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Supporting Information

Ni^{II}, Cu^{II} and Zn^{II} Complexes with a Sterically Hindered Scorpionate Ligand ($Tpms^{Ph}$) and Catalytic Application in the Diasteroselective Nitroaldol (Henry) Reaction

Bruno G.M. Rocha,[a] Tatiana C.O. Mac Leod,[a] M. Fátima C. Guedes da Silva,[a] Konstantin V. Luzyanin,[a] Luísa M.D.R.S. Martins,[a,b] Armando J.L. Pombeiro[a]**

[a] Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049–001 Lisboa, Portugal. E-mail: pombeiro@tecnico.ulisboa.pt

[b] Chemical Engineering Department, ISEL, R. Conselheiro Emídio Navarro, 1959-007 Lisboa, Portugal. E-mail: lmartins@deq.isel.ipl.pt

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Table S1 DFT calculated energies E (Hartree) for N_3 and N_2O coordination modes [and their differences, ΔE = E (N_2O) - E (N_3) (kJ/mol)] in [NiCl(Tpms^{Ph})] (**2**) (entries 1-3), [ZnCl(Tpms^{Ph})] (**3**) (entries 4-6) and [CuCl(Tpms^{Ph})(H_2O)] (**4**) (entries 7-9) using B3LYP as functional and 3-21G and 6-31G** as basis.

Entries		B3LYP/6-31G**	B3LYP/3-21G
1	E (N_3)	-4000.34	-3979.99
2	E (N_2O)	-4000.33	-3979.99
3	ΔE	10.29	-0.795
4	E (N_3)	-4271.38	-4249.76
5	E (N_2O)	-4271.38	-4249.77
6	ΔE	7.155	-9.247
7	E (N_3)	-4208.94	-4187.56
8	E (N_2O)	-4208.94	-4187.57
9	ΔE	0.879	-12.68

FIGURES

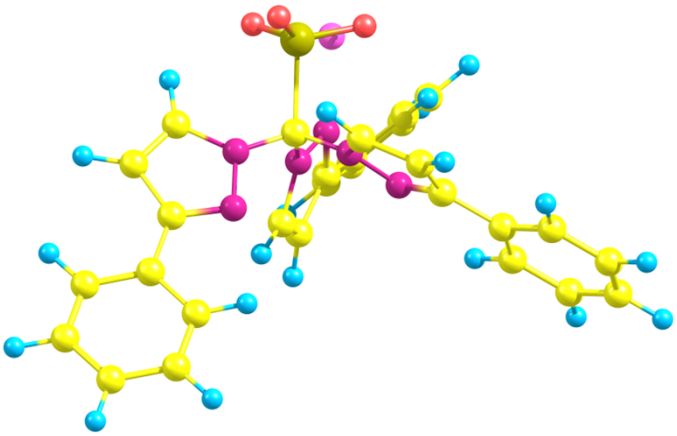

Figure S1: Li(Tpms^{Ph}) (**1**) geometry optimization (B3LYP/6-31G**).

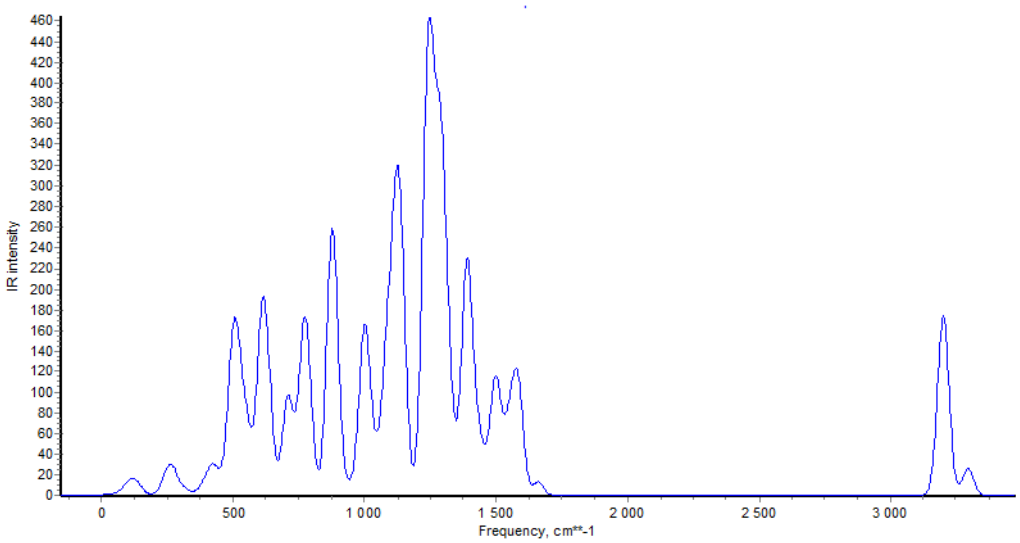

Figure S2: Theoretical IR spectrum (B3LYP/6-31G**) of Li(Tpms^{Ph}) (**1**).

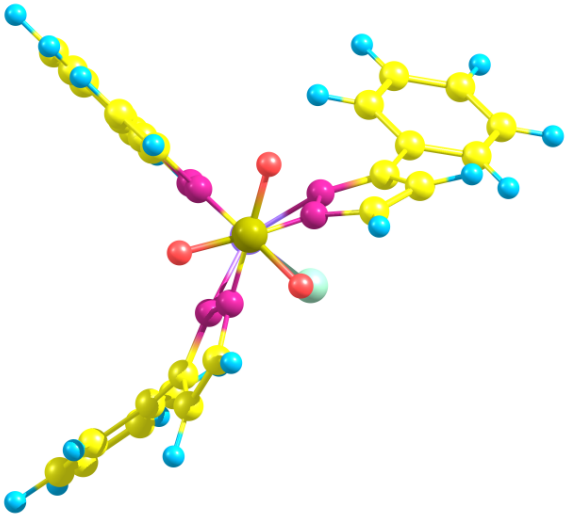

Figure S3: [NiCl(Tpms^{Ph})] (**2**) geometry optimization in N_3 coordination mode (B3LYP/6-31G**).

