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Electronic Supplementary Material (ESM) for

Enhancing the Charge Transport and Luminescent Properties of Ethyl 4-[(E)-(2-hydroxy-4-methoxyphenyl)methyleneamino]benzoate Through Complexation: A DFT and TD-DFT study

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A. Cartesian coordinates of atoms in the optimized geometries of EMAB, $[Ir(EMAB)_2]^+$, $[Pd(EMAB)_2]$, $[Rh(EMAB)_2]^+$, $[Zn(EMAB)_2]$, $[Pt(EMAB)_2]$, [Ni(EMAB)2] and $Cu[EMAB]_2$ in gas phase at the PBE0-D3(BJ)/def2-TZVP level of theory

ESM Table S1 Cartesian coordinates of atoms in the optimized geometries of EMAB in gas phase

C	4.793718	1.174157	-0.292323
C	3.418777	0.989931	-0.226238
C	2.887329	-0.293323	0.104518
C	3.787714	-1.338908	0.359959
C	5.155734	-1.164479	0.294412
C	5.654835	0.108980	-0.036077
H	5.196912	2.149066	-0.543129
H	3.387414	-2.317494	0.615302
H	5.816398	-1.997679	0.496289
O	6.975378	0.400674	-0.129559
C	7.916494	-0.642104	0.121769

H	7.797575	-1.466656	-0.592537
H	7.824834	-1.022815	1.146950
H	8.899743	-0.188254	-0.009400
O	2.617461	2.030938	-0.472895
H	1.676564	1.702110	-0.362416
C	1.475900	-0.524535	0.183712
N	0.610783	0.417358	-0.027421
H	1.154958	-1.540386	0.458598
C	-0.759317	0.146544	-0.009361
C	-1.620060	1.138595	0.481213
C	-1.305706	-1.049431	-0.503197
C	-2.986900	0.925305	0.520886
H	-1.191296	2.068561	0.842366
C	-2.673776	-1.254826	-0.469299
H	-0.656161	-1.797364	-0.948611
C	-3.527943	-0.277029	0.050025
H	-3.644718	1.691976	0.914443
H	-3.108654	-2.171407	-0.855595
C	-4.982980	-0.559361	0.059287
O	-5.481470	-1.588604	-0.349497
O	-5.697412	0.463038	0.585241
C	-7.137107	0.283051	0.613597
C	-7.757724	0.627867	-0.725158
H	-7.359334	-0.748978	0.902427
H	-7.475448	0.963913	1.399687
H	-7.417691	-0.065299	-1.498594
H	-8.848181	0.555617	-0.653305

H	-7.499149	1.649073	-1.021048

ESM Table S2 Cartesian coordinates of atoms in the optimized geometries of [Ir(EMAB)2]+ in gas phase

H	-6.04543	-2.17159	-0.81777
C	-6.11235	-3.01076	-0.11801
H	-6.02540	-2.65116	0.91312
H	-7.05966	-3.53160	-0.25039
O	-5.09514	-3.99742	-0.39222
C	-3.81520	-3.63349	-0.34178
C	-3.38002	-2.35164	-0.01009
C	-2.88239	-4.65876	-0.65804
C	-1.54937	-4.37227	-0.65801
C	-2.01633	-2.05110	-0.03251
C	-1.05934	-3.06530	-0.37293
H	-4.06358	-1.55252	0.24989
H	-3.25744	-5.64793	-0.89502
H	-0.83288	-5.15345	-0.89765
O	-1.68130	-0.82143	0.27969
C	0.33056	-2.86393	-0.36202
N	0.97587	-1.72047	-0.16374
H	0.95253	-3.75190	-0.49490
C	2.40560	-1.80503	-0.11953
C	3.07914	-1.30839	0.99537
C	3.10937	-2.36109	-1.18792
C	4.49279	-2.42136	-1.13416
C	4.46214	-1.38466	1.04953
C	5.17729	-1.93785	-0.01673
C	6.66608	-2.03784	-0.02100

C	8.65968	-1.63519	1.21364
C	9.08437	-3.01122	1.67967
O	7.20699	-1.54445	1.10745
O	7.29910	-2.50459	-0.94295
H	8.91751	-0.86328	1.94308
H	9.09650	-1.38519	0.24226
H	8.61215	-3.26217	2.63399
H	10.17002	-3.02722	1.81964
H	8.82486	-3.77121	0.93858
H	2.51091	-0.87728	1.81387
H	4.99285	-1.01693	1.92032
H	2.57702	-2.70820	-2.06921
H	5.06619	-2.83493	-1.95760
N	-0.92500	1.83007	-0.08203
O	1.77326	0.93669	-0.36274
C	-2.35934	1.81539	-0.11487
C	-3.09108	2.31573	0.95840
C	-2.99999	1.20319	-1.19152
C	-4.47226	2.16240	0.97536
C	-4.37299	1.03786	-1.16237
C	-5.11491	1.49541	-0.06931
C	-6.56797	1.17139	-0.03166
C	-8.66159	1.65540	0.99405
C	-8.89219	0.50149	1.94589
O	-7.23559	1.93292	0.84660
O	-7.06929	0.30038	-0.71643
H	-5.04840	2.52300	1.82029

