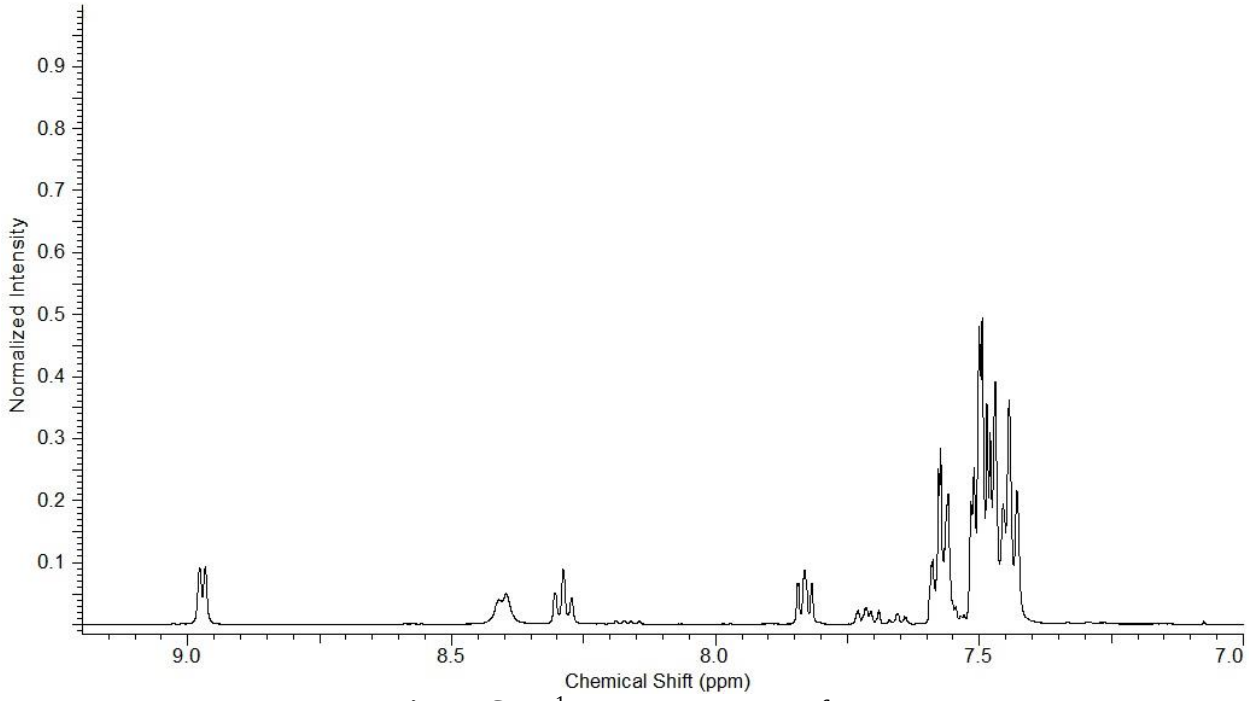

Figure S11. ^{1}H NMR spectrum of **1.**

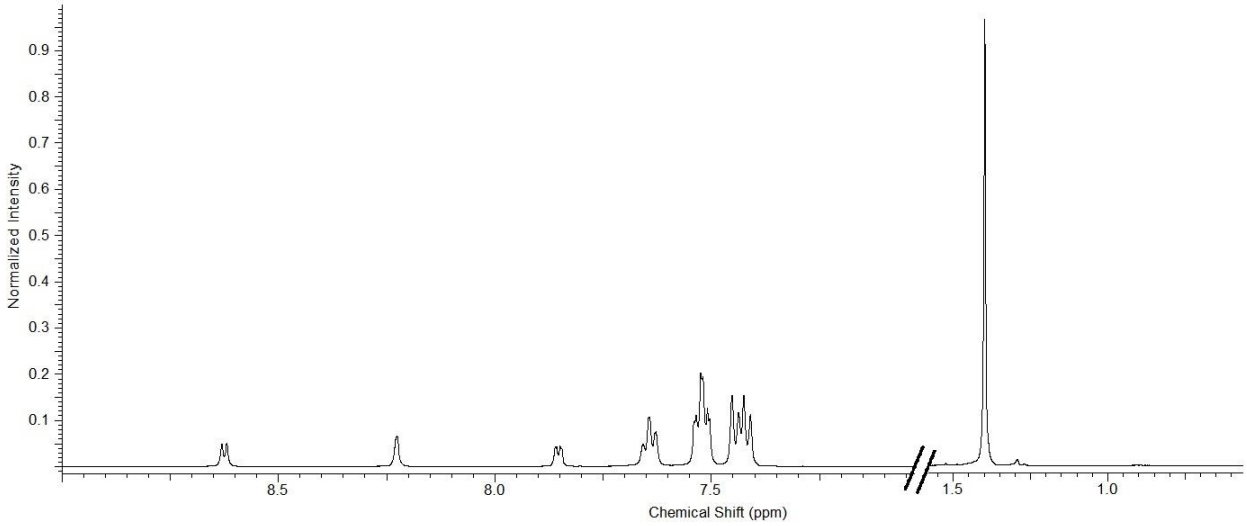

Figure S12. ^{1}H NMR spectrum of **2**.

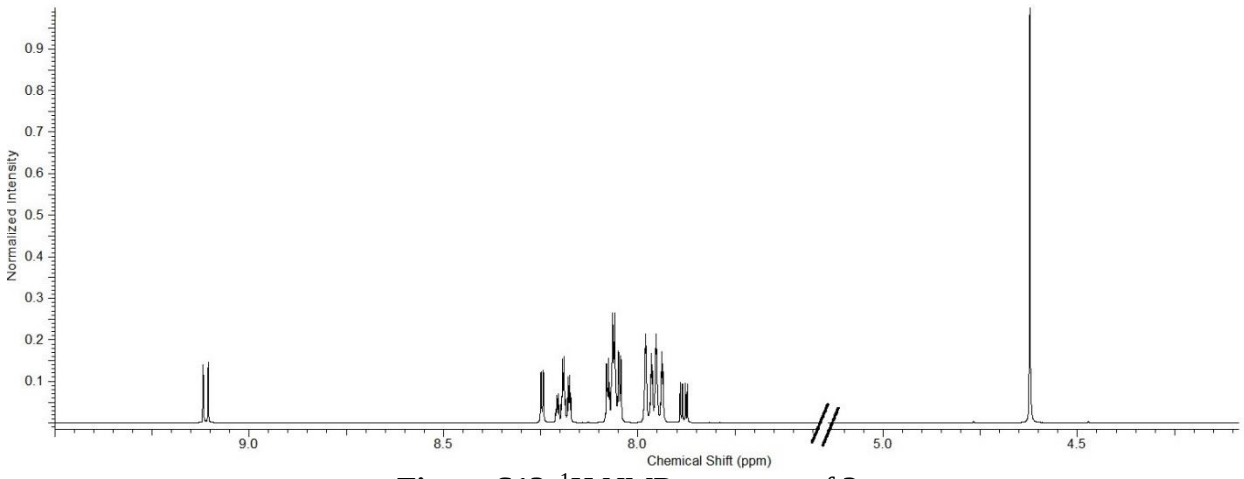

Figure S13. ^{1}H NMR spectrum of **3**.

