Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

for

Constrained formation of 2-(1-(arylimino)ethyl)-7-arylimino-6,6-dimethylcyclopentapyridines and their cobalt(II) chloride complexes: synthesis, characterization and ethylene polymerization

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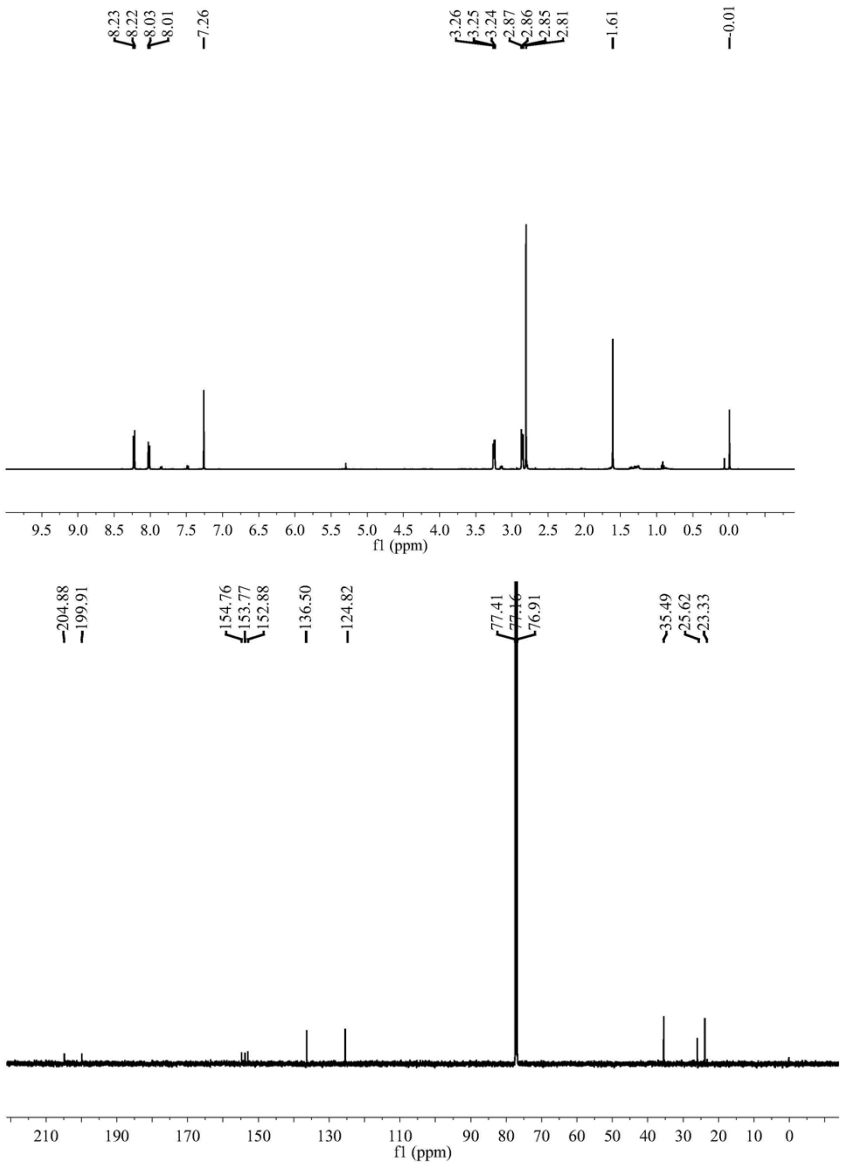
NMR spectra for 2-acetyl-cyclopentapyridin-7-one