H	-4.88914	0.53761	-1.97573
H	-2.57738	2.76689	1.80273
H	-2.41052	0.83128	-2.02412
H	-9.07060	2.59011	1.38446
H	-9.08122	1.45496	0.00414
H	-9.96771	0.36590	2.09792
H	-8.43203	0.69940	2.91845
H	-8.48700	-0.42807	1.53732
C	-0.32944	3.00416	-0.02564
C	1.05939	3.24372	-0.06945
C	2.04935	2.22422	-0.26972
C	3.38748	2.58557	-0.38812
C	3.77710	3.92658	-0.29899
C	1.49551	4.58898	0.00265
C	2.81759	4.94406	-0.09816
C	5.58463	5.49534	-0.35244
H	5.16253	6.10330	-1.15990
H	5.35967	5.94199	0.62214
H	6.66337	5.41241	-0.47955
O	5.08994	4.14627	-0.42030
H	4.13338	1.81475	-0.55028
H	0.74928	5.36622	0.14654
H	3.10459	5.98548	-0.03135
H	-0.97962	3.88193	0.01381
Ir	0.04678	0.05839	-0.05805

ESM Table S3 Cartesian coordinates of atoms in the optimized geometries of [Pd(EMAB)2]in gas phase

H	-6.056745	-2.069830	-0.883104

C	-6.149741	-2.897464	-0.169784
H	-6.059250	-2.510226	0.853345
H	-7.120247	-3.379760	-0.293551
O	-5.177044	-3.917286	-0.420501
C	-3.870840	-3.569358	-0.358775
C	-3.423546	-2.301932	-0.033435
C	-2.957892	-4.608137	-0.662964
C	-1.617675	-4.334885	-0.647265
C	-2.041803	-2.004848	-0.029452
C	-1.108818	-3.042460	-0.356259
H	-4.095755	-1.488926	0.211630
H	-3.341661	-5.593137	-0.902734
H	-0.909467	-5.128280	-0.875553
O	-1.706343	-0.796298	0.301349
C	0.295792	-2.866969	-0.332157
N	0.963174	-1.753188	-0.165670
H	0.890044	-3.780182	-0.439129
C	2.379294	-1.821572	-0.156654
C	3.084519	-1.247349	0.903120
C	3.071799	-2.434545	-1.203931
C	4.456157	-2.489288	-1.178343
C	4.466697	-1.307784	0.928753
C	5.165627	-1.929263	-0.113489
C	6.646021	-2.012984	-0.145197
C	8.661362	-1.477115	0.997840
C	9.134360	-2.802818	1.558995
O	7.213064	-1.422959	0.933153

O	7.281743	-2.542531	-1.034001
H	8.930221	-0.644749	1.654301
H	9.067422	-1.299927	-0.003008
H	8.695661	-2.985393	2.544688
H	10.224443	-2.789243	1.664065
H	8.863760	-3.623353	0.889827
H	2.532429	-0.752389	1.695705
H	5.012768	-0.868826	1.755896
H	2.520157	-2.836179	-2.049128
H	5.010616	-2.953089	-1.987866
N	-0.926957	1.840970	-0.135380
O	1.799646	0.942476	-0.474357
C	-2.345739	1.809645	-0.143803
C	-3.078170	2.297411	0.937860
C	-3.002018	1.204886	-1.218766
C	-4.458600	2.150350	0.961654
C	-4.375024	1.057500	-1.192717
C	-5.114747	1.510527	-0.093276
C	-6.568078	1.222793	-0.070541
C	-8.611446	1.535360	1.105195
C	-8.829248	0.209279	1.805554
O	-7.196057	1.825235	0.964067
O	-7.134093	0.513524	-0.880297
H	-5.026594	2.500234	1.816350
H	-4.896563	0.567667	-2.008740
H	-2.555488	2.736507	1.782789
H	-2.414107	0.818897	-2.045835

H	-8.996040	2.369745	1.697966
H	-9.076211	1.545401	0.114453
H	-9.900078	0.053489	1.973494
H	-8.322807	0.194945	2.775408
H	-8.455191	-0.616111	1.194094
C	-0.319779	2.992674	-0.055359
C	1.077714	3.227160	-0.073629
C	2.064271	2.202639	-0.303865
C	3.416122	2.590829	-0.372830
C	3.796303	3.912386	-0.213705
C	1.512801	4.563933	0.068369
C	2.836694	4.925583	0.013142
C	5.588627	5.492237	-0.130392
H	5.185240	6.149063	-0.911628
H	5.326226	5.888612	0.858836
H	6.674590	5.444937	-0.224313
O	5.130567	4.151167	-0.291166
H	4.166533	1.828143	-0.551850
H	0.761884	5.334478	0.228556
H	3.120628	5.962925	0.132992
H	-0.956168	3.882365	-0.002846
Pd	0.044483	0.061658	-0.111510