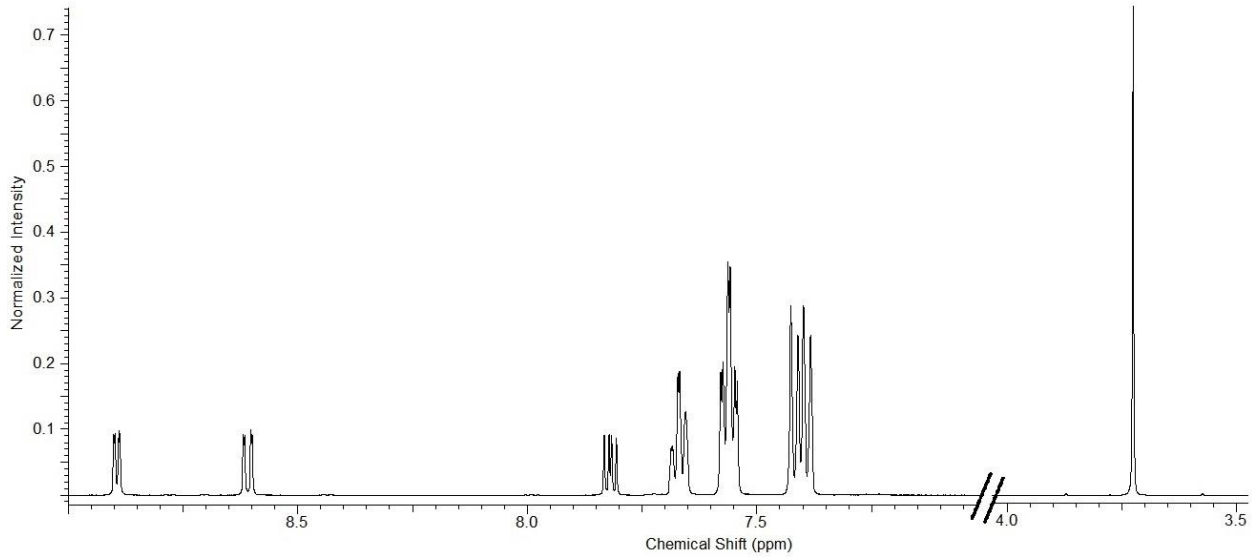

Figure S14. ^{1}H NMR spectrum of **4**.

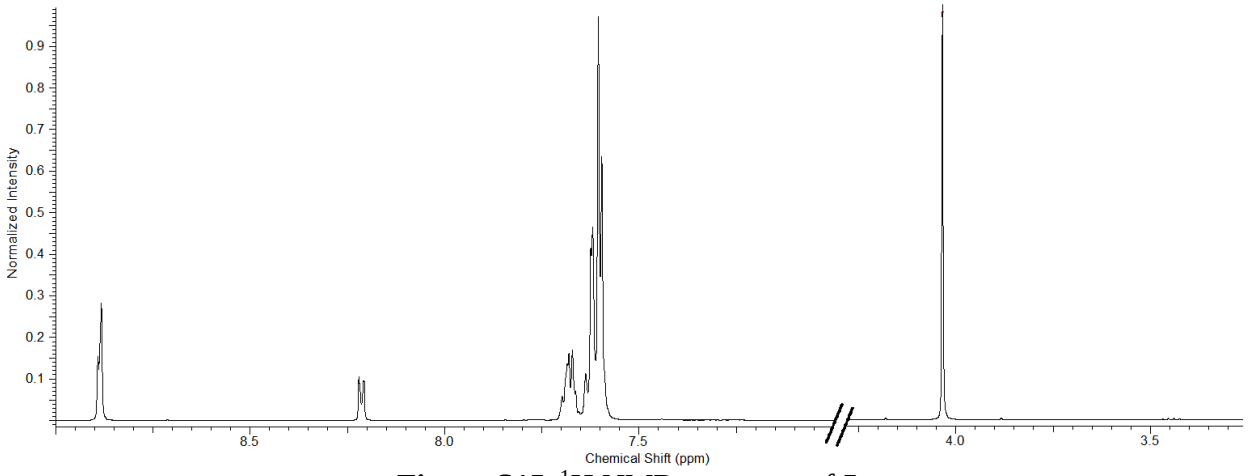

Figure S15. ^{1}H NMR spectrum of **5**.