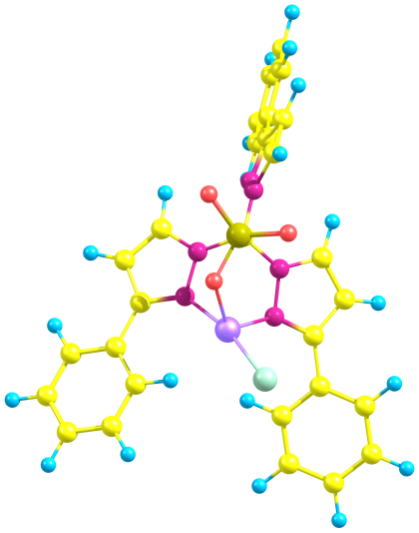

Figure S4: [NiCl Tpms^{Ph})] (**2**) geometry optimization in N_2O coordination mode (B3LYP/6-31G**).

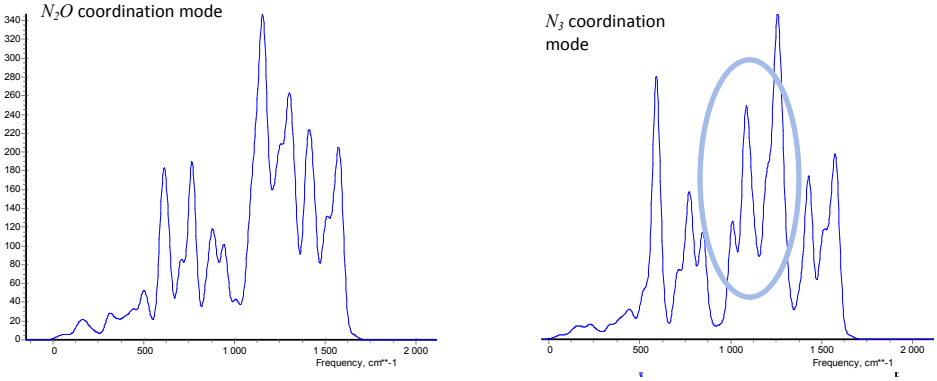

Figure S5: Theoretical IR spectrum of [NiCl(Tpms^{Ph})] (**2**) in N_2O and N_3 coordination modes (B3LYP/6 31G**).

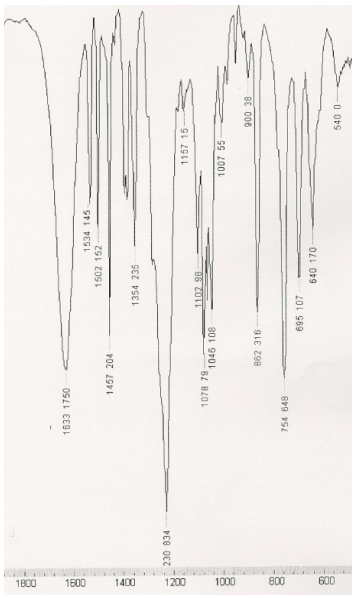

Figure S6: Experimental IR spectrum of [NiCl(Tpms^{Ph})] (**2**).

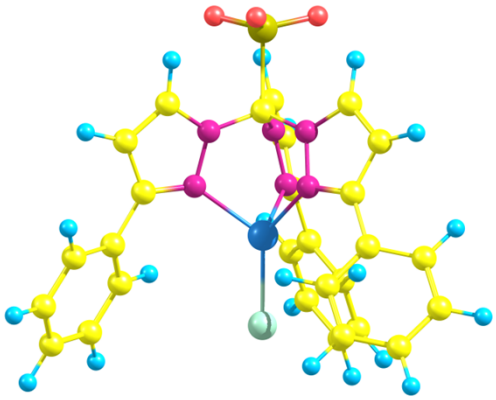

Figure S7: [ZnCl(Tpms^{Ph})] (**3**) geometry optimization in N_3 coordination mode (B3LYP/6-31G**).

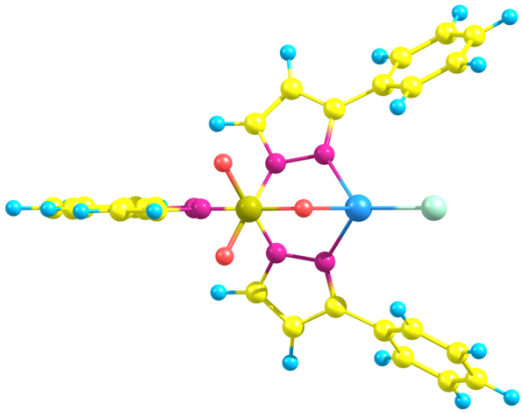

Figure S8: [ZnCl(Tpms^{Ph})] (**3**) geometry optimization in N_2O coordination mode (B3LYP/6-31G**).

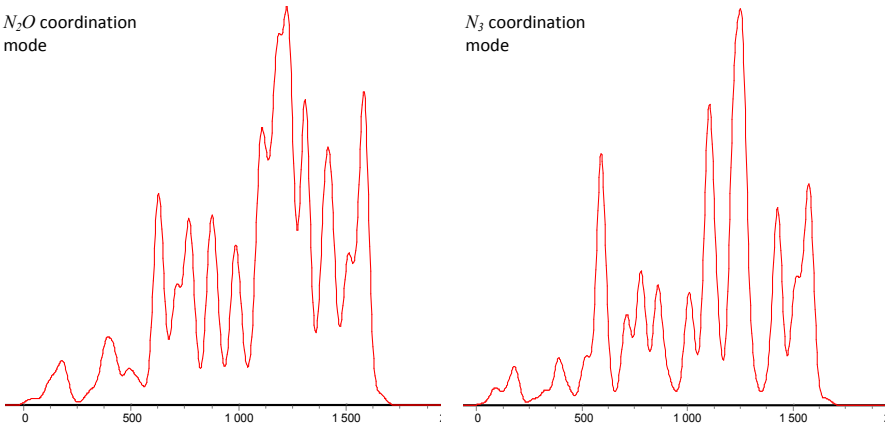

Figure S9: Theoretical IR spectra of [ZnCl(Tpms^{Ph})] (**3**) in N_2O and N_3 coordination modes (B3LYP/6 31G**).