ESM Table S4 Cartesian coordinates of atoms in the optimized geometries of [Rh(EMAB)2]+ in gas phase

H	-6.068506	-2.170429	-0.890843
C	-6.138620	-2.977990	-0.154155
H	-6.033586	-2.571383	0.858540
H	-7.097794	-3.485188	-0.250853

O	-5.143550	-3.990974	-0.396183
C	-3.856528	-3.629680	-0.364938
C	-3.401139	-2.349308	-0.094297
C	-2.931017	-4.672283	-0.637966
C	-1.583561	-4.414853	-0.653883
C	-2.021684	-2.076276	-0.137975
C	-1.077036	-3.116073	-0.428576
H	-4.064557	-1.522025	0.126744
H	-3.318491	-5.667129	-0.830575
H	-0.887134	-5.224691	-0.853741
O	-1.657084	-0.849272	0.109206
C	0.324272	-2.914102	-0.413691
N	0.946866	-1.769158	-0.240889
H	0.943783	-3.809619	-0.507676
C	2.369620	-1.818407	-0.203574
C	3.038488	-1.228753	0.871499
C	3.086920	-2.426076	-1.237469
C	4.470803	-2.441213	-1.190045
C	4.422358	-1.267944	0.923981
C	5.147394	-1.867709	-0.109969
C	6.638638	-1.922916	-0.119791
C	8.626479	-1.377784	1.068600
C	9.100956	-2.707438	1.613992
O	7.170506	-1.341761	0.970065
O	7.279210	-2.428807	-1.015438
H	8.862909	-0.554160	1.746915
H	9.047376	-1.173350	0.079680

H	8.644860	-2.915226	2.586391
H	10.187523	-2.678101	1.744372
H	8.862475	-3.519976	0.923299
H	2.462798	-0.763885	1.665866
H	4.946809	-0.831515	1.766414
H	2.560979	-2.842165	-2.092046
H	5.052262	-2.888248	-1.990082
N	-0.919110	1.819660	-0.117258
O	1.712312	0.928373	-0.463592
C	-2.345099	1.799496	-0.132969
C	-3.073238	2.285070	0.952592
C	-2.996510	1.203158	-1.214821
C	-4.453213	2.132425	0.975610
C	-4.370047	1.047795	-1.184072
C	-5.104777	1.489028	-0.079565
C	-6.560569	1.176340	-0.044106
C	-8.644920	1.648236	1.005583
C	-8.884991	0.463790	1.916739
O	-7.216442	1.915316	0.861984
O	-7.073139	0.332910	-0.754134
H	-5.023939	2.478744	1.830156
H	-4.892917	0.565273	-2.003917
H	-2.554249	2.722595	1.800728
H	-2.412669	0.845336	-2.057410
H	-9.041909	2.572959	1.430652
H	-9.070525	1.487700	0.010936
H	-9.961408	0.335739	2.068962

H	-8.418245	0.621350	2.893538
H	-8.493029	-0.455389	1.473254
C	-0.330662	2.982700	0.006137
C	1.067713	3.213964	-0.022755
C	2.036048	2.185475	-0.291767
C	3.392900	2.514347	-0.404590
C	3.817542	3.827099	-0.236114
C	1.536327	4.532328	0.118849
C	2.874819	4.848451	0.029700
C	5.649107	5.367377	-0.189590
H	5.241179	6.035358	-0.956764
H	5.430032	5.755970	0.811548
H	6.727446	5.279894	-0.319126
O	5.138585	4.034108	-0.345850
H	4.110039	1.728192	-0.615359
H	0.817661	5.326400	0.303751
H	3.188372	5.877409	0.155052
H	-0.971328	3.865150	0.087568
Rh	0.032291	0.032737	-0.165804

ESM Table S5 Cartesian coordinates of atoms in the optimized geometries of [Zn(EMAB)2] in gas phase

H	-6.24169	-3.35498	1.89323
C	-6.03428	-4.42821	1.80304
H	-5.39288	-4.74908	2.63288
H	-6.97111	-4.98606	1.82697
O	-5.43619	-4.73176	0.54370
C	-4.24305	-4.16532	0.23256
C	-3.54604	-3.30126	1.06406