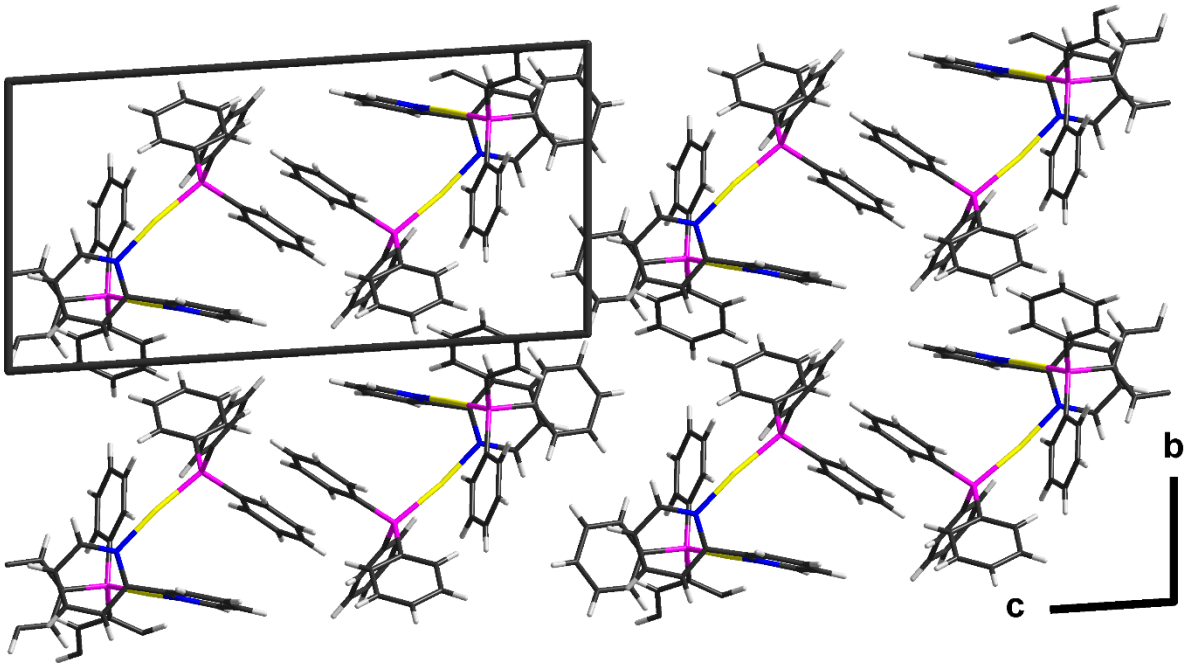

Figure S16. Crystal packing of **1**.

