# Electronic Supporting Information

## Dinuclear Tethered Pyridine, Diimine Complexes

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**Magnetic Properties of Complex 11-$NiCl_2$.**

The magnetic susceptibility data were recorded with a Quantum Design PPMS Dynacool vibrating sample magnetometer at the Fachbereich Physik of the Universität Hamburg. Upon diamagnetic corrections with the according Pascal constants the vT magnetic susceptibility data of complex **11-$Cl_2$** were fitted with the JulX program[1] for two 2independent S = 1 nickel spin centers. The fit parameters reveal a weak antiferromagnetic coupling with J = - 1.44 $cm^{-1}$, a magnetic anisotropy with a zero field splitting of D = -6.95 $cm^{-1}$ (E = 0) and a g-value of 2.268. The effective magnetic moment $\mu_{eff}$ amounts to 4.33 $\mu_B$, which is slightly larger than the anticipated theoretical value of 4 ($\mu_{eff}^2 = \Sigma\ \mu_i^2$).

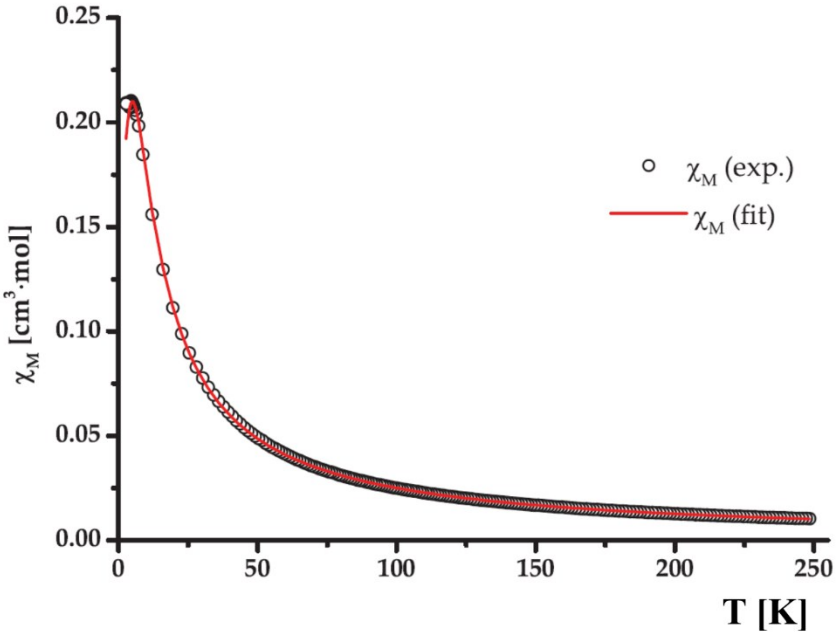



**Fig. S1.** Experimental and fitted temperature dependent magnetic susceptibility of complex **11-$NiCl_2$.**

[1] Kindly provided by Dr. Eckhard Bill, Max-Planck Institut für Chemische Energiekonversion, Mülheim, Germany. https://cec.mpg.de/en/research/molecular-theory-and-spectroscopy/dr-eckhard-bill/

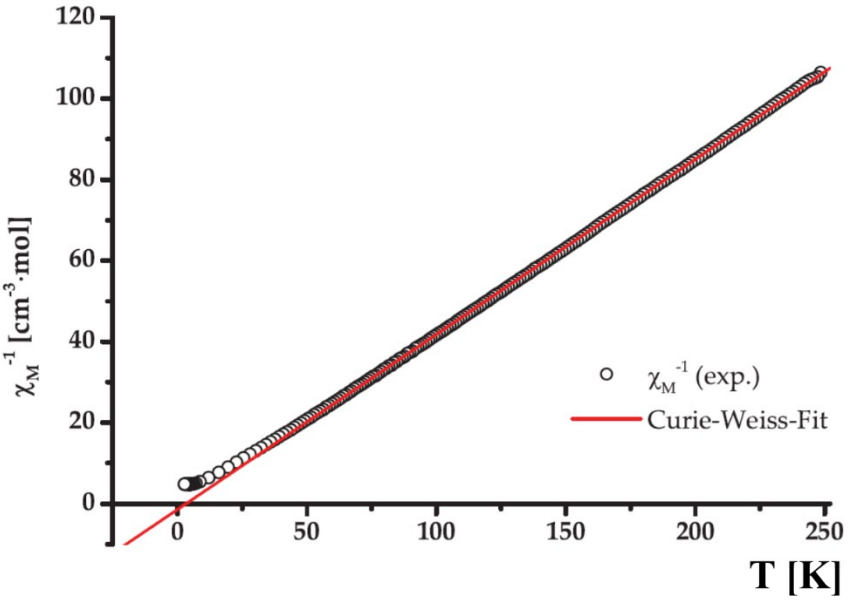



**Fig. S2.** Experimental and fitted reciprocal magnetic susceptibility vs temperature of complex **11-$NiCl_2$.**

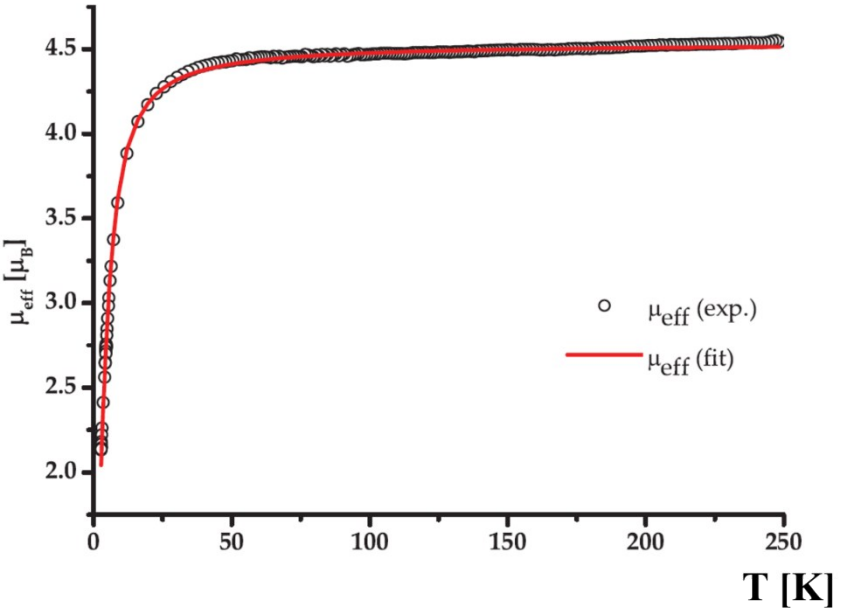
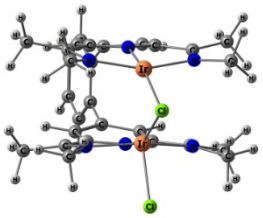



**Fig. S3.** Effective magnetic moment $\mu_{eff}$ in units of $\mu_B$ vs temperature of complex **11-$NiCl_2$.**

**70**
**phenyl_bridge short: DPLNO-CCSD(T) -2539.98550566 H**



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| C | -0.010753000 | -1.285815000 | -5.847777000 |
| C | -0.057127000 | -1.425760000 | -3.294008000 |
| N | -0.108805000 | -1.777234000 | -0.559610000 |
| C | 1.139850000 | -1.652769000 | -2.591990000 |
| C | -1.287438000 | -1.549114000 | -2.624726000 |
| C | -1.318295000 | -1.703827000 | -1.236780000 |
| C | 1.120263000 | -1.806800000 | -1.203872000 |
| H | 2.093335000 | -1.541398000 | -3.108891000 |
| H | -2.213778000 | -1.356917000 | -3.166533000 |
| C | 0.056200000 | 1.346254000 | -3.131520000 |
| N | 0.033002000 | 1.660424000 | -0.393142000 |
| C | -1.155787000 | 1.558522000 | -2.451464000 |
| C | 1.263188000 | 1.457624000 | -2.419205000 |
| C | 1.254569000 | 1.609901000 | -1.032703000 |
| C | -1.171199000 | 1.710395000 | -1.064787000 |
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| C | 2.354850000 | 1.575580000 | -0.098592000 |
| C | -2.294502000 | 1.767855000 | -0.159956000 |
| N | -1.983545000 | 1.602133000 | 1.126926000 |
| N | 1.998084000 | 1.436812000 | 1.179363000 |
| C | 2.208488000 | -1.813249000 | -0.274312000 |
| C | -2.427375000 | -1.619032000 | -0.336355000 |
| N | -2.077812000 | -1.454250000 | 0.961029000 |
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| H | -4.488975000 | -0.954819000 | -0.474236000 |
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| C | 2.842707000 | -1.778069000 | 2.058575000 |
| H | 2.402213000 | -1.477236000 | 3.014196000 |
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| C | 0.100616000 | 1.499294000 | -5.672538000 |
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| C | 0.040114000 | -0.513508000 | -7.011289000 |
| H | 0.036721000 | -1.001054000 | -7.987664000 |
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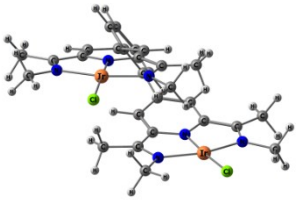
| Cl | 0.070783000 | 3.459894000 | 2.639824000 |

**70**
**phenyl bridge long: DPLNO-CCSD(T) -2540.00300155 H**



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| H | -0.408407000 | -1.357125000 | -7.654705000 |
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| C | -1.335476000 | -1.424494000 | -0.697534000 |
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| C | 0.205134000 | 1.311137000 | -3.011232000 |
| N | 0.135529000 | 2.343405000 | -0.432059000 |
| C | -0.553119000 | 2.458561000 | -2.727235000 |
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| C | -2.050559000 | 5.283011000 | 1.073653000 |
| H | -1.627335000 | 6.260786000 | 0.791937000 |
| H | -1.978517000 | 5.161371000 | 2.159221000 |
| H | -3.109440000 | 5.267948000 | 0.771207000 |
| C | 2.431222000 | -0.464228000 | 0.507292000 |
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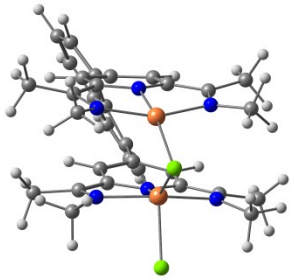
**76**
**naphthyl_bridge short: DPLNO-CCSD(T) -2693.35102091 H**