C	-3.73086	-4.52366	-1.04429
C	-2.53053	-3.99512	-1.44346
C	-2.30042	-2.74099	0.67080
C	-1.77480	-3.09582	-0.63109
H	-3.90985	-3.01363	2.04192
H	-4.30177	-5.20200	-1.66764
H	-2.13215	-4.26401	-2.41928
O	-1.70714	-1.94458	1.51030
C	-0.55205	-2.61602	-1.17877
N	0.30567	-1.78625	-0.62839
H	-0.30776	-2.99898	-2.17525
C	1.41755	-1.32395	-1.37064
C	2.63975	-1.14303	-0.69920
C	1.32054	-0.97831	-2.73141
C	2.43411	-0.49123	-3.40905
C	3.74880	-0.65313	-1.37998
C	3.65789	-0.32639	-2.74333
C	4.81160	0.20502	-3.51844
C	7.12151	0.81200	-3.43336
C	7.82994	-0.30777	-4.18258
O	5.93044	0.32408	-2.76596
O	4.76488	0.50450	-4.70022
H	7.73700	1.20590	-2.62102
H	6.84167	1.62661	-4.10712
H	8.07485	-1.13156	-3.50472
H	8.76136	0.07020	-4.61884
H	7.19862	-0.68589	-4.99061

H	2.70011	-1.39428	0.35461
H	4.68946	-0.52179	-0.85776
H	0.36705	-1.05666	-3.24481
H	2.36842	-0.21465	-4.45626
N	-0.26327	1.03916	1.11244
O	1.44573	-0.97684	2.41046
C	-1.40691	1.61855	0.51341
C	-2.01871	2.77675	1.02636
C	-1.97818	0.98043	-0.60190
C	-3.15294	3.30320	0.41316
C	-3.10972	1.50722	-1.21062
C	-3.70612	2.67713	-0.71394
C	-4.91954	3.19488	-1.40258
C	-6.60067	4.89348	-1.40883
C	-7.85293	4.18013	-0.91905
O	-5.40593	4.31710	-0.82236
O	-5.42481	2.67502	-2.38332
H	-3.62473	4.19180	0.81693
H	-3.54999	1.02264	-2.07566
H	-1.63000	3.24136	1.92703
H	-1.52043	0.07523	-0.98454
H	-6.57742	5.93661	-1.08463
H	-6.51726	4.84807	-2.49820
H	-8.74285	4.67708	-1.32123
H	-7.90844	4.20301	0.17391
H	-7.85649	3.14020	-1.25519
C	0.67178	1.81276	1.61014

C	1.84002	1.42278	2.33072
C	2.17101	0.06334	2.71347
C	3.35823	-0.14007	3.45139
C	4.19853	0.91171	3.79671
C	2.72754	2.46505	2.70819
C	3.88719	2.24442	3.42148
C	6.22841	1.59080	4.89128
H	6.65308	2.10256	4.01866
H	5.75275	2.32458	5.55377
H	7.02430	1.07767	5.43256
O	5.31109	0.57187	4.50061
H	3.61304	-1.15132	3.74743
H	2.47763	3.48343	2.41847
H	4.53020	3.07435	3.68327
H	0.56805	2.89073	1.44865
Zn	-0.06447	-0.99096	1.21442

ESM Table S6 Cartesian coordinates of atoms in the optimized geometries of [Pt(EMAB)2] in gas phase

H	-6.064355	-2.150529	-0.933160
C	-6.155336	-2.948507	-0.186270
H	-6.075820	-2.517117	0.819954
H	-7.120370	-3.444884	-0.296218
O	-5.171284	-3.968143	-0.386433
C	-3.869019	-3.604084	-0.326963
C	-3.437972	-2.318304	-0.060590
C	-2.941248	-4.646854	-0.567190
C	-1.604367	-4.359362	-0.546877
C	-2.059783	-2.009857	-0.052692

C	-1.110050	-3.048996	-0.311252
H	-4.119963	-1.499230	0.132579
H	-3.311539	-5.646804	-0.762211
H	-0.885621	-5.155970	-0.725433
O	-1.750413	-0.776143	0.215818
C	0.292952	-2.865110	-0.280238
N	0.956057	-1.741172	-0.144305
H	0.895598	-3.774558	-0.353879
C	2.377336	-1.823214	-0.119292
C	3.076502	-1.272051	0.955119
C	3.069070	-2.436294	-1.165051
C	4.452568	-2.511574	-1.126095
C	4.457675	-1.353020	0.994012
C	5.158123	-1.973250	-0.047841
C	6.637864	-2.079343	-0.064487
C	8.648235	-1.591155	1.108122
C	9.094737	-2.932665	1.653184
O	7.201598	-1.513719	1.028266
O	7.274931	-2.606053	-0.953839
H	8.922128	-0.773477	1.780733
H	9.068160	-1.404277	0.114788
H	8.642103	-3.124144	2.630845
H	10.183615	-2.937215	1.770648
H	8.819543	-3.738235	0.967925
H	2.522021	-0.778024	1.746370
H	5.001497	-0.932156	1.831953
H	2.518945	-2.822263	-2.018495