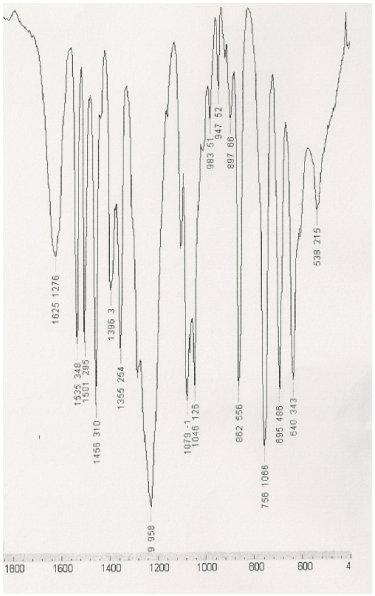

Figure S10: Experimental IR spectrum of [ZnCl(Tpms^{Ph})] (**3**).

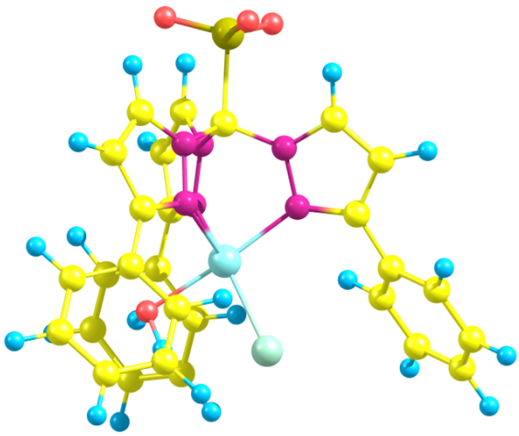

Figure S11: [CuCl(Tpms^{Ph})(H_2O)] (**4**) geometry optimization in N_3 coordination mode (B3LYP/6-31G**).

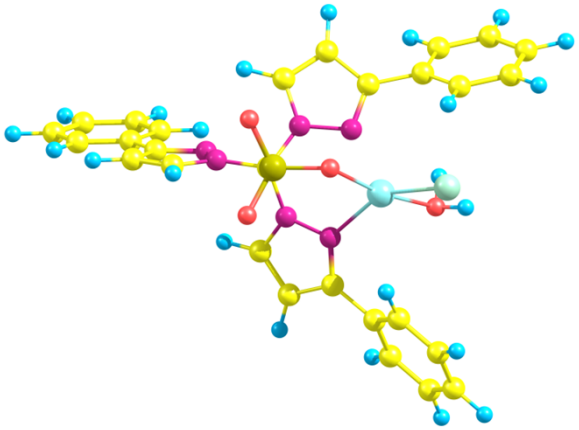

Figure S12: [CuCl(Tpms^{Ph})(H$_2$O)] (**4**) geometry optimization in *N$_2$O* coordination mode (B3LYP/6-31G**).

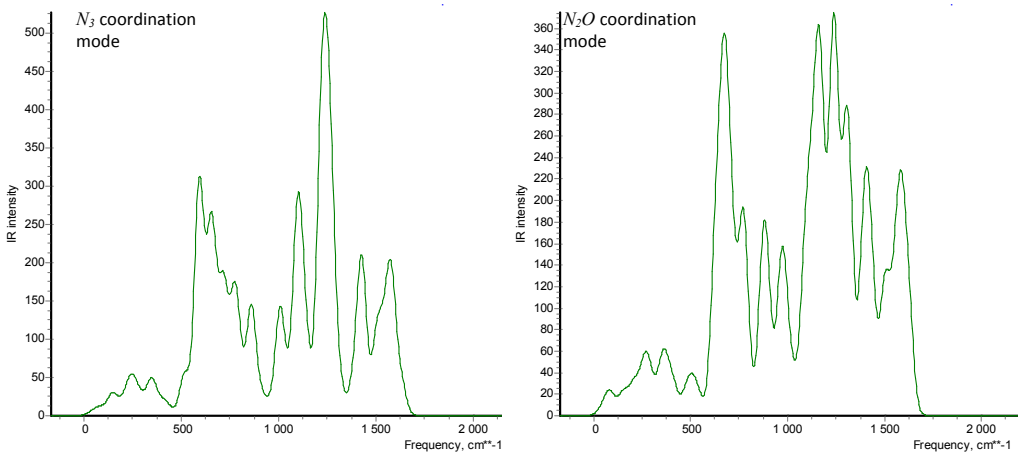

Figure S13: Theoretical IR spectra of [CuCl(Tpms^{Ph})(H$_2$O)] (**4**) in *N$_3$* and *N$_2$O* coordination modes (B3LYP/6 31G**).