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| H | 2.380131000 | -1.617182000 | 3.301051000 |
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| H | -3.926126000 | 1.831203000 | 2.289675000 |
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| C | 3.598696000 | 1.483730000 | -0.747921000 |
| H | 3.575061000 | 1.439517000 | -1.842332000 |
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| H | 4.064091000 | 2.440648000 | -0.461592000 |
| C | 3.028800000 | 1.432784000 | 2.106956000 |
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| H | 3.109692000 | 2.496056000 | 2.385663000 |
| H | 4.002123000 | 1.080971000 | 1.737217000 |
| C | -0.479055000 | 1.139827000 | -4.486593000 |
| C | -1.066437000 | 2.187685000 | -5.187202000 |
| H | -1.424184000 | 3.049381000 | -4.620257000 |
| C | -1.143495000 | 2.204799000 | -6.592344000 |
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| H | -0.570862000 | 1.195712000 | -8.402832000 |
| Ir | -0.013328000 | -1.323902000 | 1.402845000 |
| Ir | 0.000008000 | 1.297368000 | 1.604892000 |
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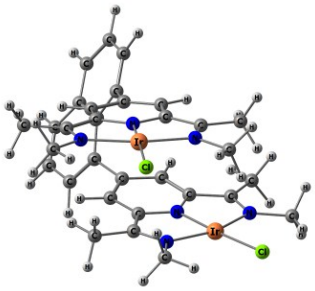
| Cl | 0.224728000 | 3.399449000 | 2.708457000 |

**76**
**naphthyl_bridge long : DPLNO-CCSD(T)-2693.36218032**



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| N | 0.575536000 | 1.910783000 | -0.375517000 |
| C | 0.019347000 | 2.027097000 | -2.699376000 |
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| C | 1.534365000 | 0.947148000 | -0.621425000 |
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| H | -0.587719000 | 2.425126000 | -3.511576000 |
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| C | 2.113323000 | 0.466295000 | 0.614005000 |
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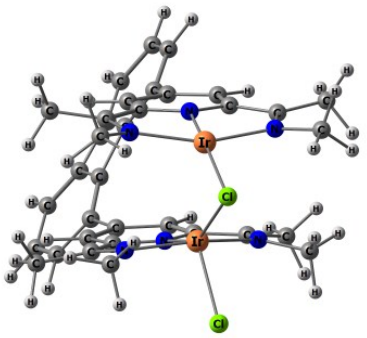
| H | -3.189942000 | -0.478193000 | 3.070988000 |
| H | -1.695503000 | 0.501306000 | 3.200884000 |
| C | -3.138899000 | 0.624912000 | 0.652941000 |
| H | -2.838290000 | 1.430946000 | 1.337487000 |
| H | -4.110663000 | 0.233704000 | 0.996305000 |
| H | -3.278796000 | 1.057926000 | -0.343630000 |
| C | 2.008154000 | -4.250758000 | -1.730246000 |
| H | 3.068527000 | -4.038174000 | -1.516117000 |
| H | 1.825877000 | -4.028320000 | -2.787141000 |
| H | 1.866637000 | -5.333062000 | -1.583585000 |
| C | 1.991442000 | -4.568925000 | 1.093765000 |
| H | 1.876033000 | -4.510668000 | 2.180933000 |
| H | 3.039316000 | -4.358265000 | 0.824613000 |
| H | 1.752228000 | -5.590696000 | 0.758479000 |
| C | -2.011089000 | 4.235973000 | -1.769004000 |
| H | -3.070705000 | 4.020646000 | -1.553881000 |
| H | -1.827420000 | 4.007192000 | -2.824301000 |
| H | -1.874093000 | 5.319838000 | -1.629696000 |
| C | -1.998861000 | 4.570371000 | 1.053141000 |
| H | -1.766462000 | 5.591303000 | 0.710541000 |
| H | -1.883012000 | 4.520493000 | 2.140655000 |
| H | -3.045367000 | 4.350895000 | 0.785683000 |
| C | 3.148487000 | -0.608743000 | 0.649758000 |
| H | 3.346035000 | -0.998299000 | -0.354951000 |
| H | 2.804620000 | -1.442189000 | 1.280535000 |
| H | 4.098777000 | -0.238654000 | 1.066714000 |
| C | 2.094260000 | 0.542031000 | 3.016542000 |
| H | 1.704763000 | -0.477652000 | 3.186496000 |
| H | 1.708358000 | 1.204072000 | 3.797243000 |
| H | 3.193543000 | 0.510444000 | 3.063566000 |
| C | 1.108568000 | 0.598503000 | -4.394765000 |
| C | 2.231936000 | 0.959986000 | -5.122156000 |
| H | 3.063829000 | 1.437379000 | -4.600352000 |
| C | 2.277540000 | 0.814736000 | -6.525922000 |
| H | 3.175011000 | 1.113248000 | -7.069820000 |
| C | 1.161712000 | 0.381565000 | -7.207884000 |
| H | 1.154091000 | 0.346722000 | -8.299310000 |
| Ir | -0.205790000 | -2.399885000 | 1.440939000 |
| Ir | 0.209323000 | 2.414899000 | 1.414785000 |
| Cl | 0.322923000 | -2.938777000 | 3.629539000 |
| Cl | -0.327943000 | 2.960163000 | 3.599850000 |

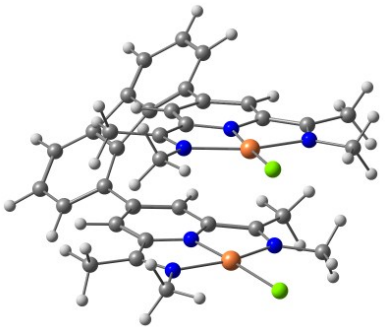
**78**
**biphenylene_bridge short (Ir..Ir 2.63 Å): DPLNO-CCSD(T) -2769.35752439 H**



| | | | |
|---|---|---|---|
| C | -0.111071000 | -0.898787000 | -3.426537000 |
| N | -0.197666000 | -1.500326000 | -0.728181000 |
| C | 1.082983000 | -1.130430000 | -2.709822000 |
| C | -1.345597000 | -0.998248000 | -2.770213000 |
| C | -1.394589000 | -1.254637000 | -1.394684000 |
| C | 1.041708000 | -1.447569000 | -1.355609000 |
| H | 2.039897000 | -1.026444000 | -3.220982000 |
| H | -2.263638000 | -0.776975000 | -3.315388000 |
| C | 1.636216000 | 2.262930000 | -2.241090000 |
| N | 0.811107000 | 1.670174000 | 0.330164000 |
| C | 0.265337000 | 2.224029000 | -1.921141000 |
| C | 2.581714000 | 2.031186000 | -1.229928000 |
| C | 2.165956000 | 1.706051000 | 0.063416000 |
| C | -0.154818000 | 1.960582000 | -0.618530000 |
| H | -0.468731000 | 2.404205000 | -2.705656000 |
| H | 3.643758000 | 2.046991000 | -1.473535000 |
| C | 2.952510000 | 1.361549000 | 1.219707000 |
| C | -1.482341000 | 1.939035000 | -0.057219000 |
| N | -1.544170000 | 1.553531000 | 1.220743000 |
| N | 2.241904000 | 0.967526000 | 2.280404000 |
| C | 2.111676000 | -1.684592000 | -0.433367000 |
| C | -2.513270000 | -1.270942000 | -0.509301000 |
| N | -2.186251000 | -1.389264000 | 0.802208000 |
| N | 1.719647000 | -1.775651000 | 0.854680000 |
| C | -3.254185000 | -1.621932000 | 1.768229000 |
| H | -2.836934000 | -1.548354000 | 2.777357000 |
| H | -3.683470000 | -2.628804000 | 1.636518000 |
| H | -4.073104000 | -0.892166000 | 1.663578000 |
| C | -3.930220000 | -1.256006000 | -0.985762000 |
| H | -3.972834000 | -1.164995000 | -2.077378000 |
| H | -4.510002000 | -0.420040000 | -0.558360000 |
| H | -4.464479000 | -2.180713000 | -0.711288000 |
| C | 3.525218000 | -1.908520000 | -0.866079000 |
| H | 4.226292000 | -1.224996000 | -0.362028000 |
| H | 3.627592000 | -1.757255000 | -1.946664000 |
| H | 3.860368000 | -2.934964000 | -0.641842000 |
| C | 2.692380000 | -2.191664000 | 1.856361000 |
| H | 2.229538000 | -2.114798000 | 2.844774000 |
| H | 3.601260000 | -1.568882000 | 1.832426000 |
| H | 2.998242000 | -3.237446000 | 1.689985000 |
| C | -2.671269000 | 2.436401000 | -0.817113000 |
| H | -3.505475000 | 1.721080000 | -0.781612000 |
| H | -2.417056000 | 2.599041000 | -1.870215000 |
| H | -3.037805000 | 3.391047000 | -0.407229000 |
| C | -2.765221000 | 1.711649000 | 1.990678000 |
| H | -3.667975000 | 1.559261000 | 1.381958000 |
| H | -2.790521000 | 2.723985000 | 2.425278000 |
| H | -2.751363000 | 0.997896000 | 2.820523000 |
| C | 4.442522000 | 1.506218000 | 1.241134000 |
| H | 4.818589000 | 1.798863000 | 0.254901000 |
| H | 4.944786000 | 0.568465000 | 1.525733000 |
| H | 4.760554000 | 2.276013000 | 1.961455000 |
| C | 2.877115000 | 0.760329000 | 3.572215000 |
| H | 2.327473000 | -0.020142000 | 4.110485000 |
| H | 2.785426000 | 1.690042000 | 4.156456000 |
| H | 3.936245000 | 0.482756000 | 3.486868000 |
| Ir | -0.222595000 | -1.385255000 | 1.168402000 |
| Ir | 0.242393000 | 1.050128000 | 2.032484000 |
| Cl | -0.329033000 | -0.804979000 | 3.594027000 |
| Cl | 0.060034000 | 2.766787000 | 3.680654000 |
| H | -1.263782000 | -1.990607000 | -5.706893000 |
| C | -0.645179000 | -1.116806000 | -5.921424000 |
| C | -0.018024000 | -0.447736000 | -4.829263000 |
| C | 0.374924000 | 0.373555000 | -7.598340000 |
| C | 0.736919000 | 0.652594000 | -5.192085000 |
| C | -0.460811000 | -0.720133000 | -7.242141000 |
| C | 0.965125000 | 1.035378000 | -6.546814000 |
| H | -0.957753000 | -1.284048000 | -8.033369000 |
| H | 0.521581000 | 0.648443000 | -8.643409000 |
| C | 1.570141000 | 1.810264000 | -4.717090000 |
| C | 2.051305000 | 2.525525000 | -3.635171000 |
| C | 1.856057000 | 2.161919000 | -6.071836000 |
| H | 2.940563000 | 3.480957000 | -7.420721000 |
| C | 2.944429000 | 3.586000000 | -3.976889000 |
| H | 3.363558000 | 4.189530000 | -3.169230000 |
| C | 3.258216000 | 3.902012000 | -5.293553000 |

| | | | |
|---|---|---|---|
| H | 3.936767000 | 4.734595000 | -5.486341000 |
| C | 2.700207000 | 3.197582000 | -6.395480000 |