H	5.008731	-2.975269	-1.934444
Pt	0.039933	0.068630	-0.111297
N	-0.921817	1.846941	-0.137490
O	1.830055	0.936157	-0.403965
C	-2.347628	1.831734	-0.146601
C	-3.066643	2.284926	0.956577
C	-3.011681	1.274966	-1.240929
C	-4.448244	2.144807	0.984827
C	-4.385508	1.131909	-1.209326
C	-5.114004	1.545588	-0.087453
C	-6.568107	1.257946	-0.061505
C	-8.601965	1.541835	1.138053
C	-8.814084	0.200553	1.810634
O	-7.187624	1.834890	0.992429
O	-7.139797	0.568767	-0.884039
H	-5.008573	2.465890	1.855664
H	-4.915933	0.674206	-2.038198
H	-2.533982	2.689692	1.812312
H	-2.430183	0.916104	-2.084324
H	-8.981979	2.362869	1.752023
H	-9.074302	1.573436	0.151389
H	-9.883451	0.041238	1.984472
H	-8.299118	0.164597	2.775414
H	-8.445746	-0.611056	1.177636
C	-0.313420	3.002619	-0.094813
C	1.084119	3.235537	-0.121385
C	2.078817	2.210128	-0.294409

C	3.429262	2.598514	-0.367296
C	3.803187	3.927208	-0.267751
C	1.514036	4.579502	-0.036210
C	2.836523	4.944690	-0.097406
C	5.586691	5.518560	-0.247437
H	5.185523	6.133475	-1.063189
H	5.314283	5.961670	0.719004
H	6.673602	5.473190	-0.330762
O	5.137250	4.168585	-0.345085
H	4.183489	1.830557	-0.502260
H	0.758600	5.353073	0.082370
H	3.114204	5.988029	-0.023628
H	-0.952934	3.889520	-0.065669

ESM Table S7 Cartesian coordinates of atoms in the optimized geometries of [Ni(EMAB)2] in gas phase

H	-6.24169	-3.35498	1.89323
C	-6.03428	-4.42821	1.80304
H	-5.39288	-4.74908	2.63288
H	-6.97111	-4.98606	1.82697
O	-5.43619	-4.73176	0.54370
C	-4.24305	-4.16532	0.23256
C	-3.54604	-3.30126	1.06406
C	-3.73086	-4.52366	-1.04429
C	-2.53053	-3.99512	-1.44346
C	-2.30042	-2.74099	0.67080
C	-1.77480	-3.09582	-0.63109
H	-3.90985	-3.01363	2.04192
H	-4.30177	-5.20200	-1.66764

H	-2.13215	-4.26401	-2.41928
O	-1.70714	-1.94458	1.51030
C	-0.55205	-2.61602	-1.17877
N	0.30567	-1.78625	-0.62839
H	-0.30776	-2.99898	-2.17525
C	1.41755	-1.32395	-1.37064
C	2.63975	-1.14303	-0.69920
C	1.32054	-0.97831	-2.73141
C	2.43411	-0.49123	-3.40905
C	3.74880	-0.65313	-1.37998
C	3.65789	-0.32639	-2.74333
C	4.81160	0.20502	-3.51844
C	7.12151	0.81200	-3.43336
C	7.82994	-0.30777	-4.18258
O	5.93044	0.32408	-2.76596
O	4.76488	0.50450	-4.70022
H	7.73700	1.20590	-2.62102
H	6.84167	1.62661	-4.10712
H	8.07485	-1.13156	-3.50472
H	8.76136	0.07020	-4.61884
H	7.19862	-0.68589	-4.99061
H	2.70011	-1.39428	0.35461
H	4.68946	-0.52179	-0.85776
H	0.36705	-1.05666	-3.24481
H	2.36842	-0.21465	-4.45626
N	-0.26327	1.03916	1.11244
O	1.44573	-0.97684	2.41046

C	-1.40691	1.61855	0.51341
C	-2.01871	2.77675	1.02636
C	-1.97818	0.98043	-0.60190
C	-3.15294	3.30320	0.41316
C	-3.10972	1.50722	-1.21062
C	-3.70612	2.67713	-0.71394
C	-4.91954	3.19488	-1.40258
C	-6.60067	4.89348	-1.40883
C	-7.85293	4.18013	-0.91905
O	-5.40593	4.31710	-0.82236
O	-5.42481	2.67502	-2.38332
H	-3.62473	4.19180	0.81693
H	-3.54999	1.02264	-2.07566
H	-1.63000	3.24136	1.92703
H	-1.52043	0.07523	-0.98454
H	-6.57742	5.93661	-1.08463
H	-6.51726	4.84807	-2.49820
H	-8.74285	4.67708	-1.32123
H	-7.90844	4.20301	0.17391
H	-7.85649	3.14020	-1.25519
C	0.67178	1.81276	1.61014
C	1.84002	1.42278	2.33072
C	2.17101	0.06334	2.71347
C	3.35823	-0.14007	3.45139
C	4.19853	0.91171	3.79671
C	2.72754	2.46505	2.70819
C	3.88719	2.24442	3.42148

C	6.22841	1.59080	4.89128
H	6.65308	2.10256	4.01866
H	5.75275	2.32458	5.55377
H	7.02430	1.07767	5.43256
O	5.31109	0.57187	4.50061
H	3.61304	-1.15132	3.74743
H	2.47763	3.48343	2.41847
H	4.53020	3.07435	3.68327
H	0.56805	2.89073	1.44865
Ni	-0.06447	-0.99096	1.21442