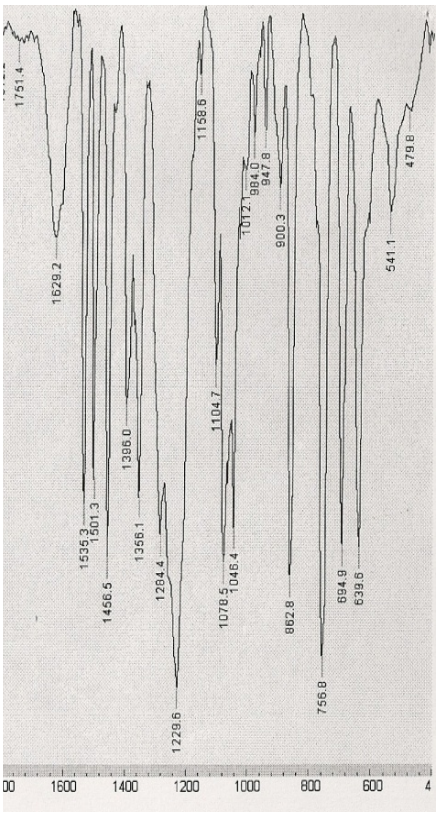

Figure S14: Experimental IR spectrum of [CuCl(Tpms^{Ph})(H_2O)] (**4**).

Cartesian coordinates of optimized structures

Li(Tpms^{Ph}) (1) (B3LYP/6-31G)**

6	-0.187848000	-1.052084000	-1.428344000
6	0.337881000	-0.645236000	0.990212000
7	-0.527543000	-1.067283000	-0.108541000
7	-1.845266000	-1.354756000	0.056827000
6	-2.334442000	-1.549850000	-1.171435000
6	-1.318601000	-1.374670000	-2.142340000
7	1.676468000	-1.157858000	0.776262000
7	2.553275000	-0.444913000	0.012486000
6	3.614684000	-1.240403000	-0.133359000
6	3.406984000	-2.488111000	0.523362000
6	2.158254000	-2.405106000	1.082330000
6	1.120937000	1.551874000	1.933187000
6	0.746479000	2.854809000	1.728610000
6	-0.265208000	2.804654000	0.725651000
7	-0.494645000	1.546811000	0.345034000
7	0.361610000	0.795814000	1.080945000
16	-0.326104000	-1.333423000	2.683238000
8	0.772079000	-1.115595000	3.622536000
8	-1.590931000	-0.558381000	2.896580000
8	-0.708536000	-2.758298000	2.378224000
6	-1.008564000	3.919012000	0.113456000
6	-3.751867000	-1.908985000	-1.345608000
6	4.793575000	-0.783380000	-0.889501000
6	-4.153133000	-2.770791000	-2.377187000
6	-5.493892000	-3.124343000	-2.520245000
6	-6.452000000	-2.626481000	-1.634840000
6	5.837818000	-1.668304000	-1.197896000
6	6.951074000	-1.231932000	-1.914388000
6	7.038274000	0.095116000	-2.336484000
6	6.002731000	0.983433000	-2.035398000
6	4.891110000	0.551318000	-1.317637000
6	-6.064503000	-1.760616000	-0.610182000
6	-4.725619000	-1.397572000	-0.469444000
6	-1.852268000	3.694549000	-0.987571000
6	-2.554774000	4.746901000	-1.567681000
6	-2.428657000	6.043916000	-1.063572000
6	-1.593469000	6.277369000	0.029398000
6	-0.890460000	5.224751000	0.613456000
1	0.813522000	-0.791714000	-1.734343000
1	-1.411474000	-1.444195000	-3.214983000
1	4.085874000	-3.322973000	0.602343000
1	1.582236000	-3.106042000	1.665546000
1	1.837457000	1.097597000	2.598180000
1	1.155533000	3.721988000	2.223416000
1	-3.408321000	-3.178881000	-3.053760000
1	-5.790024000	-3.796363000	-3.320132000
1	-7.495291000	-2.904921000	-1.747787000
1	5.779643000	-2.705752000	-0.883294000
1	7.749815000	-1.931093000	-2.144268000
1	7.905793000	0.435165000	-2.894308000
1	6.063702000	2.018894000	-2.357796000
1	4.088677000	1.239646000	-1.075521000
1	-6.807550000	-1.350950000	0.067603000
1	-4.433119000	-0.674312000	0.287696000
1	-1.943516000	2.687168000	-1.378760000
1	-3.201840000	4.555574000	-2.419179000
1	-2.976200000	6.864104000	-1.518616000
1	-1.489746000	7.280956000	0.431849000
1	-0.252172000	5.420281000	1.469532000
3	-2.476831000	-1.954979000	1.855214000