Cartesian coordinates of selected optimized structures

53
C1'.log E(UB3LYP) = -2158.28974397

C	-3.745869	2.655039	-0.286906
H	-4.661105	2.111945	-0.519041
H	-3.556404	3.384709	-1.080547
H	-3.906638	3.214260	0.642163
C	-2.573528	1.714784	-0.163348
C	-1.199136	2.306460	-0.147587
C	-0.919091	3.683550	-0.120816
H	-1.728636	4.403549	-0.124164
C	0.407408	4.133569	-0.072953
H	0.615581	5.199423	-0.042397
C	1.432752	3.188667	-0.058929
C	1.057101	1.849430	-0.095786
C	2.936896	3.289351	-0.005444
H	3.270064	3.880765	0.854853
H	3.321802	3.794746	-0.899293
C	3.481078	1.805397	0.078773
C	2.206166	0.933951	-0.052304
C	4.509571	1.559492	-1.041408
H	4.938838	0.558774	-0.973198
H	5.323603	2.288054	-0.956356
H	4.057714	1.671881	-2.032592
C	4.123572	1.547227	1.459189
H	4.444893	0.506961	1.551147
H	3.420560	1.757138	2.271924
H	4.999845	2.191540	1.589427
C	2.912025	-1.360778	0.012433
C	3.009341	-2.119826	1.188149
C	3.900748	-3.190098	1.242660
H	3.980845	-3.767383	2.159284
C	4.667483	-3.536572	0.127198
H	5.349926	-4.379959	0.173084
C	4.530138	-2.808158	-1.055148
H	5.098011	-3.087466	-1.938061
C	3.655717	-1.722525	-1.119679
H	2.367307	-1.873934	2.027209
H	3.516416	-1.177683	-2.047195
C	-3.842948	-0.309036	-0.032486
C	-3.993531	-1.404967	-0.896122
C	-5.152416	-2.174905	-0.831774
H	-5.270534	-3.014557	-1.510053
C	-6.144416	-1.889180	0.110082
H	-7.037219	-2.504760	0.166198
C	-5.972785	-0.824037	0.995987
H	-6.725098	-0.613703	1.750473
C	-4.829440	-0.029147	0.926278
H	-3.197231	-1.636876	-1.597191
H	-4.677233	0.774672	1.639331
Cl	-0.523176	-1.684970	-2.058754
Cl	-0.529161	-1.344318	2.119789
Co	-0.618267	-0.616388	-0.042503
N	-0.193824	1.415995	-0.133561
N	1.955434	-0.318264	-0.041826
N	-2.633523	0.426860	-0.103950

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C0.log E(UB3LYP) = -2118.98517408

Co	0.284902	-0.533126	0.011796
Cl	0.615560	-1.305764	-2.119667
Cl	0.262938	-1.559532	2.058832
N	-0.070738	1.513587	0.096892
N	-1.998790	-0.320488	-0.066077
N	2.358179	0.441721	0.141764
C	-1.337739	1.949186	0.053746
C	0.970744	2.355312	0.149007
C	3.552418	-0.316778	0.081864
C	-2.869436	-1.435805	-0.063286
C	-0.559635	4.210058	0.094565
H	-0.746650	5.280614	0.080396
C	-2.399237	0.899968	0.015079
C	4.519247	-0.096605	-0.911708
C	-3.864615	-1.611898	0.911400
H	2.924779	-1.560331	1.718054
C	3.710070	-1.371904	0.993015
C	-2.655117	-2.429264	-1.031810
C	-1.640240	3.323965	0.046489
C	0.748930	3.739066	0.150624
H	1.578075	4.434966	0.181593
C	-3.832733	1.390161	0.041826
H	-4.153899	1.499218	1.087491
H	-4.482199	0.632114	-0.403196
C	2.329228	1.727556	0.180562
C	5.650453	-0.909568	-0.970490
H	6.386511	-0.745889	-1.752237
C	-3.072587	3.798291	-0.023926
H	-3.120291	4.745835	-0.571653
H	-3.428570	4.013888	0.994429
H	-3.980854	-0.881109	1.704743
H	-1.845997	-2.299012	-1.743634
C	3.522881	2.644717	0.292858
H	4.431763	2.077924	0.489564
H	3.371719	3.360482	1.107631
H	3.671383	3.220612	-0.627930
C	-4.474375	-3.726684	-0.094046
H	-5.095950	-4.617156	-0.105596
H	4.358030	0.674133	-1.658633
C	-4.656658	-2.759035	0.895468
H	-5.411847	-2.898201	1.663607
C	4.857871	-2.159098	0.938996
H	4.981905	-2.967046	1.653986
C	5.830648	-1.933106	-0.038549
H	6.714166	-2.562835	-0.085716
C	-3.980895	2.744788	-0.667922
H	-5.024619	3.070851	-0.624686
H	-3.723162	2.635309	-1.728351
C	-3.472624	-3.556344	-1.053605
H	-3.311267	-4.315543	-1.813151

50
ligand-C1'.log E(RB3LYP) = -1092.67819785

C	-4.007856	2.001158	-0.645536
H	-4.892895	1.427171	-0.920426
H	-3.688206	2.597988	-1.505565
H	-4.297318	2.702048	0.146338
C	-2.888920	1.080744	-0.192073
C	-1.512235	1.674387	-0.076307
C	-1.339514	3.071003	0.022690
H	-2.198627	3.731452	0.006051
C	-0.060951	3.609130	0.156756
H	0.081318	4.682919	0.245984
C	1.013726	2.726767	0.172627
C	0.739955	1.357982	0.051694
C	2.488780	2.973684	0.327245
H	2.713297	3.280277	1.357374
H	2.852801	3.777378	-0.323032