ESM Table S8 Cartesian coordinates of atoms in the optimized geometries of Cu[EMAB]2 in gas phase

H	-6.01040	-1.89528	0.06196
C	-6.06813	-2.75033	0.74660
H	-5.89804	-2.41917	1.77897
H	-7.05368	-3.21180	0.66926
O	-5.13666	-3.76985	0.37251
C	-3.82275	-3.44773	0.34731
C	-3.31336	-2.22353	0.74584
C	-2.97298	-4.47058	-0.13824
C	-1.63116	-4.22382	-0.23589
C	-1.92821	-1.95562	0.65235
C	-1.06603	-2.97616	0.12776
H	-3.93976	-1.42405	1.12209
H	-3.40797	-5.41918	-0.43146
H	-0.97035	-5.00056	-0.61469
O	-1.49675	-0.79969	1.04464
C	0.33220	-2.80652	-0.00775

N	1.02334	-1.71865	0.22095
H	0.89058	-3.69747	-0.32155
C	2.42235	-1.78323	0.00939
C	3.29203	-1.44775	1.05026
C	2.93998	-2.16366	-1.23275
C	4.31109	-2.22236	-1.42462
C	4.66103	-1.51496	0.85811
C	5.18363	-1.90024	-0.38259
C	6.64033	-1.97917	-0.64711
C	8.81484	-1.70214	0.27584
C	9.31610	-3.11770	0.47963
O	7.37493	-1.62974	0.43555
O	7.12548	-2.31214	-1.70939
H	9.20302	-1.02485	1.04178
H	9.08092	-1.32403	-0.71621
H	9.01514	-3.49797	1.46053
H	10.40985	-3.13228	0.42483
H	8.92421	-3.78034	-0.29606
H	2.87855	-1.13636	2.00327
H	5.33460	-1.26627	1.67043
H	2.25902	-2.38943	-2.04880
H	4.72847	-2.51013	-2.38430
N	-0.88966	1.69954	-0.01847
O	1.76837	0.99244	0.64595
C	-2.28591	1.59063	-0.20225
C	-3.17604	2.34663	0.56690
C	-2.78349	0.67499	-1.13524

C	-4.54415	2.18269	0.41204
C	-4.14666	0.51070	-1.28675
C	-5.04187	1.25662	-0.50958
C	-6.48947	0.99135	-0.66784
C	-8.68277	1.60973	0.01298
C	-9.08586	0.50724	0.97162
O	-7.25105	1.84257	0.05740
O	-6.94899	0.10372	-1.36086
H	-5.23170	2.75520	1.02447
H	-4.54312	-0.20664	-1.99819
H	-2.78737	3.02536	1.32079
H	-2.08645	0.08307	-1.72124
H	-9.11795	2.57041	0.30160
H	-8.97228	1.37100	-1.01508
H	-10.17636	0.40737	0.97994
H	-8.75335	0.73664	1.98857
H	-8.65726	-0.44936	0.66129
C	-0.35747	2.89376	-0.04935
C	1.00125	3.22593	0.16047
C	2.01419	2.25354	0.48260
C	3.33949	2.70530	0.62617
C	3.66327	4.04402	0.48167
C	1.37758	4.57993	0.01828
C	2.67355	5.00702	0.17443
C	5.37705	5.71143	0.50067
H	5.16905	6.07957	-0.51198
H	4.88553	6.35815	1.23863

H	6.45421	5.71964	0.67379
O	4.97429	4.35123	0.65146
H	4.11467	1.98191	0.85567
H	0.60593	5.30696	-0.22571
H	2.91639	6.05510	0.05752
H	-1.01990	3.73329	-0.29427
Cu	0.12226	0.05304	0.49811