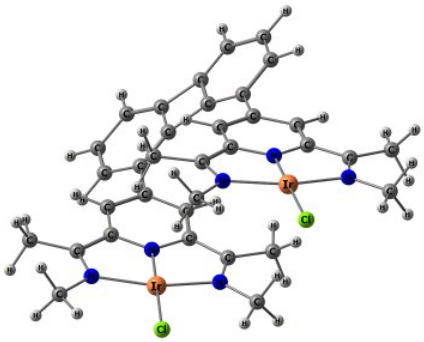
**78**
**biphenylene_bridge intermediate (Ir..Ir 3.53 Å) : DPLNO-CCSD(T)-2769.3620248 H**



| | | | |
|---|---|---|---|
| C | 0.286888000 | -1.862646000 | -2.916059000 |
| N | 0.770944000 | -1.618004000 | -0.188294000 |
| C | 1.254452000 | -0.958918000 | -2.435562000 |
| C | -0.396927000 | -2.680167000 | -1.998392000 |
| C | -0.159850000 | -2.545285000 | -0.626711000 |
| C | 1.505867000 | -0.848654000 | -1.072159000 |
| H | 1.806768000 | -0.346140000 | -3.146281000 |
| H | -1.146584000 | -3.385747000 | -2.356947000 |
| C | -0.296394000 | 1.881678000 | -2.895182000 |
| N | -0.762538000 | 1.608494000 | -0.166988000 |
| C | -1.260975000 | 0.973119000 | -2.417826000 |
| C | 0.393441000 | 2.689610000 | -1.973522000 |
| C | 0.165266000 | 2.540465000 | -0.601793000 |
| C | -1.503411000 | 0.848566000 | -1.054029000 |
| H | -1.817925000 | 0.367757000 | -3.131283000 |
| H | 1.141098000 | 3.398559000 | -2.329584000 |
| C | 0.775460000 | 3.214604000 | 0.519167000 |
| C | -2.447258000 | 0.004189000 | -0.362195000 |
| N | -2.414366000 | 0.098242000 | 0.969133000 |
| N | 0.342134000 | 2.815889000 | 1.722013000 |
| C | 2.454282000 | -0.011518000 | -0.377743000 |
| C | -0.762887000 | -3.231006000 | 0.491125000 |
| N | -0.321021000 | -2.845566000 | 1.695169000 |
| N | 2.430737000 | -0.120202000 | 0.952676000 |
| C | -0.871178000 | -3.489732000 | 2.886174000 |
| H | -0.361207000 | -3.080988000 | 3.764085000 |
| H | -0.725264000 | -4.580851000 | 2.848742000 |
| H | -1.951287000 | -3.289737000 | 2.974187000 |
| C | -1.780816000 | -4.312042000 | 0.318618000 |
| H | -2.693880000 | -4.110940000 | 0.900794000 |
| H | -1.395160000 | -5.284367000 | 0.666270000 |
| H | -2.066002000 | -4.424061000 | -0.733385000 |
| C | 3.406853000 | 0.887445000 | -1.095267000 |
| H | 3.309830000 | 1.928159000 | -0.751094000 |
| H | 3.227455000 | 0.873440000 | -2.175299000 |
| H | 4.451580000 | 0.585705000 | -0.917203000 |
| C | 3.375885000 | 0.668467000 | 1.737975000 |
| H | 3.165563000 | 0.500452000 | 2.799249000 |
| H | 3.282158000 | 1.740616000 | 1.504828000 |
| H | 4.412053000 | 0.362526000 | 1.521750000 |
| C | -3.405447000 | -0.886248000 | -1.082872000 |
| H | -3.305338000 | -1.931071000 | -0.752398000 |
| H | -3.234953000 | -0.858888000 | -2.164096000 |
| H | -4.448753000 | -0.587075000 | -0.892539000 |
| C | -3.355015000 | -0.697880000 | 1.752299000 |
| H | -4.392128000 | -0.386914000 | 1.548051000 |
| H | -3.136015000 | -0.543090000 | 2.813820000 |
| H | -3.265755000 | -1.767336000 | 1.505453000 |
| C | 1.790712000 | 4.298856000 | 0.351293000 |
| H | 2.066876000 | 4.424097000 | -0.701638000 |
| H | 2.708977000 | 4.091942000 | 0.923201000 |
| H | 1.406803000 | 5.266316000 | 0.714098000 |
| C | 0.899206000 | 3.448520000 | 2.915996000 |
| H | 1.981029000 | 3.253220000 | 2.992669000 |
| H | 0.398494000 | 3.026966000 | 3.793190000 |
| H | 0.747418000 | 4.539243000 | 2.892700000 |
| Ir | 1.081451000 | -1.421198000 | 1.669627000 |
| Ir | -1.059597000 | 1.390855000 | 1.690825000 |
| Cl | 1.566988000 | -1.267481000 | 3.922952000 |
| Cl | -1.527098000 | 1.209807000 | 3.945996000 |
| H | -0.081735000 | -4.046925000 | -4.594133000 |
| C | -0.106498000 | -3.091932000 | -5.123065000 |
| C | 0.027484000 | -1.889504000 | -4.364349000 |
| C | -0.164054000 | -1.890738000 | -7.274985000 |
| C | -0.016681000 | -0.729954000 | -5.122776000 |
| C | -0.205467000 | -3.089716000 | -6.509391000 |
| C | -0.059521000 | -0.727766000 | -6.549408000 |
| H | -0.286003000 | -4.045240000 | -7.030359000 |
| H | -0.208644000 | -1.921038000 | -8.364092000 |
| C | -0.007127000 | 0.771478000 | -5.115194000 |
| C | -0.046240000 | 1.923270000 | -4.344755000 |
| C | 0.026457000 | 0.783759000 | -6.542018000 |
| H | 0.163938000 | 1.995383000 | -8.345426000 |
| C | 0.083024000 | 3.133333000 | -5.092074000 |
| H | 0.061848000 | 4.082928000 | -4.553340000 |
| C | 0.173001000 | 3.145168000 | -6.478971000 |

| | | | |
|---|---|---|---|
| H | 0.250250000 | 4.105928000 | -6.990724000 |
| C | 0.126419000 | 1.954031000 | -7.256414000 |

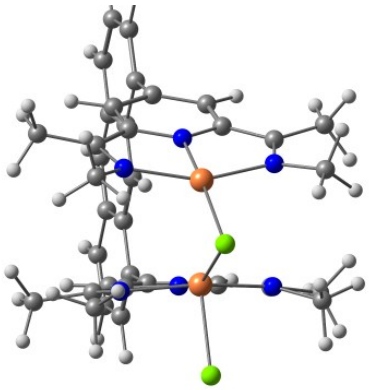
**78**
**biphenylene_bridge long (Ir..Ir 5.21 Å) : DPLNO-CCSD(T)-2769.36824786**



| | | | |
|---|---|---|---|
| C | -0.676106000 | -1.973679000 | -2.930418000 |
| N | -0.713582000 | -2.305918000 | -0.168483000 |
| C | 0.384197000 | -1.493329000 | -2.138787000 |
| C | -1.748860000 | -2.634281000 | -2.301311000 |
| C | -1.766241000 | -2.797377000 | -0.917039000 |
| C | 0.361652000 | -1.665312000 | -0.753381000 |
| H | 1.231094000 | -1.001462000 | -2.614785000 |
| H | -2.585488000 | -2.990623000 | -2.901096000 |
| C | 0.678307000 | 1.973703000 | -2.930479000 |
| N | 0.712294000 | 2.307365000 | -0.168578000 |
| C | -0.382878000 | 1.493639000 | -2.139890000 |
| C | 1.750248000 | 2.634631000 | -2.300334000 |
| C | 1.765903000 | 2.798433000 | -0.916175000 |
| C | -0.362051000 | 1.666196000 | -0.754559000 |
| H | -1.229095000 | 1.001377000 | -2.616690000 |
| H | 2.587577000 | 2.990755000 | -2.899276000 |
| C | 2.765225000 | 3.412345000 | -0.072652000 |
| C | -1.318259000 | 1.239086000 | 0.244026000 |
| N | -0.985628000 | 1.529472000 | 1.503389000 |
| N | 2.493497000 | 3.382472000 | 1.235675000 |
| C | 1.316748000 | -1.237981000 | 0.246189000 |
| C | -2.766559000 | -3.411039000 | -0.074527000 |
| N | -2.496332000 | -3.380798000 | 1.234104000 |
| N | 0.982507000 | -1.527720000 | 1.505290000 |
| C | -3.453008000 | -3.983605000 | 2.161023000 |
| H | -3.079960000 | -3.841710000 | 3.180156000 |
| H | -3.563460000 | -5.061461000 | 1.961407000 |
| H | -4.445021000 | -3.514189000 | 2.064446000 |
| C | -4.008690000 | -4.033243000 | -0.624140000 |
| H | -4.912722000 | -3.531881000 | -0.243170000 |
| H | -4.087720000 | -5.092839000 | -0.334204000 |
| H | -4.028900000 | -3.980802000 | -1.717774000 |
| C | 2.583547000 | -0.531180000 | -0.104943000 |
| H | 2.709408000 | 0.362855000 | 0.523041000 |
| H | 2.584037000 | -0.215636000 | -1.153972000 |
| H | 3.458827000 | -1.181784000 | 0.057918000 |
| C | 1.869381000 | -1.094180000 | 2.582704000 |
| H | 1.500261000 | -1.508565000 | 3.525247000 |
| H | 1.855012000 | 0.009904000 | 2.644888000 |
| H | 2.903725000 | -1.426412000 | 2.404866000 |
| C | -2.584582000 | 0.532117000 | -0.108437000 |
| H | -2.711742000 | -0.361089000 | 0.520434000 |
| H | -2.583272000 | 0.215187000 | -1.157042000 |
| H | -3.460016000 | 1.183111000 | 0.052009000 |
| C | -1.873827000 | 1.096351000 | 2.579881000 |
| H | -2.907510000 | 1.430485000 | 2.401635000 |
| H | -1.504705000 | 1.509426000 | 3.522997000 |
| H | -1.861306000 | -0.007798000 | 2.641203000 |
| C | 4.008313000 | 4.033843000 | -0.620922000 |
| H | 4.031024000 | 3.978893000 | -1.714388000 |
| H | 4.911656000 | 3.533769000 | -0.236684000 |
| H | 4.086191000 | 5.094181000 | -0.333320000 |
| C | 3.449568000 | 3.984670000 | 2.163603000 |
| H | 4.439139000 | 3.508794000 | 2.073420000 |
| H | 3.071738000 | 3.849521000 | 3.181897000 |
| H | 3.567465000 | 5.060836000 | 1.959201000 |
| Ir | -0.766564000 | -2.487961000 | 1.717563000 |
| Ir | 0.763071000 | 2.489999000 | 1.717350000 |
| Cl | -0.852769000 | -2.700701000 | 4.014576000 |
| Cl | 0.846995000 | 2.702622000 | 4.014781000 |
| H | -1.429601000 | -3.839792000 | -4.700230000 |
| C | -1.118631000 | -2.924593000 | -5.206890000 |
| C | -0.669129000 | -1.832485000 | -4.395790000 |
| C | -0.692430000 | -1.752181000 | -7.313038000 |
| C | -0.252388000 | -0.717203000 | -5.112799000 |
| C | -1.131564000 | -2.892581000 | -6.592290000 |
| C | -0.261343000 | -0.700794000 | -6.543328000 |
| H | -1.473515000 | -3.773501000 | -7.137919000 |
| H | -0.702103000 | -1.732152000 | -8.403072000 |
| C | 0.257251000 | 0.716259000 | -5.112817000 |
| C | 0.673018000 | 1.831860000 | -4.395784000 |
| C | 0.267905000 | 0.699224000 | -6.543322000 |
| H | 0.710695000 | 1.729860000 | -8.402993000 |
| C | 1.123307000 | 2.923701000 | -5.206819000 |
| H | 1.433504000 | 3.839181000 | -4.700197000 |
| C | 1.137794000 | 2.891130000 | -6.592184000 |