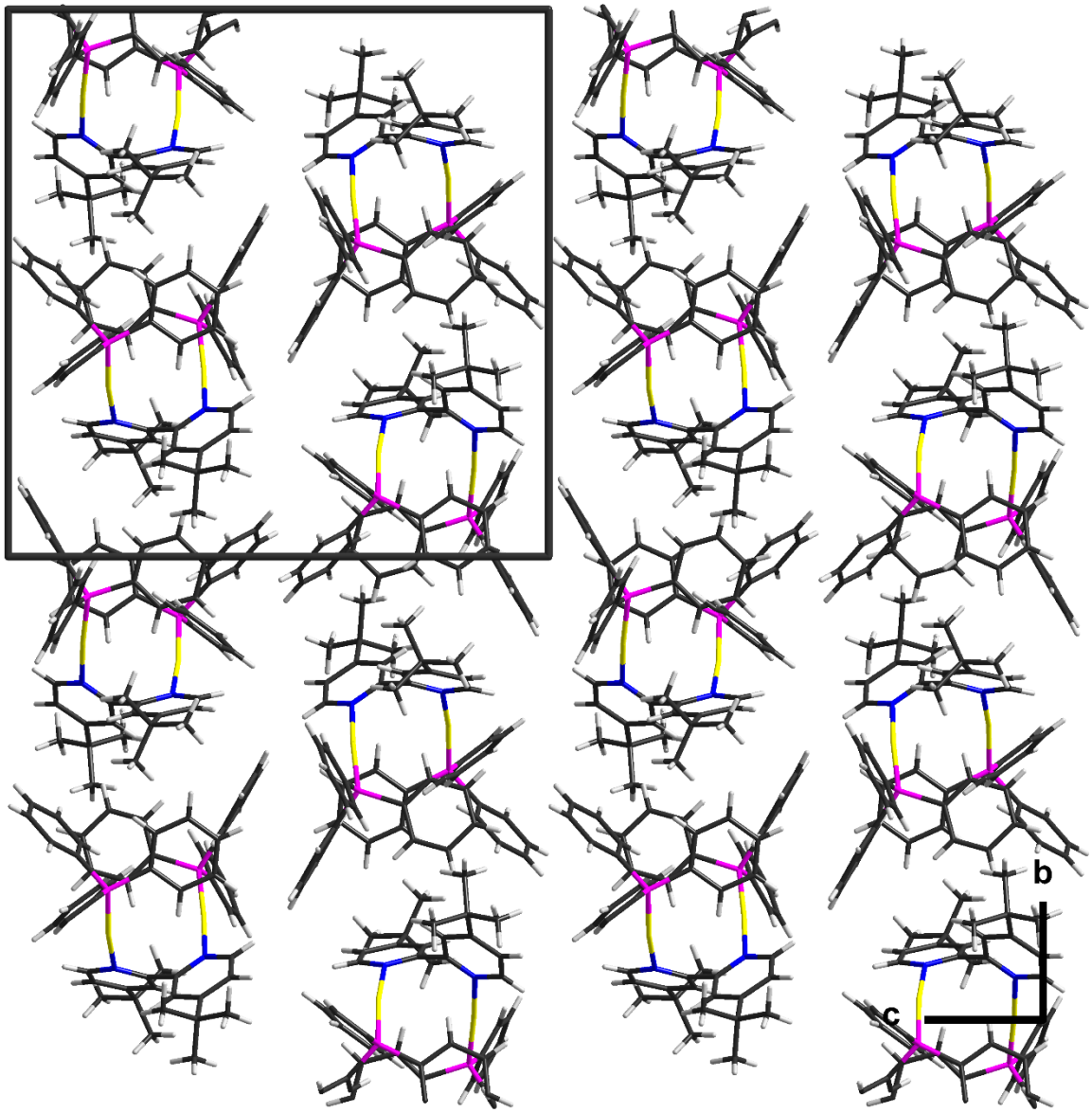

Figure S17. Crystal packing of **2**.