[NiCl(Tpms^{Ph})] (2) in N_3 coordination mode (B3LYP/6-31G)**

6	-1.884824000	2.959859000	-0.843581000
6	0.236513000	2.194764000	0.364615000
7	-1.060122000	2.023015000	-0.300664000
7	-1.625796000	0.767598000	-0.413593000
6	-2.813096000	0.935003000	-1.011281000
6	-3.003643000	2.304838000	-1.303547000
7	1.361656000	1.765458000	-0.480727000
7	1.610790000	0.416428000	-0.695808000
6	2.820559000	0.345671000	-1.270830000
6	3.337954000	1.651762000	-1.449082000
6	2.403142000	2.515679000	-0.938384000
6	0.362052000	1.673832000	2.897705000
6	0.288349000	0.482081000	3.584252000
6	0.113783000	-0.536245000	2.615544000
7	0.088995000	0.040787000	1.406825000
7	0.237799000	1.378276000	1.574954000
6	-0.032905000	-1.987331000	2.782753000
6	-3.745773000	-0.176525000	-1.243088000
6	3.536736000	-0.907549000	-1.578568000
6	-4.600843000	-0.149830000	-2.354753000
6	-5.510832000	-1.182409000	-2.569040000
6	-5.580879000	-2.251933000	-1.674880000
6	4.924746000	-0.940458000	-1.353065000
6	5.661134000	-2.090047000	-1.626715000
6	5.024085000	-3.224643000	-2.132832000
6	3.648592000	-3.197517000	-2.364178000
6	2.904682000	-2.049304000	-2.092383000
6	-4.736509000	-2.283215000	-0.563272000
6	-3.825914000	-1.252419000	-0.345693000
6	-0.193667000	-2.832737000	1.672049000
6	-0.337298000	-4.206553000	1.837090000
6	-0.322645000	-4.762689000	3.117721000
6	-0.163403000	-3.933363000	4.229367000
6	-0.019945000	-2.557903000	4.065231000
28	-0.131176000	-0.479743000	-0.363288000
17	-0.533520000	-1.425955000	-2.262275000
1	-1.608656000	4.001664000	-0.849731000
1	-3.875556000	2.758025000	-1.748152000
1	4.274742000	1.916011000	-1.913274000
1	2.381373000	3.590781000	-0.876346000
1	0.496404000	2.687188000	3.234277000
1	0.354466000	0.363531000	4.653712000
1	-4.533300000	0.669061000	-3.064209000
1	-6.160765000	-1.154778000	-3.438341000
1	-6.290699000	-3.056410000	-1.842504000
1	5.421642000	-0.068127000	-0.939927000
1	6.730760000	-2.100605000	-1.439629000
1	5.597404000	-4.121635000	-2.347835000
1	3.147123000	-4.071146000	-2.769964000
1	1.843055000	-2.027850000	-2.307540000
1	-4.792201000	-3.108400000	0.140293000
1	-3.188607000	-1.265915000	0.532619000
1	-0.207394000	-2.419157000	0.664598000
1	-0.459495000	-4.839629000	0.964051000
1	-0.433757000	-5.834708000	3.247854000
1	-0.150762000	-4.357755000	5.228532000
1	0.101829000	-1.925580000	4.938479000
16	0.453049000	4.090755000	0.909180000
8	1.737260000	4.028905000	1.626130000
8	-0.754466000	4.267609000	1.730149000
8	0.468730000	4.778682000	-0.397147000

[NiCl(Tpms^{Ph})] (2) in N_2O coordination mode (B3LYP/6-31G)**

6	-3.224208000	-0.017589000	2.115299000
6	-0.969635000	-0.243237000	0.978857000
7	-2.398482000	-0.211413000	1.031992000
7	-3.091800000	-0.164264000	-0.150908000
6	-4.364241000	0.023044000	0.198437000
6	-4.490400000	0.127951000	1.615855000
7	-0.490252000	1.051666000	0.464732000
7	0.812799000	1.235102000	0.072540000
6	0.920297000	2.514579000	-0.318484000
6	-0.324025000	3.162678000	-0.140903000
6	-1.186307000	2.213600000	0.356378000
6	-1.133228000	-2.374646000	-0.460377000
6	-0.156251000	-3.150785000	-1.043383000
6	1.078817000	-2.506316000	-0.785662000
7	0.833312000	-1.390853000	-0.081175000
7	-0.506736000	-1.307381000	0.100015000
6	2.439387000	-2.900643000	-1.171973000
6	-5.420981000	0.102091000	-0.825185000
6	2.147904000	3.073032000	-0.900574000
6	-6.774567000	0.136878000	-0.457946000
6	-7.771626000	0.214886000	-1.428921000
6	-7.432379000	0.257696000	-2.781597000
6	2.996350000	2.285952000	-1.693678000
6	4.136077000	2.841705000	-2.268491000
6	4.441534000	4.188476000	-2.062493000
6	3.599569000	4.979094000	-1.278835000
6	2.458189000	4.426672000	-0.702479000
6	-6.087069000	0.221703000	-3.157094000
6	-5.089317000	0.145288000	-2.189768000
6	2.640469000	-4.002542000	-2.018690000
6	3.927319000	-4.390658000	-2.382543000
6	5.035515000	-3.686384000	-1.908526000
6	4.847743000	-2.588119000	-1.067350000
6	3.562684000	-2.199631000	-0.702665000
28	1.861564000	-0.144546000	0.872892000
17	3.395086000	1.045819000	1.774254000
8	-1.087042000	-1.801619000	3.197568000
16	-0.260713000	-0.659897000	2.788932000
8	-0.428338000	0.616821000	3.492925000
8	1.178305000	-1.065077000	2.515280000
1	-2.847229000	0.000345000	3.123841000
1	-5.385353000	0.289098000	2.196159000
1	-0.564335000	4.182801000	-0.395073000
1	-2.231793000	2.266598000	0.610229000
1	-2.204065000	-2.473380000	-0.419891000
1	-0.314663000	-4.070203000	-1.583382000
1	-7.054062000	0.094316000	0.590071000
1	-8.814437000	0.239362000	-1.126964000
1	-8.209420000	0.318371000	-3.537663000
1	2.749230000	1.244707000	-1.872549000
1	4.784349000	2.223567000	-2.882082000
1	5.331726000	4.619558000	-2.510614000
1	3.835481000	6.025166000	-1.108991000
1	1.818630000	5.037860000	-0.073225000
1	-5.814754000	0.256117000	-4.207931000
1	-4.043921000	0.121740000	-2.477842000
1	1.789131000	-4.557198000	-2.399517000
1	4.063964000	-5.245376000	-3.037896000
1	6.038205000	-3.991768000	-2.191226000
1	5.699665000	-2.033490000	-0.687350000
1	3.443798000	-1.341131000	-0.044133000