| | | | |
|---|---|---|---|
| H | 1.480150000 | 3.771903000 | -7.137792000 |
| C | 0.699714000 | 1.750340000 | -7.312984000 |

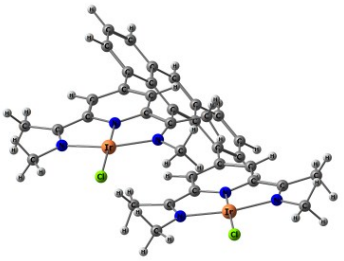
**82**
**anthracene_bridge short : DPLNO-CCSD(T)-2846.70082449 H**



| | | | |
|---|---|---|---|
| C | 0.270931000 | -1.551356000 | -3.494900000 |
| N | -0.082691000 | -1.642335000 | -0.753740000 |
| C | 1.350607000 | -1.871977000 | -2.654869000 |
| C | -0.992575000 | -1.293016000 | -2.938132000 |
| C | -1.176934000 | -1.331845000 | -1.552649000 |
| C | 1.179511000 | -1.915325000 | -1.268096000 |
| H | 2.337978000 | -2.027792000 | -3.089255000 |
| H | -1.815058000 | -1.001846000 | -3.591141000 |
| C | 1.244359000 | 2.950833000 | -2.154750000 |
| N | 0.673515000 | 1.868604000 | 0.319683000 |
| C | -0.067897000 | 2.978757000 | -1.655465000 |
| C | 2.268760000 | 2.394254000 | -1.371544000 |
| C | 1.984950000 | 1.854094000 | -0.114982000 |
| C | -0.358466000 | 2.440499000 | -0.399471000 |
| H | -0.864942000 | 3.393421000 | -2.271643000 |
| H | 3.282964000 | 2.356347000 | -1.768173000 |
| C | 2.872631000 | 1.281164000 | 0.861511000 |
| C | -1.604766000 | 2.399250000 | 0.317373000 |
| N | -1.555921000 | 1.769130000 | 1.496631000 |
| N | 2.273306000 | 0.811451000 | 1.961126000 |
| C | 2.122891000 | -2.200405000 | -0.234950000 |
| C | -2.349624000 | -1.091958000 | -0.775027000 |
| N | -2.149884000 | -1.139897000 | 0.563617000 |
| N | 1.628694000 | -2.078010000 | 1.019875000 |
| C | -3.317989000 | -1.163439000 | 1.435758000 |
| H | -2.980447000 | -1.124631000 | 2.475684000 |
| H | -3.892600000 | -2.092353000 | 1.287513000 |
| H | -3.996694000 | -0.317504000 | 1.243602000 |
| C | -3.705021000 | -0.909499000 | -1.378579000 |
| H | -3.645429000 | -0.908191000 | -2.472817000 |
| H | -4.172989000 | 0.039831000 | -1.068073000 |
| H | -4.397964000 | -1.715577000 | -1.085676000 |
| C | 3.506318000 | -2.696839000 | -0.507626000 |
| H | 4.274560000 | -2.060897000 | -0.036650000 |
| H | 3.706021000 | -2.717329000 | -1.584782000 |
| H | 3.660374000 | -3.718542000 | -0.122471000 |
| C | 2.424446000 | -2.590410000 | 2.128669000 |
| H | 1.917498000 | -2.346436000 | 3.067136000 |
| H | 3.439353000 | -2.162912000 | 2.143772000 |
| H | 2.524309000 | -3.685934000 | 2.058737000 |
| C | -2.833753000 | 3.095107000 | -0.176368000 |
| H | -3.693195000 | 2.408676000 | -0.231814000 |
| H | -2.672816000 | 3.508258000 | -1.177866000 |
| H | -3.122099000 | 3.925240000 | 0.487687000 |
| C | -2.648537000 | 1.905400000 | 2.446565000 |
| H | -3.634062000 | 1.909588000 | 1.959692000 |
| H | -2.518025000 | 2.847214000 | 3.003734000 |
| H | -2.593875000 | 1.083410000 | 3.167161000 |
| C | 4.359740000 | 1.304218000 | 0.698968000 |
| H | 4.639114000 | 1.687520000 | -0.288249000 |
| H | 4.794439000 | 0.297328000 | 0.801566000 |
| H | 4.838470000 | 1.944894000 | 1.456239000 |
| C | 3.057944000 | 0.485499000 | 3.141356000 |
| H | 2.471680000 | -0.179613000 | 3.782466000 |
| H | 3.246622000 | 1.412486000 | 3.707198000 |
| H | 4.019755000 | 0.014217000 | 2.893097000 |
| Ir | -0.242033000 | -1.376231000 | 1.119593000 |
| Ir | 0.267624000 | 1.052322000 | 1.987801000 |
| Cl | -0.377039000 | -0.770092000 | 3.534449000 |
| Cl | 0.495672000 | 2.735883000 | 3.662106000 |
| H | 0.114018000 | -3.222437000 | -5.682968000 |
| C | 0.403415000 | -2.200848000 | -5.935985000 |
| C | 0.518128000 | -1.263059000 | -4.934825000 |
| C | 1.025617000 | -0.580867000 | -7.643498000 |
| C | 0.900112000 | 0.082968000 | -5.273058000 |
| C | 0.658270000 | -1.857329000 | -7.294002000 |
| C | 1.159786000 | 0.433486000 | -6.649589000 |
| C | 1.026385000 | 1.066148000 | -4.286235000 |
| H | 0.558914000 | -2.625607000 | -8.062709000 |
| H | 1.730635000 | 2.019993000 | -7.995395000 |
| H | 1.220927000 | -0.324284000 | -8.687083000 |
| C | 1.397547000 | 2.379793000 | -4.587877000 |
| H | 0.829427000 | 0.797806000 | -3.250803000 |
| C | 1.522796000 | 3.373513000 | -3.555842000 |
| C | 1.660120000 | 2.737288000 | -5.962612000 |
| H | 2.240388000 | 4.358480000 | -7.290066000 |

| | | | |
|---|---|---|---|
| C | 1.532609000 | 1.752154000 | -6.953813000 |
| C | 1.892534000 | 4.656224000 | -3.892844000 |
| H | 1.988313000 | 5.411245000 | -3.110373000 |
| C | 2.151641000 | 5.009992000 | -5.247264000 |
| H | 2.443131000 | 6.035300000 | -5.480868000 |
| C | 2.039575000 | 4.081334000 | -6.252898000 |