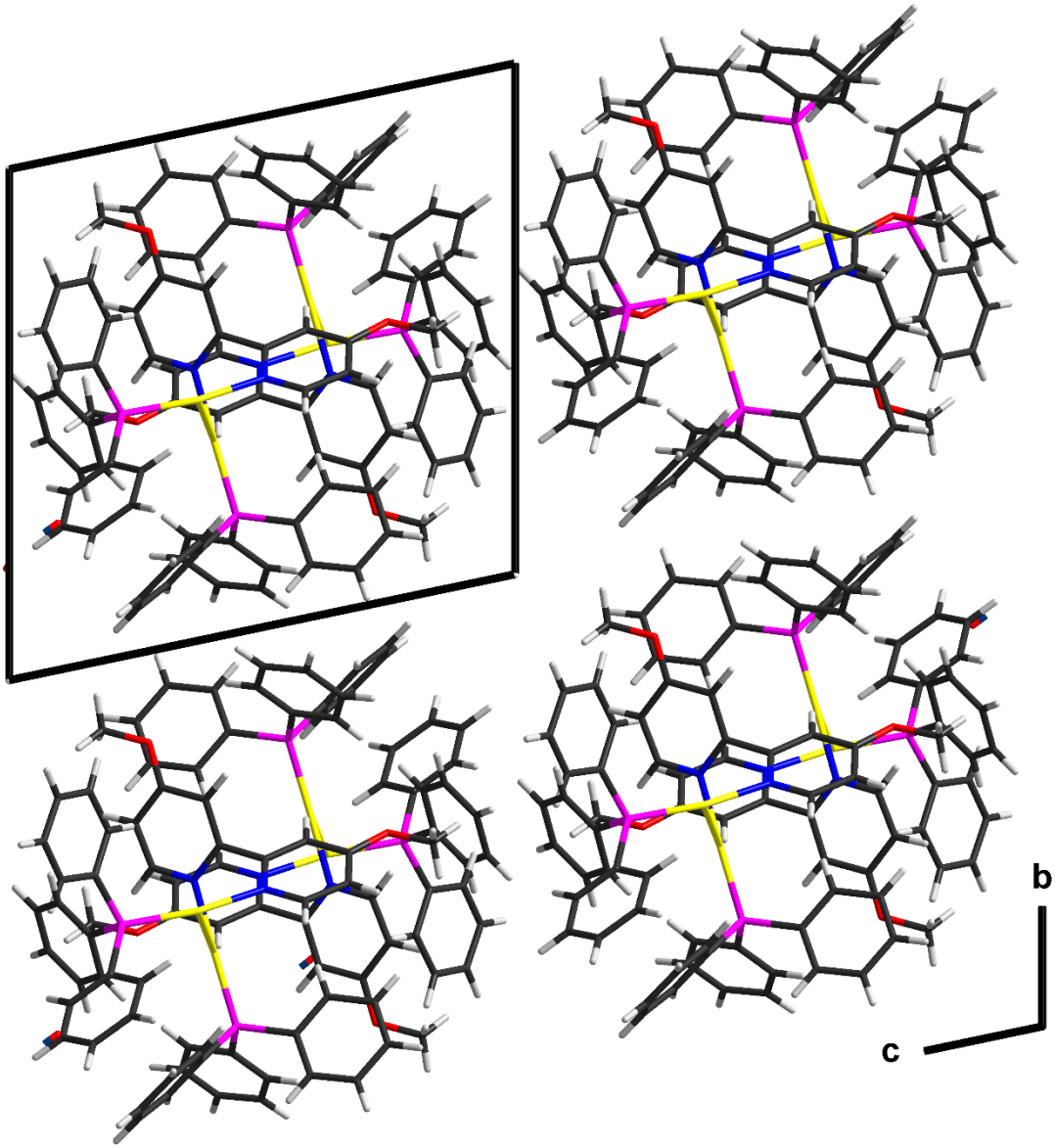

Figure S18. Crystal packing of **3**.