C	3.178612	1.606023	-0.000619
C	2.011536	0.580761	0.056969
C	3.733137	1.645992	-1.443493
H	4.186888	0.690632	-1.715770
H	4.499920	2.424531	-1.526842
H	2.943149	1.870186	-2.168112
C	4.314193	1.317058	0.993611
H	4.843684	0.394286	0.751596
H	3.935586	1.231611	2.017349
H	5.038645	2.139452	0.971157
C	3.117161	-1.542351	0.067453
C	3.581113	-2.115971	1.264419
C	4.618451	-3.045355	1.242719
H	4.972059	-3.468552	2.178943
C	5.196840	-3.441007	0.034223
H	6.000721	-4.170407	0.022376
C	4.717232	-2.897976	-1.158309
H	5.145376	-3.206580	-2.108111
C	3.683832	-1.961324	-1.148954
H	3.118537	-1.822724	2.201453
H	3.292430	-1.562107	-2.079233
C	-4.232593	-0.851460	0.063076
C	-4.343272	-1.993795	-0.749313
C	-5.514073	-2.746219	-0.748145
H	-5.589890	-3.616845	-1.393574
C	-6.579634	-2.401638	0.088556
H	-7.485000	-3.000837	0.098032
C	-6.462300	-1.289696	0.922729
H	-7.277318	-1.019838	1.588702
C	-5.303253	-0.513490	0.909205
H	-3.500389	-2.269600	-1.374648
H	-5.207581	0.341248	1.571919
N	-0.474213	0.823307	-0.063810
N	2.001711	-0.691632	0.084274
N	-3.011355	-0.163122	0.078208

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ligand-C0.log E(RB3LYP) = -1053.36708367

N	-0.125960	1.052817	-0.018726
N	2.007561	-0.623556	0.167336
N	-2.603597	-0.045609	-0.181948
C	1.105261	1.575472	-0.053054
C	-1.189595	1.860902	0.013264
C	-3.785824	-0.796516	-0.127158
C	2.977212	-1.634026	0.112175
C	0.227416	3.803840	-0.015863
H	0.361238	4.882887	-0.006967
C	2.254837	0.607311	-0.079477
C	-4.481321	-1.002023	1.077491
C	3.685501	-1.940948	-1.063387
H	-3.666689	-1.324059	-2.207362
C	-4.224015	-1.460313	-1.286118
C	3.163753	-2.444517	1.246254
C	1.345666	2.969249	-0.065221
C	-1.049268	3.260203	0.027178
H	-1.912862	3.913105	0.068019
C	3.625937	1.204279	-0.358714
H	3.737098	1.358493	-1.442165
H	4.401482	0.494302	-0.062325
C	-2.547446	1.212588	0.039007
C	-5.598823	-1.835932	1.111404
H	-6.120673	-1.989520	2.052016
C	2.742395	3.545997	-0.130857
H	2.784467	4.477545	0.445470
H	2.962147	3.824098	-1.172791
H	3.512665	-1.348953	-1.956925
H	2.589138	-2.225784	2.140557
C	-3.743098	2.113454	0.287353
H	-4.668594	1.539338	0.302334
H	-3.820833	2.869913	-0.501820
H	-3.647644	2.647838	1.238862
C	4.778698	-3.795184	0.048074
H	5.473018	-4.629533	0.023797
H	-4.122415	-0.524160	1.984030
C	4.571860	-3.017366	-1.091596
H	5.103987	-3.246223	-2.010903
C	-5.353572	-2.273060	-1.245951
H	-5.687137	-2.767786	-2.153947
C	-6.047393	-2.468327	-0.048539
H	-6.919481	-3.114331	-0.019043
C	3.799832	2.552512	0.353487
H	4.804499	2.948113	0.170920
H	3.705117	2.408759	1.437038
C	4.070538	-3.499857	1.216561
H	4.214133	-4.106030	2.106680

3
CoCl2-quartet.log E(UB3LYP) = -1065.51898368

Cl	2.115372	-0.023452	0.000000
Cl	-2.115372	0.021845	0.000000
Co	0.000000	0.001011	0.000000