B. Supplementary data for the calculation of reorganization energies for the hole and the electron

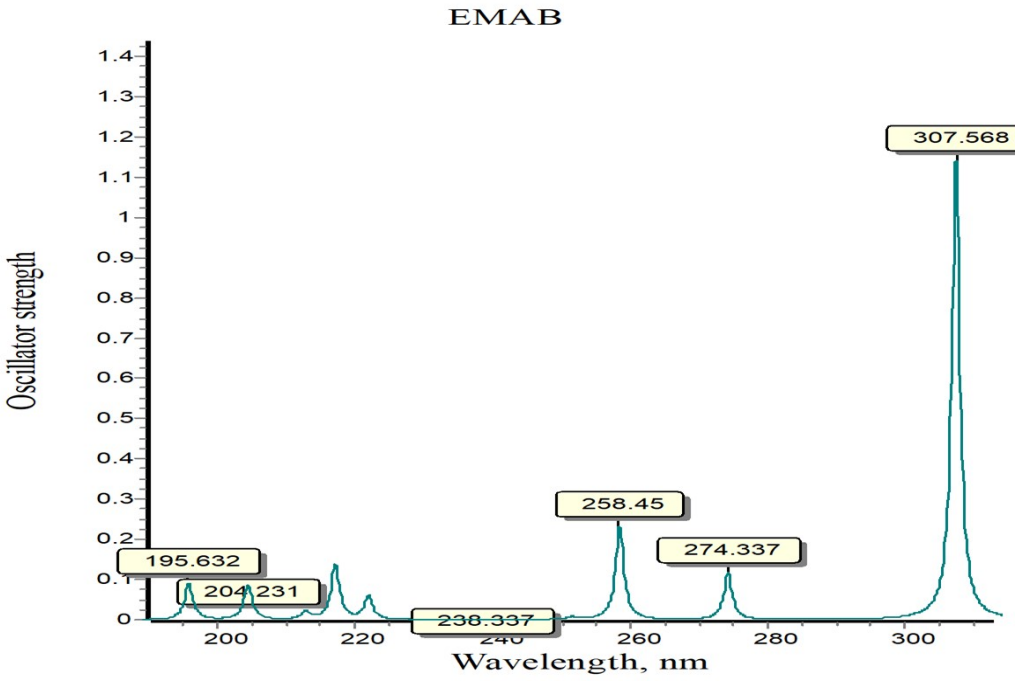
Reorganization Energies for the electron

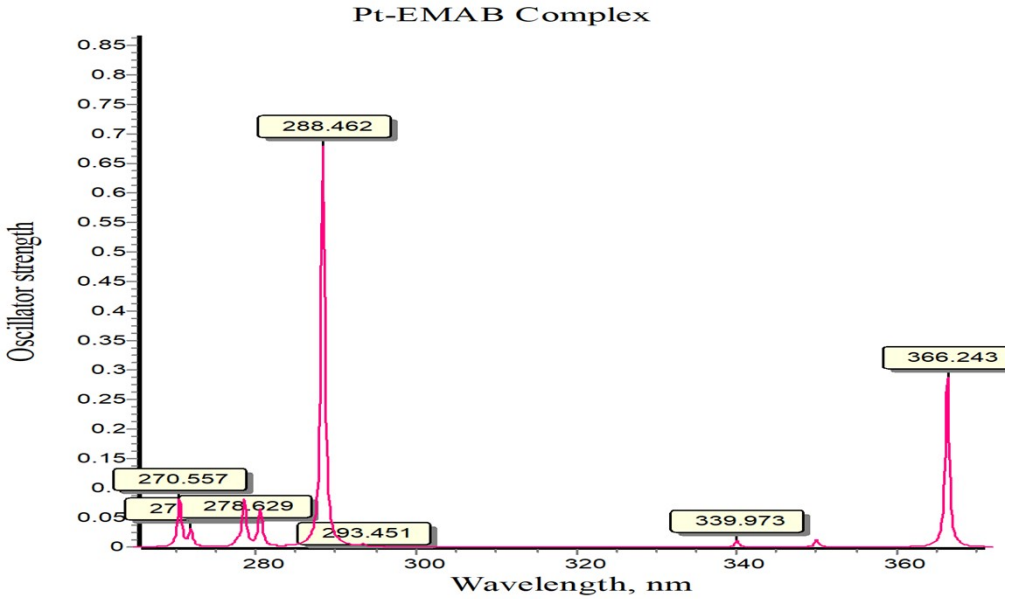
		EMAB	Pt	Pd	Zn	Ir	Rh	Ni
	E_+^-	-1013.001178	-2144.216271	-2152.754726	-3804.038896	-2129.097256	-2135.384028	-3532.977333
	E_-^-	-1013.012075	-2144.223632	-2152.762351	-3804.0497	-2129.108999	-2135.386626	-3533.053
	$E_0^- - E_-^-$	0.010897	0.007361	0.007625	0.010804	0.011743	0.002598	0.075667
	E_-^0	-1012.959224	-2144.17257	-2152.711174	-3803.998766	-2128.917858	-2135.137567	-3532.977332
	E_0^0	-1012.970821	-2144.182911	-2152.721563	-3805.096064	-2128.939729	-2135.142873	-3532.94296
	$E_-^0 - E_0^0$	0.011597	0.010341	0.010389	1.097298	0.021871	0.005306	-0.034372
λ_e	$(E_0^- - E_-^-) + (E_-^0 - E_0^0)$	0.022494	0.017702	0.018014	1.108102	0.033614	0.007904	0.041295
		EMAB	Pt	Pd	Zn	Ir	Rh	Ni
Multiplied by 27.21138		0.612092782	0.481695849	0.490185799	30.15256352	0.914683327	0.215078748	1.123693937