[ZnCl(Tpms^{Ph})] (3) in N_3 coordination mode (B3LYP/6-31G)**

6	-2.480851000	-1.982069000	-1.607822000
6	-2.291492000	-0.016495000	0.006077000
7	-1.807512000	-0.980170000	-0.982196000
7	-0.485770000	-0.976094000	-1.359718000
6	-0.344674000	-1.975985000	-2.246754000
6	-1.582646000	-2.633299000	-2.420685000
7	-1.823050000	1.324243000	-0.340944000
7	-0.503547000	1.665074000	-0.159487000
6	-0.382188000	2.935849000	-0.581072000
6	-1.629647000	3.399204000	-1.054628000
6	-2.513722000	2.358456000	-0.890335000
6	-2.476749000	-0.442438000	2.513321000
6	-1.574872000	-0.814793000	3.482755000
6	-0.333468000	-0.970543000	2.827726000
7	-0.475800000	-0.692691000	1.520223000
7	-1.802138000	-0.383250000	1.334459000
6	0.943470000	-1.392370000	3.423009000
6	0.927343000	-2.275163000	-2.921394000
6	0.881292000	3.684659000	-0.508884000
6	1.210894000	-3.596530000	-3.305166000
6	2.396168000	-3.899807000	-3.969691000
6	3.314580000	-2.888670000	-4.259880000
6	1.139851000	4.696355000	-1.448755000
6	2.317479000	5.436168000	-1.384212000
6	3.253602000	5.176354000	-0.381102000
6	3.004549000	4.173881000	0.557146000
6	1.825390000	3.434752000	0.498707000
6	3.040501000	-1.573332000	-3.883009000
6	1.853836000	-1.265254000	-3.221642000
6	1.882805000	-2.136312000	2.692935000
6	3.073483000	-2.544823000	3.289320000
6	3.338844000	-2.224813000	4.621455000
6	2.408009000	-1.488683000	5.357322000
6	1.218812000	-1.074452000	4.763322000
30	0.702949000	0.008164000	-0.004307000
17	2.871642000	0.043672000	-0.017538000
1	-3.530386000	-2.144416000	-1.428514000
1	-1.798936000	-3.448411000	-3.092765000
1	-1.861933000	4.385616000	-1.423356000
1	-3.563478000	2.269023000	-1.114590000
1	-3.529516000	-0.221699000	2.564629000
1	-1.790120000	-0.997906000	4.523468000
1	0.508438000	-4.388442000	-3.063971000
1	2.605379000	-4.926125000	-4.255778000
1	4.239756000	-3.125586000	-4.776567000
1	0.424205000	4.888779000	-2.242225000
1	2.506958000	6.211242000	-2.120625000
1	4.173052000	5.751915000	-0.332100000
1	3.727696000	3.964882000	1.338968000
1	1.632506000	2.670010000	1.242251000
1	3.749647000	-0.782147000	-4.104320000
1	1.640869000	-0.237997000	-2.949034000
1	1.676742000	-2.404487000	1.663113000
1	3.792620000	-3.115488000	2.710460000
1	4.267007000	-2.546425000	5.084184000
1	2.610732000	-1.231394000	6.392513000
1	0.506675000	-0.485030000	5.332709000
16	-4.283768000	-0.032640000	0.016674000
8	-4.570545000	1.056199000	0.967361000
8	-4.551562000	-1.402710000	0.488970000
8	-4.577007000	0.240276000	-1.401658000

[ZnCl(Tpms^{Ph})] (3) in N_2O coordination mode (B3LYP/6-31G)**

6	-3.194255000	-0.058912000	2.214513000
6	-0.945430000	-0.010502000	1.013055000
7	-2.379213000	-0.017994000	1.106560000
7	-3.107443000	0.004156000	-0.056998000
6	-4.383768000	-0.020123000	0.328185000
6	-4.481729000	-0.060415000	1.750274000
7	-0.518565000	1.213589000	0.323891000
7	0.802352000	1.455490000	0.054486000
6	0.857334000	2.684907000	-0.485965000
6	-0.442317000	3.232663000	-0.552189000
6	-1.282231000	2.285613000	-0.019221000
6	-1.268868000	-2.279394000	-0.080971000
6	-0.422337000	-3.215035000	-0.623596000
6	0.876704000	-2.670257000	-0.527033000
7	0.814647000	-1.453182000	0.039828000
7	-0.509243000	-1.216299000	0.297321000
6	2.127925000	-3.311372000	-0.964447000
6	-5.468332000	-0.005208000	-0.669310000
6	2.102082000	3.335200000	-0.928866000
6	-6.812666000	-0.009541000	-0.268099000
6	-7.835821000	0.004148000	-1.214624000
6	-7.532329000	0.022479000	-2.576318000
6	3.278606000	3.277955000	-0.169128000
6	4.427436000	3.935330000	-0.605695000
6	4.413006000	4.663038000	-1.795733000
6	3.241997000	4.733104000	-2.553701000
6	2.092833000	4.075414000	-2.123230000
6	-6.196438000	0.027219000	-2.985538000
6	-5.172721000	0.013504000	-2.042831000
6	2.136322000	-4.032152000	-2.170631000
6	3.292582000	-4.680652000	-2.595987000
6	4.453066000	-4.620704000	-1.821138000
6	4.449954000	-3.912276000	-0.619421000
6	3.294020000	-3.264118000	-0.188011000
30	2.098519000	0.001863000	0.686749000
17	4.260837000	0.007100000	0.517568000
8	-0.648816000	-1.299101000	3.362499000
16	-0.178578000	-0.024776000	2.808534000
8	-0.679278000	1.223349000	3.393872000
8	1.309228000	-0.002793000	2.524827000
1	-2.800183000	-0.084925000	3.215505000
1	-5.371909000	-0.088108000	2.358823000
1	-0.714259000	4.211546000	-0.913763000
1	-2.347457000	2.285603000	0.127775000
1	-2.336048000	-2.282212000	0.051902000
1	-0.689985000	-4.185401000	-1.010416000
1	-7.064800000	-0.022613000	0.787537000
1	-8.870922000	0.000754000	-0.886391000
1	-8.329757000	0.033030000	-3.313249000
1	3.298510000	2.731317000	0.765763000
1	5.332646000	3.876537000	-0.010128000
1	5.309973000	5.174448000	-2.131993000
1	3.225071000	5.295012000	-3.482682000
1	1.187497000	4.116171000	-2.721582000
1	-5.951891000	0.041374000	-4.043619000
1	-4.134822000	0.016787000	-2.357663000
1	1.239357000	-4.064868000	-2.781959000
1	3.289452000	-5.227436000	-3.534092000
1	5.355562000	-5.124916000	-2.153434000
1	5.346978000	-3.861390000	-0.010886000
1	3.299860000	-2.732347000	0.755654000