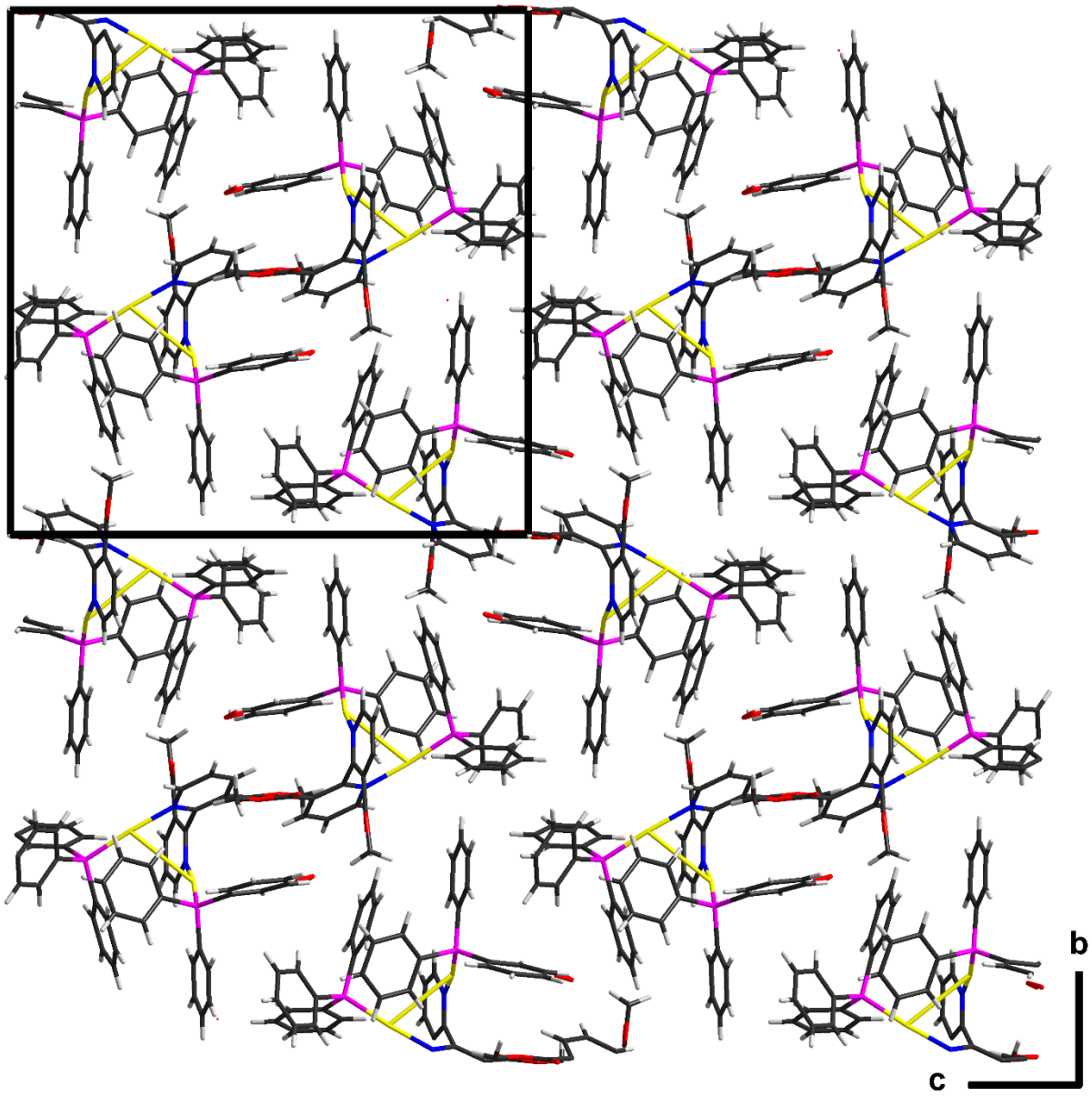

Figure S19. Crystal packing of **4**.