**82**
**anthracene_bridge long : DPLNO-CCSD(T)-2846.7107633**



| | | | |
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| C | -0.229144000 | -0.389518000 | -4.577437000 |
| C | -0.146558000 | -0.637769000 | -7.355929000 |
| C | -0.661601000 | -1.589986000 | -5.154890000 |
| C | 0.242991000 | 0.691974000 | -5.331703000 |
| C | 0.283805000 | 0.560988000 | -6.772071000 |
| C | -0.616542000 | -1.716540000 | -6.595481000 |
| H | -0.114117000 | -0.735129000 | -8.444433000 |
| C | -1.085402000 | -2.681007000 | -2.887092000 |
| N | -0.939156000 | -2.660650000 | -0.104445000 |
| C | -0.431635000 | -3.715831000 | -2.193473000 |
| C | -1.682300000 | -1.643736000 | -2.143135000 |
| C | -1.595667000 | -1.630763000 | -0.750183000 |
| C | -0.363395000 | -3.706364000 | -0.799444000 |
| H | 0.050473000 | -4.512057000 | -2.759612000 |
| H | -2.228889000 | -0.854396000 | -2.656311000 |
| C | 0.537341000 | 2.170197000 | -3.272155000 |
| N | 0.221179000 | 2.639802000 | -0.544122000 |
| C | -0.149789000 | 3.309093000 | -2.813264000 |
| C | 1.080973000 | 1.282638000 | -2.322125000 |
| C | 0.907689000 | 1.514007000 | -0.956762000 |
| C | -0.301661000 | 3.545722000 | -1.446225000 |
| H | -0.593127000 | 3.989725000 | -3.539220000 |
| H | 1.653766000 | 0.418166000 | -2.653799000 |
| C | 1.341694000 | 0.723942000 | 0.176116000 |
| C | -0.971098000 | 4.631375000 | -0.767458000 |
| N | -0.965052000 | 4.550571000 | 0.566453000 |
| N | 1.014959000 | 1.224840000 | 1.369289000 |
| C | 0.261045000 | -4.649569000 | 0.099490000 |
| C | -2.099096000 | -0.658784000 | 0.197307000 |
| N | -1.850474000 | -0.940762000 | 1.477639000 |
| N | 0.170430000 | -4.336902000 | 1.395521000 |
| C | -2.327422000 | -0.011291000 | 2.501473000 |
| H | -2.050584000 | -0.403726000 | 3.483978000 |
| H | -3.421879000 | 0.098728000 | 2.444183000 |
| H | -1.870707000 | 0.983970000 | 2.364184000 |
| C | -2.820160000 | 0.578560000 | -0.221796000 |
| H | -2.328736000 | 1.468345000 | 0.210398000 |
| H | -3.863194000 | 0.575652000 | 0.133560000 |
| H | -2.829983000 | 0.684974000 | -1.312097000 |
| C | 0.952712000 | -5.882758000 | -0.383064000 |
| H | 2.007157000 | -5.902739000 | -0.065378000 |
| H | 0.927877000 | -5.950453000 | -1.475775000 |
| H | 0.481275000 | -6.791476000 | 0.023617000 |
| C | 0.771767000 | -5.238696000 | 2.376709000 |
| H | 0.588592000 | -4.831436000 | 3.375950000 |
| H | 1.857748000 | -5.328186000 | 2.212933000 |
| H | 0.331202000 | -6.245766000 | 2.305889000 |
| C | -1.617655000 | 5.760586000 | -1.501314000 |
| H | -2.696507000 | 5.815775000 | -1.284854000 |
| H | -1.496088000 | 5.651806000 | -2.584237000 |
| H | -1.184761000 | 6.729384000 | -1.206524000 |
| C | -1.614944000 | 5.610625000 | 1.335295000 |
| H | -1.134036000 | 6.583240000 | 1.143283000 |
| H | -1.526640000 | 5.367979000 | 2.398886000 |
| H | -2.679722000 | 5.696498000 | 1.065749000 |
| C | 2.076732000 | -0.565953000 | 0.026070000 |
| H | 2.147414000 | -0.865669000 | -1.025405000 |
| H | 1.555395000 | -1.365600000 | 0.581346000 |
| H | 3.098040000 | -0.496034000 | 0.433937000 |
| C | 1.418461000 | 0.490046000 | 2.567368000 |
| H | 0.965163000 | -0.516116000 | 2.574932000 |
| H | 1.081707000 | 1.045917000 | 3.447034000 |
| H | 2.513706000 | 0.377267000 | 2.601176000 |
| C | 0.646086000 | 1.942195000 | -4.731179000 |
| C | 1.069198000 | 2.971839000 | -5.552740000 |
| H | 1.383755000 | 3.913044000 | -5.098150000 |
| C | 1.128948000 | 2.829395000 | -6.962276000 |
| H | 1.485577000 | 3.664074000 | -7.567783000 |
| C | 0.744723000 | 1.655089000 | -7.560160000 |
| H | 0.782386000 | 1.540316000 | -8.645398000 |
| Ir | -0.813669000 | -2.633360000 | 1.786859000 |
| Ir | -0.024630000 | 2.942541000 | 1.310772000 |
| Cl | -0.649535000 | -2.611060000 | 4.091616000 |
| Cl | -0.345189000 | 3.316989000 | 3.568521000 |
| H | -0.261586000 | -0.292666000 | -3.496348000 |
| C | -1.035035000 | -2.935800000 | -7.203088000 |

| | | | |
|---|---|---|---|
| H | -1.007438000 | -3.015612000 | -8.291801000 |
| C | -1.105872000 | -2.715965000 | -4.367272000 |
| C | -1.484681000 | -3.877305000 | -5.016838000 |
| H | -1.831181000 | -4.724588000 | -4.421990000 |
| C | -1.459342000 | -3.987868000 | -6.430298000 |
| H | -1.783086000 | -4.918991000 | -6.897994000 |

Transition state coordinates (RI-DFT, PBE-D3 functional; basis: C,H,N,Cl def-SV(P); Ir: def2-TZVP basis & ECP-60-MWB pseudopotential) for the conversion of the μ-Cl-bridged and unbridged iridium system with the phenyl linker ($\nu_{imag}$= -44 $cm^{-1}$). The Ir—Ir distance in Å and the scaled vectors are presented.

```
70
Energy = -2540.849936099 Hartree
H     -1.6218637   -1.4060533   -6.3884624
C     -0.3898520   -0.3910820   -4.9231511
C     -0.7853484   -0.7053740   -6.2338339
C     -1.0095224   -0.9405613   -3.6761691
N     -1.3468222   -1.1307847   -0.9357377
C     -0.2677370   -1.8912428   -2.9364607
C     -2.0596326   -0.2391828   -3.0482240
C     -2.2372294   -0.3404613   -1.6533033
C     -0.4296725   -1.9651338   -1.5440416
H      0.5484646   -2.4406853   -3.4280560
H     -2.6304194    0.5079195   -3.6210521
C      1.0542458    0.8446231   -3.2940895
N      1.1999111    0.9298653   -0.5132629
C      0.2417640    1.7373924   -2.5589231
C      2.0462332    0.1110657   -2.6099525
C      2.1281153    0.1691218   -1.2051876
C      0.3125672    1.7817542   -1.1574010
H     -0.5063813    2.3420682   -3.0908112
H      2.7046177   -0.5672137   -3.1730389
C      3.0543235   -0.4818078   -0.3001720
C     -0.4750079    2.5543554   -0.2116358
N     -0.2132678    2.3040442    1.0759494
N      2.8322263   -0.2469310    1.0029715
C      0.3658950   -2.6767612   -0.5634677
C     -3.1245217    0.3734986   -0.7723213
N     -2.8341948    0.2377636    0.5491238
N      0.1513123   -2.2969703    0.7079825
C     -3.7484931    0.8134587    1.5294325
H     -3.3631936    0.5835945    2.5421023
H     -4.7733753    0.3906431    1.4211034
H     -3.8218442    1.9198678    1.4109453
C     -4.3269398    1.1238820   -1.2613930
H     -4.3395466    2.1828989   -0.9153102
H     -5.2741996    0.6617160   -0.8979069
H     -4.3685607    1.1293091   -2.3691243
C      1.3129602   -3.7787300   -0.9375205
H      2.3681282   -3.5307680   -0.6801254
H      1.2691189   -3.9896191   -2.0247677
H      1.0648339   -4.7244494   -0.4045488
C      0.8098882   -3.0088004    1.7960312
H      0.7247948   -2.3977160    2.7165113
H      1.8800962   -3.2120080    1.5712337
H      0.3020436   -3.9852337    1.9723138
C     -1.4842899    3.5700406   -0.6653855
H     -2.4884279    3.3724166   -0.2320674
H     -1.5911844    3.5618767   -1.7674796
H     -1.1907149    4.6006029   -0.3625699
C     -0.9048064    2.9673605    2.1653814
H     -1.7004261    3.6638295    1.8287964
H     -0.1556146    3.5109152    2.7805914
H     -1.3293926    2.1733669    2.8205318
C      4.2180164   -1.2929507   -0.7902600
H      4.0892782   -1.5801183   -1.8530089
H      4.3486730   -2.2245026   -0.1983935
H      5.1748027   -0.7245218   -0.7131191
C      3.7613396   -0.7731091    1.9992968
H      3.6105139   -1.8681873    2.1363227
H      3.5582581   -0.2581996    2.9601321
H      4.8200912   -0.5980088    1.7052601
C      0.6948421    0.5184868   -4.7136853
C      1.3584303    1.0670226   -5.8248291
H      2.1931727    1.7675521   -5.6598331
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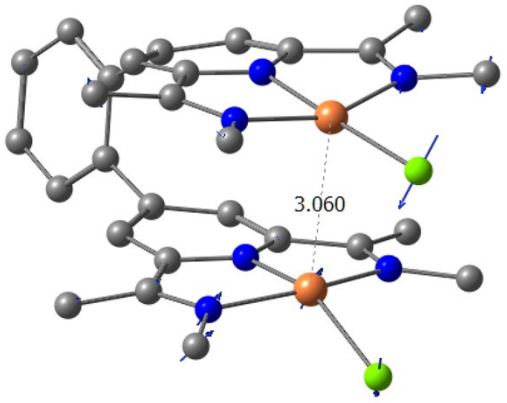

| | | | |
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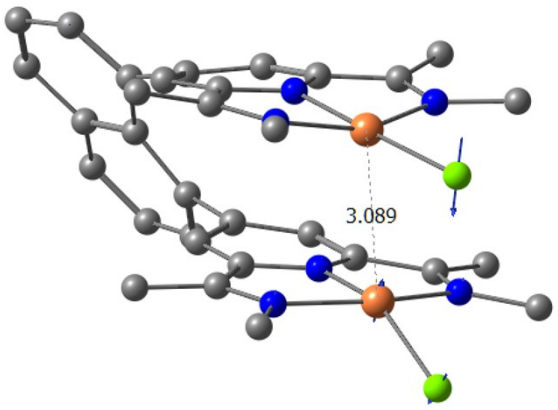
| C | 0.9564641 | 0.7375299 | -7.1308200 |
| H | 1.4836748 | 1.1763013 | -7.9936826 |
| C | -0.1166915 | -0.1428125 | -7.3348384 |
| H | -0.4346348 | -0.3985072 | -8.3588518 |
| Ir | -1.1948796 | -0.8206768 | 0.9403381 |
| Ir | 1.2573595 | 0.9540389 | 1.3851211 |
| Cl | -1.0587364 | -0.4525846 | 3.2752613 |
| Cl | 1.9915497 | 1.6590440 | 3.4875171 |

Transition state coordinates for the conversion of the μ-Cl-bridged and unbridged iridium system with the naphthyl linker ($\nu_{imag}$= -48 $cm^{-1}$). The Ir—Ir distance in Å and the scaled vectors are presented.

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76
Energy = -2696.239376759 Hartree (RI-DFT: PBE-D3, def2-TZVP basis, Ir: ECP-60-MWB)
C      0.1306175   -0.8971471   -4.7270382
C      0.4905546   -0.3493862   -7.4725213
C      0.3461621   -1.9111105   -5.6523475
C      0.1903662    0.4818208   -5.1514598
C      0.2999148    0.7293780   -6.5708166
C      0.5520184   -1.6469572   -7.0192938
H      0.2927387   -2.9446736   -5.3048683
H      0.7070405   -2.4726471   -7.7153412
H      0.5851069   -0.1234633   -8.5366865
C     -0.2160487   -1.2867661   -3.3422837
N     -0.6567313   -1.6289640   -0.6385136
C      0.6485342   -2.0962035   -2.5859722
C     -1.3920992   -0.7915529   -2.7512321
C     -1.6067972   -0.9597962   -1.3851993
C      0.4288902   -2.2627283   -1.2139133
H      1.5555017   -2.4892263   -3.0465199
H     -2.0806906   -0.1947300   -3.3478922
C      0.2933498    1.5768540   -2.8022574
N      0.5014750    1.3763626   -0.0404321
C     -0.6365569    2.2203488   -1.9654719
C      1.4003738    0.9409272   -2.2132465
C      1.5067116    0.8435155   -0.8269765
C     -0.5283758    2.1234961   -0.5754584
H     -1.4791923    2.7479472   -2.4119739
H      2.1633772    0.5010470   -2.8531826
C      2.5336317    0.2138967   -0.0243486
C     -1.3719433    2.6770589    0.4627547
N     -1.0013370    2.3693033    1.7063794
N      2.3273655    0.2688496    1.2892969
C      1.2184452   -2.9370548   -0.2188365
C     -2.6493629   -0.4275937   -0.5469426
N     -2.4359182   -0.5748042    0.7689593
N      0.8249971   -2.7155979    1.0511411
C     -3.4854227   -0.1700221    1.6991430
H     -3.1107727   -0.3088262    2.7188072
H     -4.3876932   -0.7867653    1.5602645
H     -3.7689968    0.8837520    1.5476631
C     -3.8989372    0.1744304   -1.1029763
H     -4.0678996    1.1954673   -0.7280739
H     -4.7857819   -0.4179837   -0.8240838
H     -3.8585026    0.2165000   -2.1971821
C      2.3101758   -3.8949563   -0.5718717
H      3.2476595   -3.6805560   -0.0341844
H      2.5215125   -3.8662156   -1.6472635
H      2.0330101   -4.9318020   -0.3164987
C      1.4672403   -3.4735369    2.1226940
H      1.0752841   -3.1138670    3.0799537
H      2.5620575   -3.3506714    2.1019513
H      1.2457490   -4.5483709    2.0239799
C     -2.5425587    3.5546041    0.1398390
H     -3.4718086    3.1903516    0.6021897
H     -2.7042457    3.6010977   -0.9425963
H     -2.3842570    4.5844236    0.4968090
C     -1.7493626    2.8343955    2.8649860
H     -2.5751933    3.5114437    2.6120640
H     -1.0460873    3.3297192    3.5488276
H     -2.1334427    1.9538634    3.4001621
C      3.7420464   -0.4119679   -0.6492448
H      3.6559700   -0.4132574   -1.7410756
H      3.8727298   -1.4542730   -0.3269345
H      4.6606299    0.1344126   -0.3845704
C      3.2631828   -0.3100029    2.2380842
H      2.6963354   -0.9570302    2.9206246
H      3.6814224    0.4999655    2.8531140
H      4.0747433   -0.8765913    1.7633893
C      0.1476508    1.6341634   -4.2795483
C      0.0452207    2.9042898   -4.8371740
H      0.0233958    3.7621910   -4.1624484
C      0.0517141    3.1215807   -6.2276184
H     -0.0208647    4.1375646   -6.6183991
```