Reorganization energies for the hole

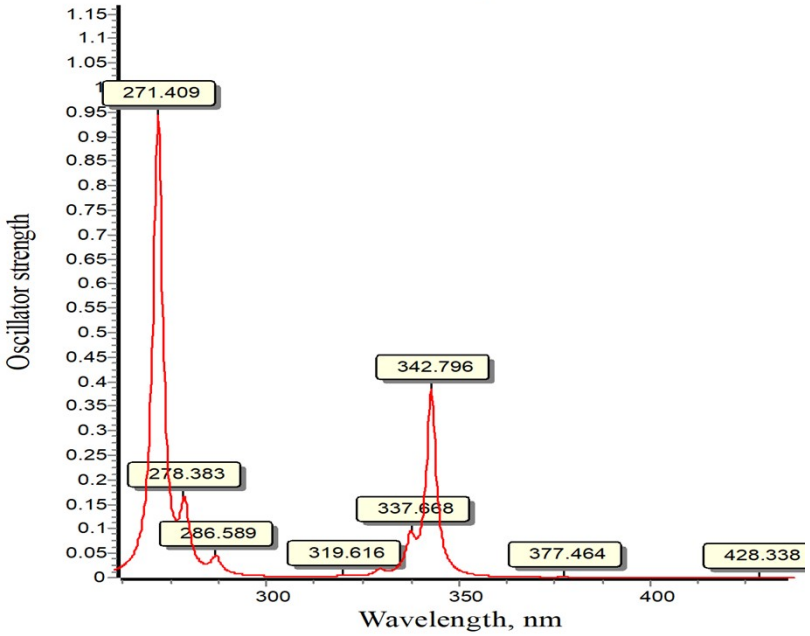
	E_0^+	-1012.692396	-2143.944635	-2152.477218	-3803.738842	-2128.565999	-2134.783638	-3532.698086
	E_+^+	-1012.699698	-2143.949284	-2152.480472	-3803.745624	-2128.579997	-2134.784273	-3532.70092
	$E_0^+ - E_+^+$	0.007302	0.004649	0.003254	0.006782	0.013998	0.000635	0.002834
	E_+^0	-1012.964319	-2144.180744	-2152.719668	-3803.991597	-2128.929047	-2135.137246	-3532.940383
	E_0^0	-1012.970821	-2144.182911	-2152.721563	-3805.094064	-2128.939027	-2135.142873	-3532.942957
	$E_+^0 - E_0^0$	0.006502	0.002167	0.001895	1.102467	0.0099797	0.005627	0.002574
λ_h	$(E_0^+ - E_+^+) + (E_+^0 - E_0^0)$	0.013804	0.006816	0.005149	1.109249	0.0239777	0.006262	0.005408
Multiplied by 27.21138		EMAB	Pt	Pd	Zn	Ir	Rh	Ni
		0.37562589	0.185472766	0.140111396	30.19241559	0.652466306	0.170397662	0.147159143

C. UV-Visible spectra for EMAB and its studied derivatives

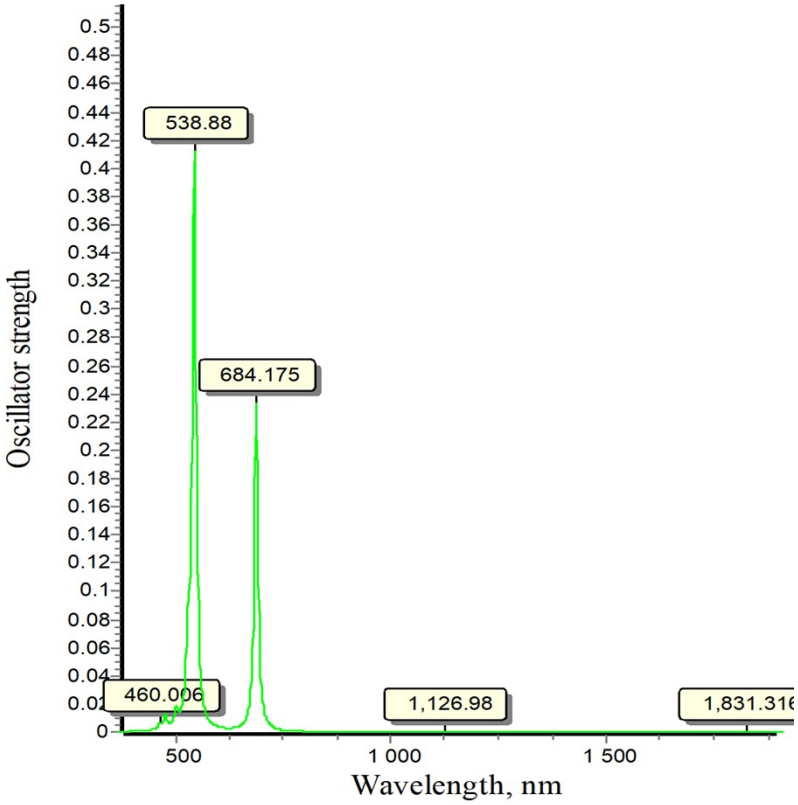




Pd-EMAB Complex



Rh-EMAB complex



Ni-EMAB complex