[CuCl(Tpms^{Ph})(H_2O)] (4) in N_3 coordination mode (B3LYP/6-31G)**

6	-1.638176000	-2.177519000	2.326288000
6	-1.982498000	-1.227362000	-0.029694000
7	-1.299118000	-1.401720000	1.260954000
7	-0.177168000	-0.673704000	1.534868000
6	0.195966000	-1.001986000	2.780568000
6	-0.709787000	-1.942350000	3.315106000
7	-1.070920000	-1.609388000	-1.105551000
7	0.251918000	-1.227825000	-1.081939000
6	0.827674000	-1.808736000	-2.149574000
6	-0.144018000	-2.518776000	-2.885222000
6	-1.326660000	-2.376122000	-2.198720000
6	-3.619398000	0.723640000	-0.021621000
6	-3.473217000	2.071361000	-0.244237000
6	-2.105427000	2.269491000	-0.554415000
7	-1.450268000	1.100833000	-0.513878000
7	-2.391343000	0.158667000	-0.199847000
6	-1.449090000	3.541915000	-0.897017000
6	1.390373000	-0.431666000	3.430525000
6	2.274732000	-1.790194000	-2.417925000
6	1.348796000	-0.118055000	4.799702000
6	2.468389000	0.409262000	5.439837000
6	3.645959000	0.636787000	4.724242000
6	3.198849000	-2.003246000	-1.385124000
6	4.561956000	-2.061773000	-1.661792000
6	5.018820000	-1.908799000	-2.972072000
6	4.104655000	-1.703917000	-4.006592000
6	2.739526000	-1.651287000	-3.733216000
6	3.700830000	0.324928000	3.364805000
6	2.584718000	-0.211425000	2.720483000
6	-0.364475000	3.591557000	-1.786333000
6	0.228420000	4.812268000	-2.105395000
6	-0.258006000	5.998585000	-1.553624000
6	-1.341561000	5.958997000	-0.673558000
6	-1.932176000	4.740704000	-0.346718000
29	0.572461000	0.426186000	0.009641000
17	2.357668000	1.323150000	-1.082006000
8	0.829672000	2.031699000	1.272396000
1	-2.500732000	-2.819959000	2.301599000
1	-0.665461000	-2.413281000	4.284437000
1	0.022181000	-3.110738000	-3.771285000
1	-2.316242000	-2.756692000	-2.389857000
1	-4.475444000	0.125769000	0.243759000
1	-4.255896000	2.813563000	-0.233246000
1	0.428927000	-0.274477000	5.354578000
1	2.418245000	0.650411000	6.497215000
1	4.516396000	1.050339000	5.224063000
1	2.839008000	-2.142731000	-0.370742000
1	5.268829000	-2.231224000	-0.855073000
1	6.082506000	-1.952616000	-3.186303000
1	4.454458000	-1.582158000	-5.027274000
1	2.029593000	-1.479755000	-4.536641000
1	4.614985000	0.485794000	2.801915000
1	2.655916000	-0.489057000	1.673662000
1	0.011885000	2.677581000	-2.230679000
1	1.069271000	4.832522000	-2.791813000
1	0.203058000	6.948395000	-1.808161000
1	-1.723850000	6.876841000	-0.236597000
1	-2.761008000	4.713041000	0.354174000
1	1.258995000	1.758721000	2.099487000
1	1.511434000	2.511048000	0.761604000
16	-3.578757000	-2.413622000	-0.077542000
8	-4.162588000	-2.060816000	-1.383242000
8	-4.326865000	-1.951334000	1.109173000
8	-2.942897000	-3.736058000	0.034407000

[CuCl(Tpms^{Ph})(H_2O)] (4) in N_2O coordination mode (B3LYP/6-31G)**

6	-3.160825000	-1.108021000	1.994739000
6	-1.020131000	-0.264094000	0.917631000
7	-2.442008000	-0.442341000	1.030168000
7	-3.238808000	-0.041828000	-0.011166000
6	-4.469884000	-0.434028000	0.320588000
6	-4.464014000	-1.112125000	1.574866000
7	-0.728573000	1.121211000	0.562411000
7	0.515330000	1.475302000	0.132272000
6	0.472517000	2.807202000	-0.020066000
6	-0.800727000	3.307149000	0.340130000
6	-1.532295000	2.209649000	0.724577000
6	-1.180934000	-2.090097000	-0.843163000
6	-0.257175000	-2.889612000	-1.473133000
6	1.008829000	-2.448859000	-1.023505000
7	0.849351000	-1.421695000	-0.177059000
7	-0.490118000	-1.203694000	-0.073935000
6	2.330348000	-3.001346000	-1.356671000
6	-5.611861000	-0.146971000	-0.565521000
6	1.618039000	3.585663000	-0.532658000
6	-6.899622000	-0.605183000	-0.249186000
6	-7.977493000	-0.329632000	-1.089022000
6	-7.786113000	0.406887000	-2.258411000
6	2.926116000	3.375648000	-0.064394000
6	3.983557000	4.135014000	-0.569234000
6	3.750963000	5.117154000	-1.532740000
6	2.451102000	5.341708000	-1.992044000
6	1.392725000	4.582642000	-1.497329000
6	-6.507120000	0.866578000	-2.582480000
6	-5.429217000	0.593887000	-1.745346000
6	2.558928000	-3.541873000	-2.631762000
6	3.799673000	-4.086407000	-2.954546000
6	4.827562000	-4.097492000	-2.009337000
6	4.606553000	-3.566876000	-0.737195000
6	3.365037000	-3.026388000	-0.408211000
29	2.132449000	-0.117393000	0.636398000
17	4.199910000	0.285720000	1.472270000
8	-0.339737000	-2.094462000	2.786434000
16	-0.175202000	-0.643974000	2.626340000
8	-0.869988000	0.249448000	3.557125000
8	1.258053000	-0.207506000	2.367314000
1	-2.693203000	-1.516662000	2.874639000
1	-5.299463000	-1.536258000	2.109412000
1	-1.123352000	4.336522000	0.342752000
1	-2.544078000	2.115623000	1.077567000
1	-2.256598000	-2.075341000	-0.883071000
1	-0.461769000	-3.713288000	-2.138597000
1	-7.063915000	-1.181357000	0.655887000
1	-8.967538000	-0.691707000	-0.828304000
1	-8.626214000	0.621714000	-2.912043000
1	3.120197000	2.644940000	0.714203000
1	4.986669000	3.964039000	-0.190384000
1	4.575240000	5.709286000	-1.918804000
1	2.261607000	6.105253000	-2.740614000
1	0.385392000	4.748239000	-1.867638000
1	-6.349903000	1.441431000	-3.490497000
1	-4.435653000	0.951906000	-1.992160000
1	1.768533000	-3.515782000	-3.375935000
1	3.965927000	-4.496436000	-3.946194000
1	5.794770000	-4.521527000	-2.261955000
1	5.396454000	-3.578763000	0.007031000
1	3.193803000	-2.651374000	0.595304000
8	2.970802000	0.322134000	-1.169737000
1	3.898587000	0.440538000	-0.886972000
1	2.661740000	1.203120000	-1.436587000