| | | | |
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| C | 0.2160839 | 2.0521867 | -7.0765214 |
| H | 0.2863350 | 2.1996226 | -8.1562155 |
| Ir | -0.7014824 | -1.4521776 | 1.2553463 |
| Ir | 0.6609999 | 1.2560000 | 1.8452310 |
| Cl | -0.7828625 | -1.2677520 | 3.6033774 |
| Cl | 1.3293203 | 1.9033574 | 3.9779754 |

## NMR-Spectra


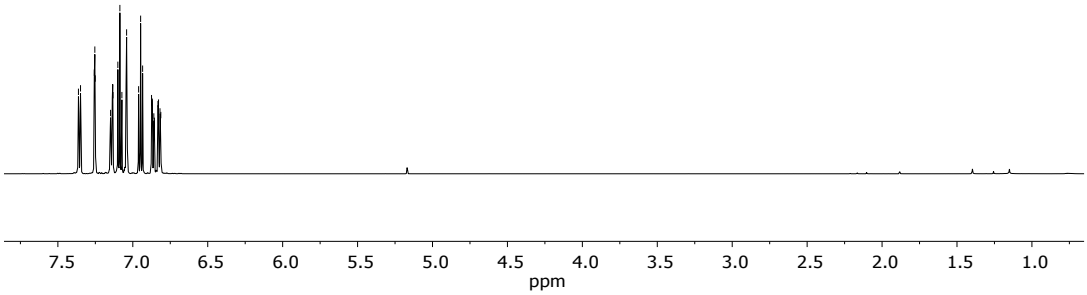


**Figure S4:** $^{1}$H-NMR spectrum of 1-iodo-3'bromodiphenyl ether in $CD_2Cl_2$, 600 MHz.

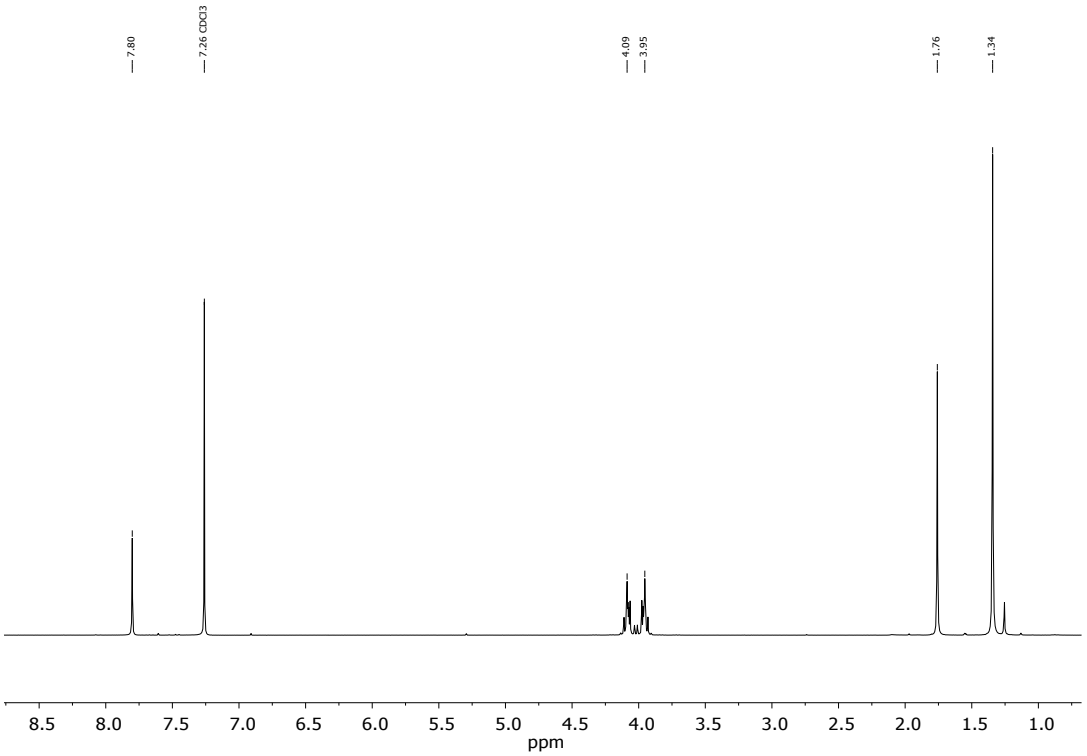