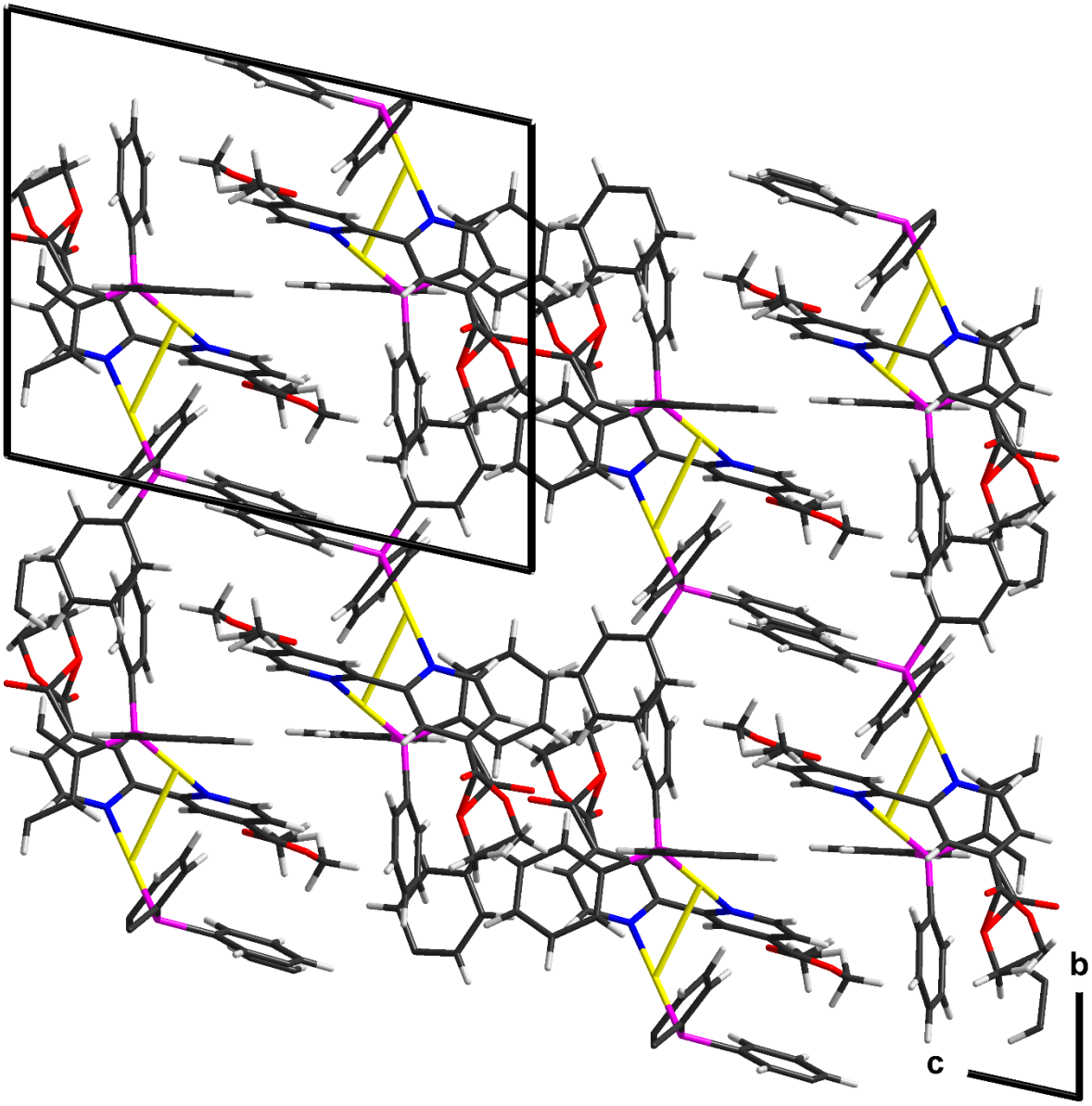

Figure S20. Crystal packing of **5**.