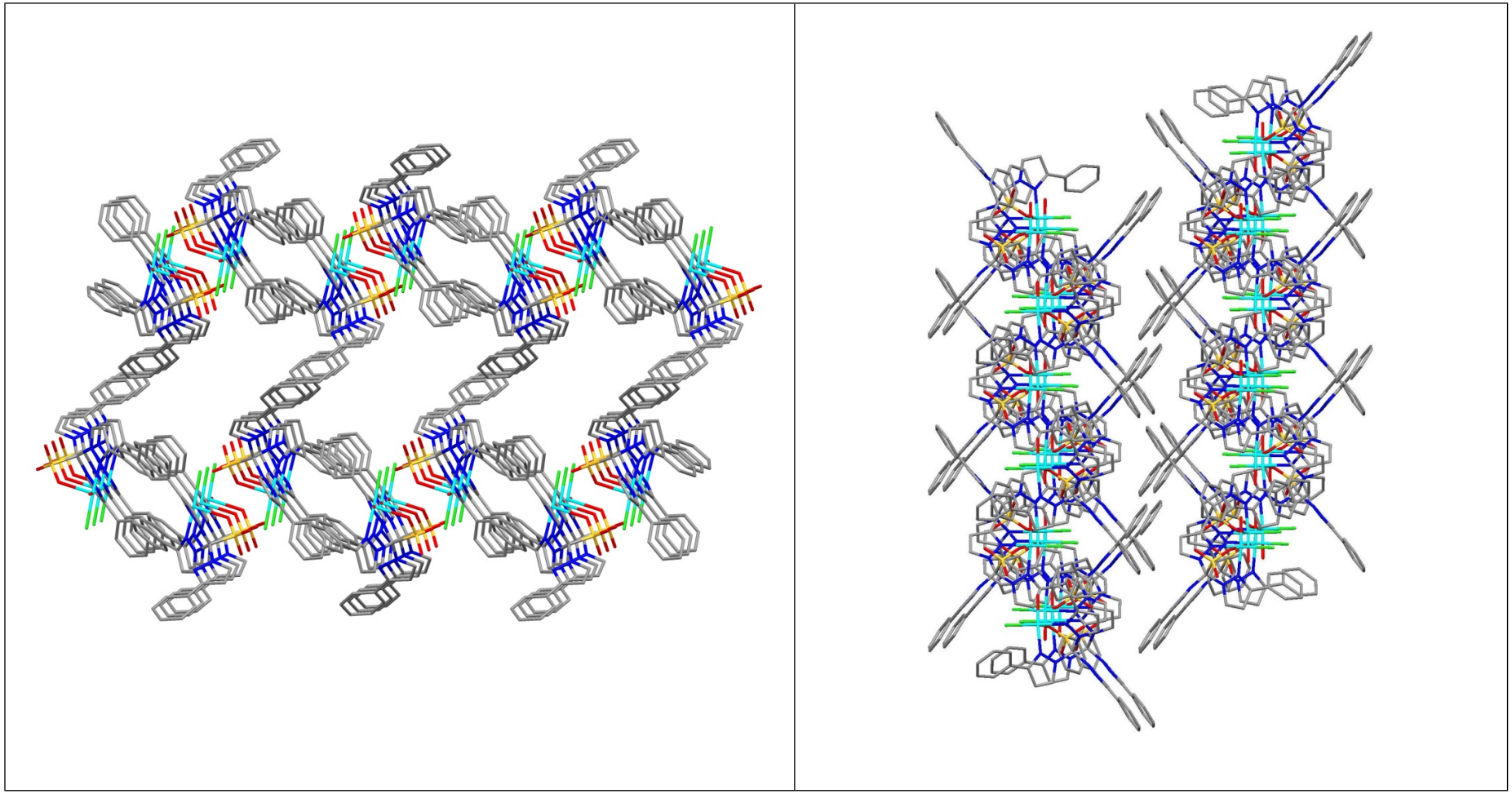

Figure S15 - Fragments of the crystal packing diagram of **4** (arbitrary views) showing the orientation of the non-coordinated phenyl pyrazolyl group towards the least crowded region of the pad.