**Figure S5:** $^{1}$H-NMR spectrum of compound **4** in $CDCl_3$, 300 MHz.

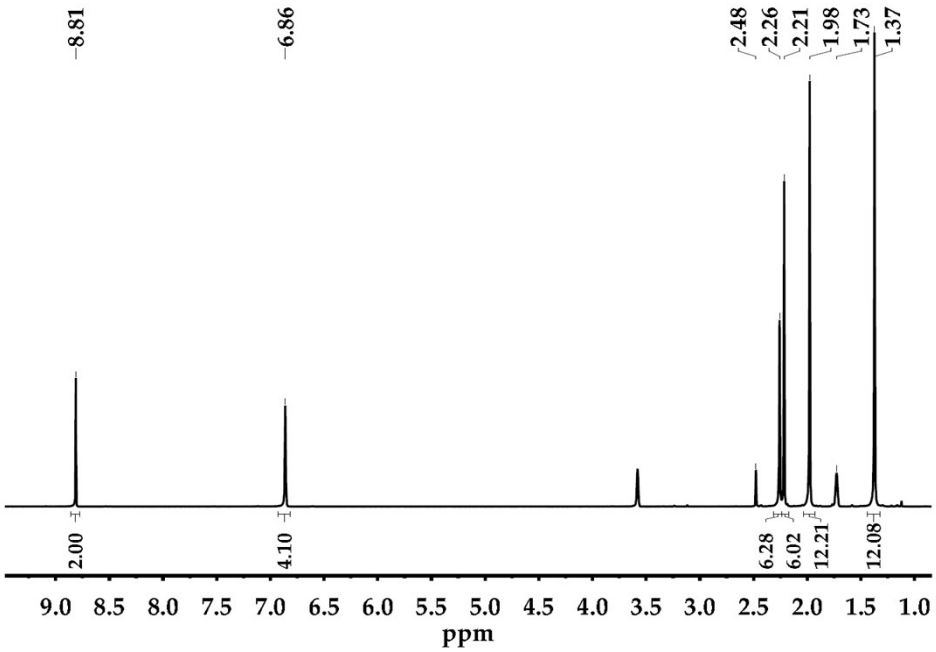


**Figure S6:** $^{1}$H-NMR spectrum of compound **5** in THF-$d_8$, 300 MHz.

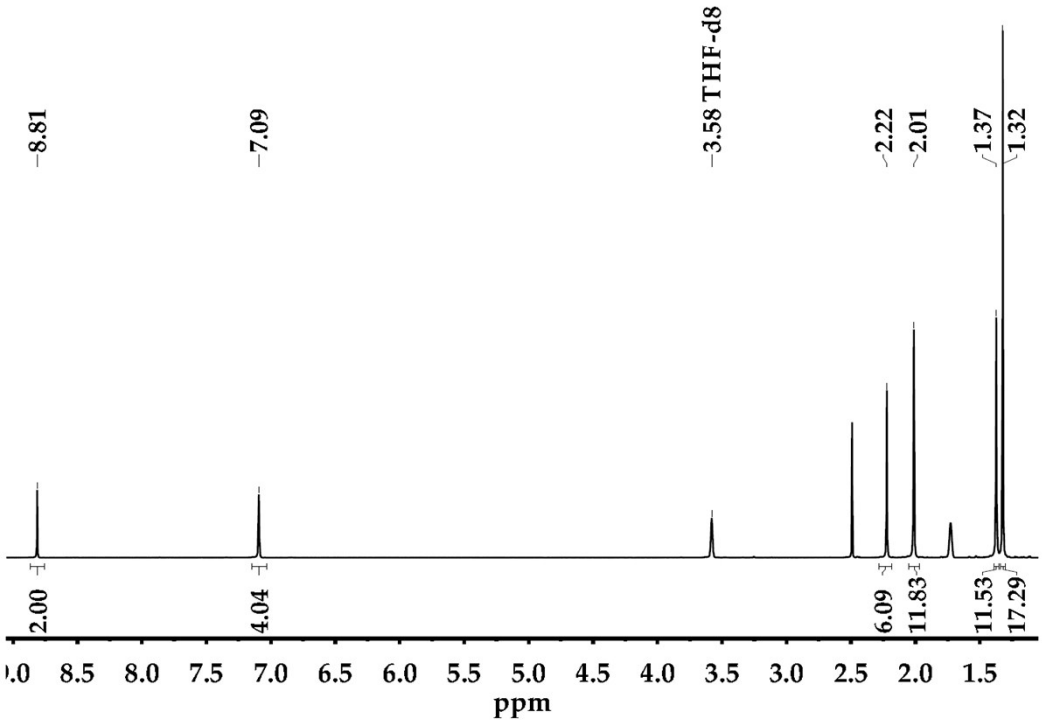


**Figure S7:** $^{1}$H-NMR spectrum of compound **6** in THF-$d_8$, 300 MHz.

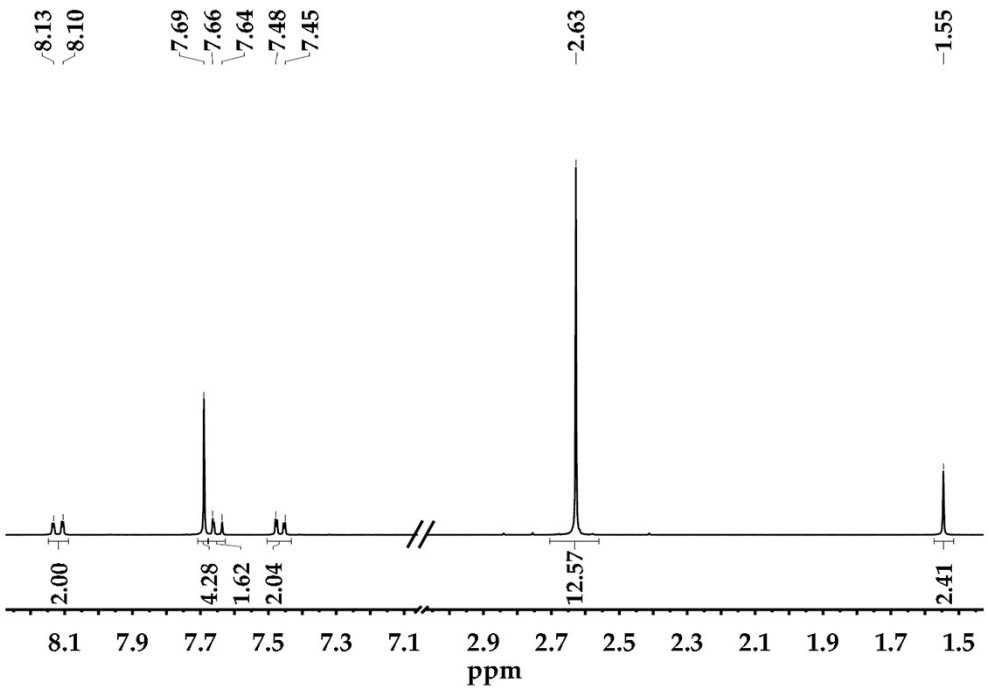


**Figure S8:** $^{1}$H-NMR spectrum of compound **7** in $CD_2Cl_2$, 300 MHz (acetone peak at 1.55 ppm).

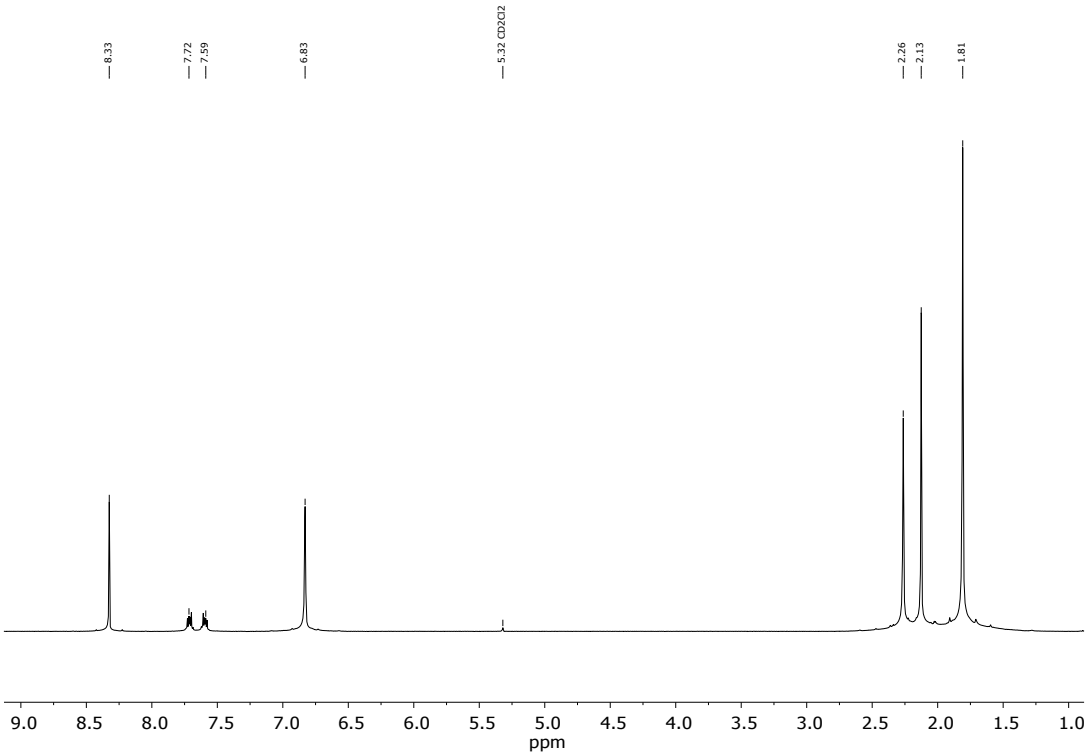


**Figure S9:** $^{1}$H-NMR spectrum of compound **8** in $CD_2Cl_2$, 300 MHz.

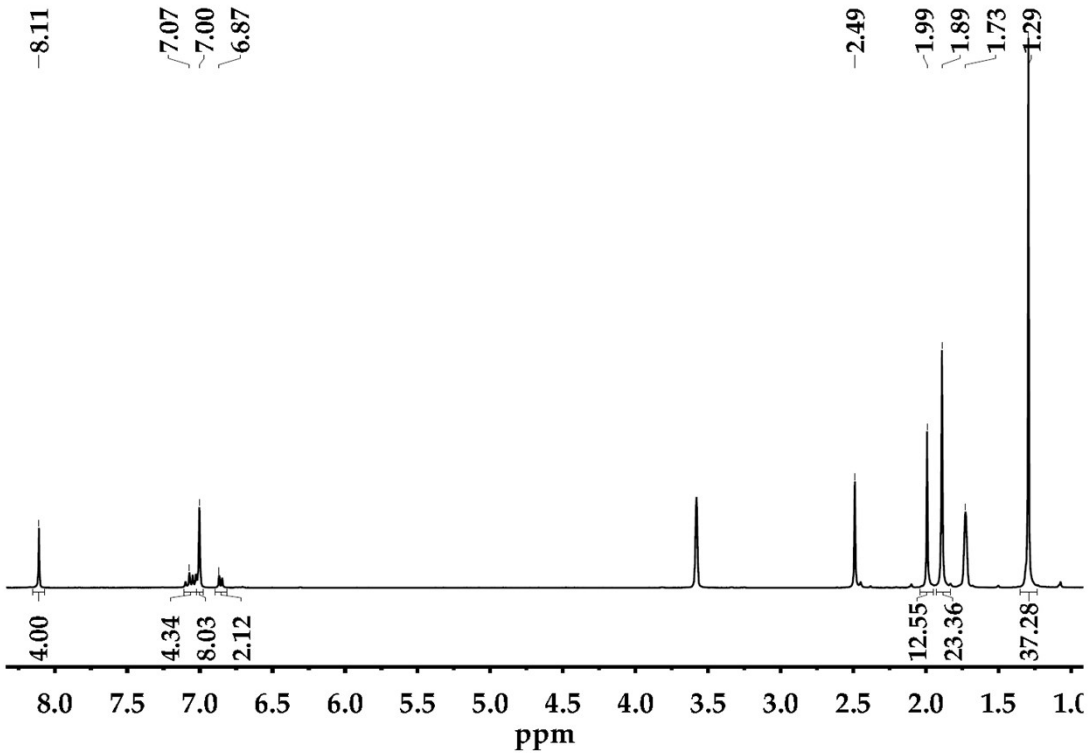


**Figure S10:** $^{1}$H-NMR spectrum of compound **9** in THF-$d_8$, 300 MHz.

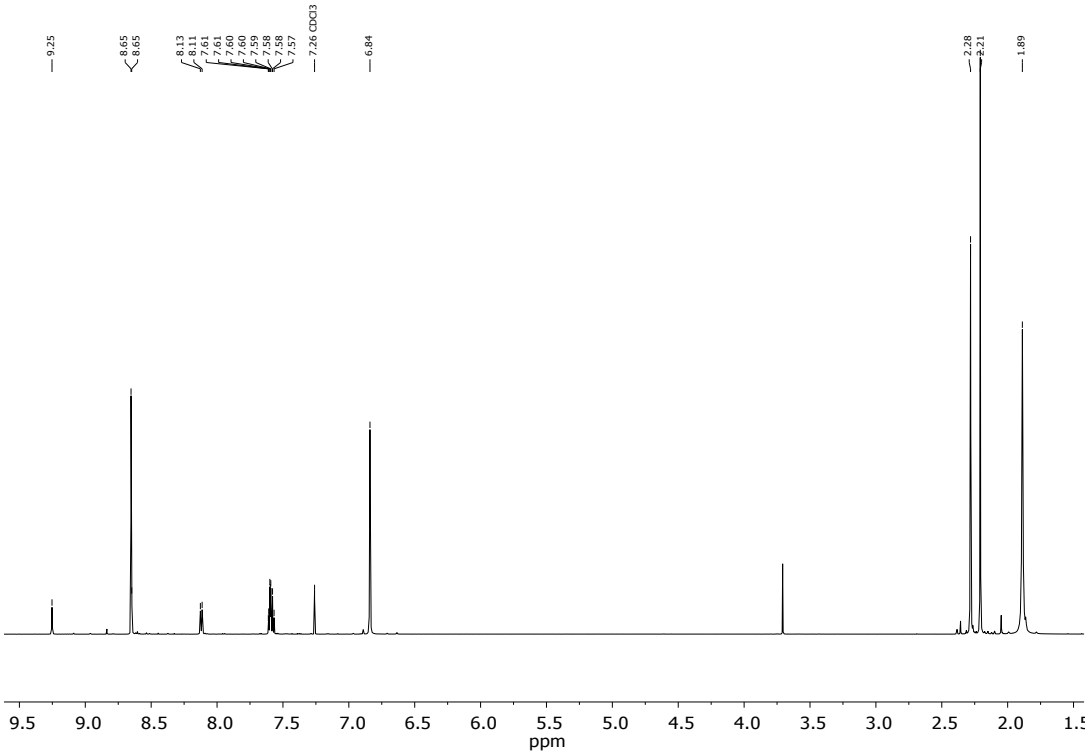


**Figure S11:** $^{1}$H-NMR spectrum of compound **10** in $CDCl_3$, 600 MHz.

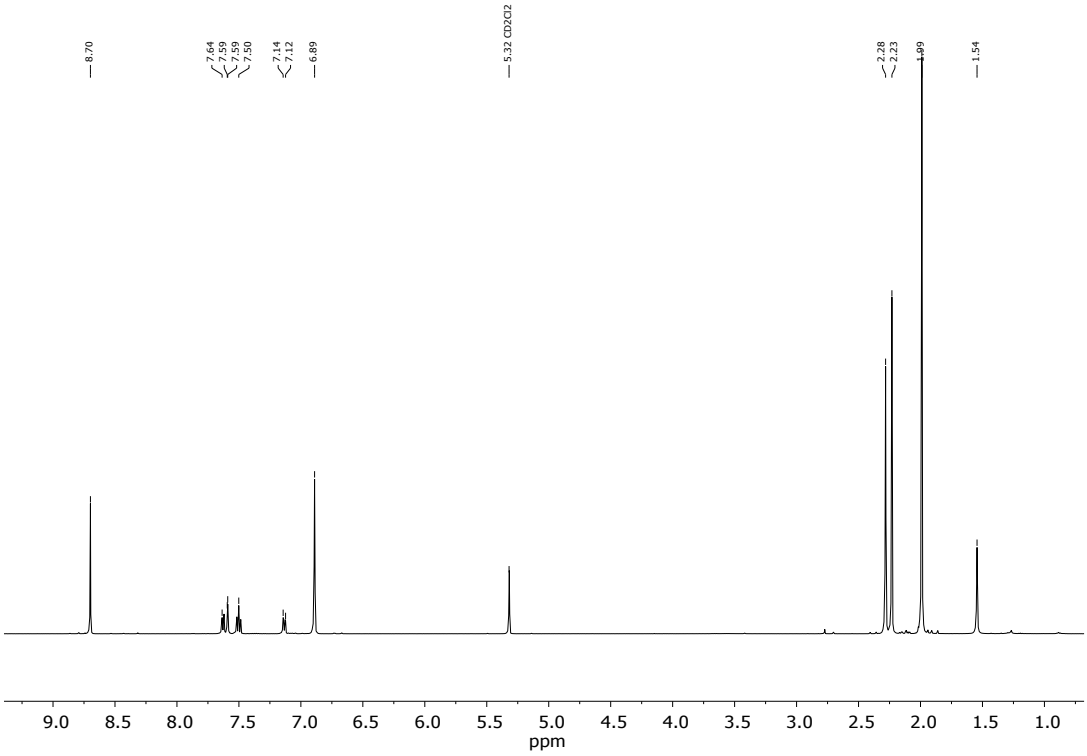


**Figure S12:** $^{1}$H-NMR spectrum of compound **11** in $CD_2Cl_2$, 500 MHz.

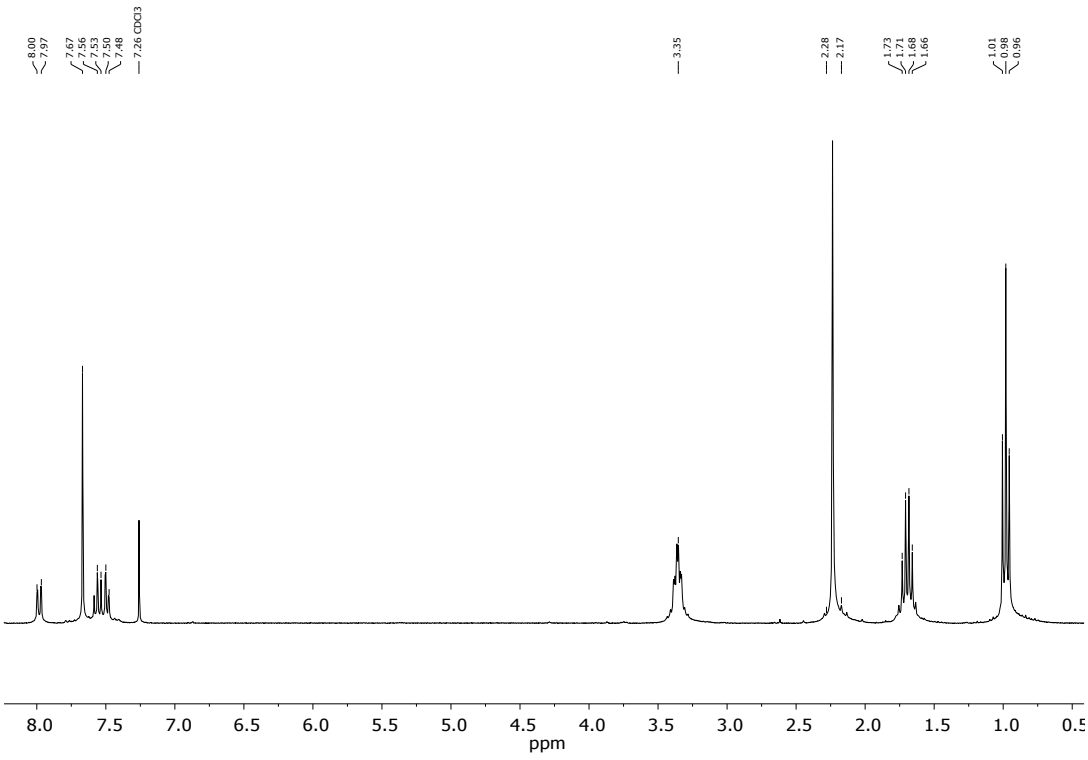


**Figure S13:** $^{1}$H-NMR spectrum of compound **12** in $CDCl_3$, 300 MHz.

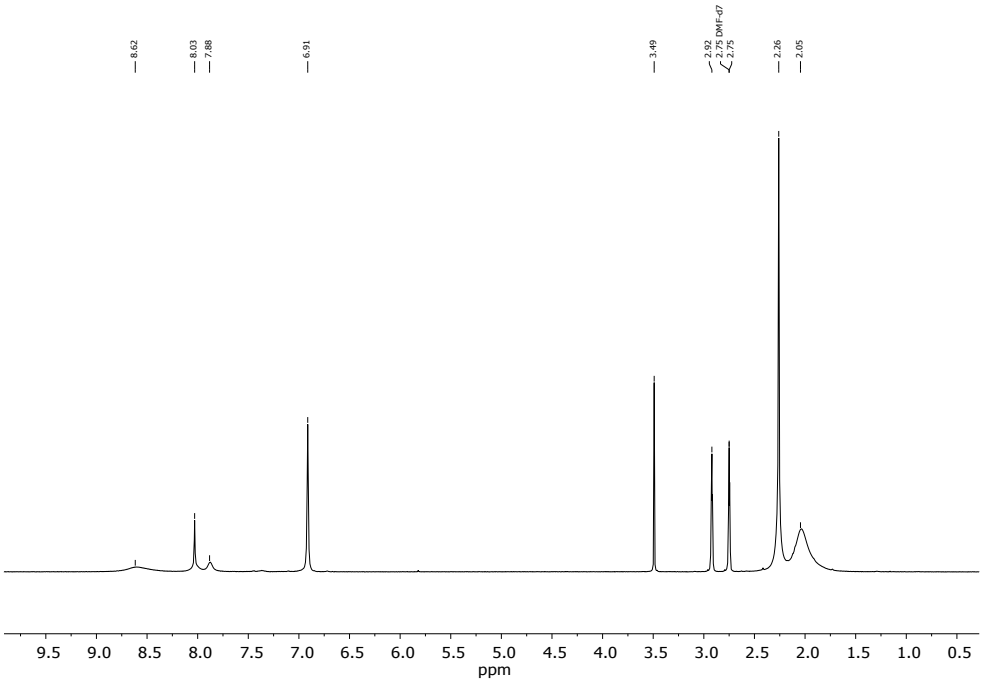


**Figure S14:** $^{1}$H-NMR spectrum of compound **8-$ZnCl_2$** in DMF-$d_7$, 400 MHz.

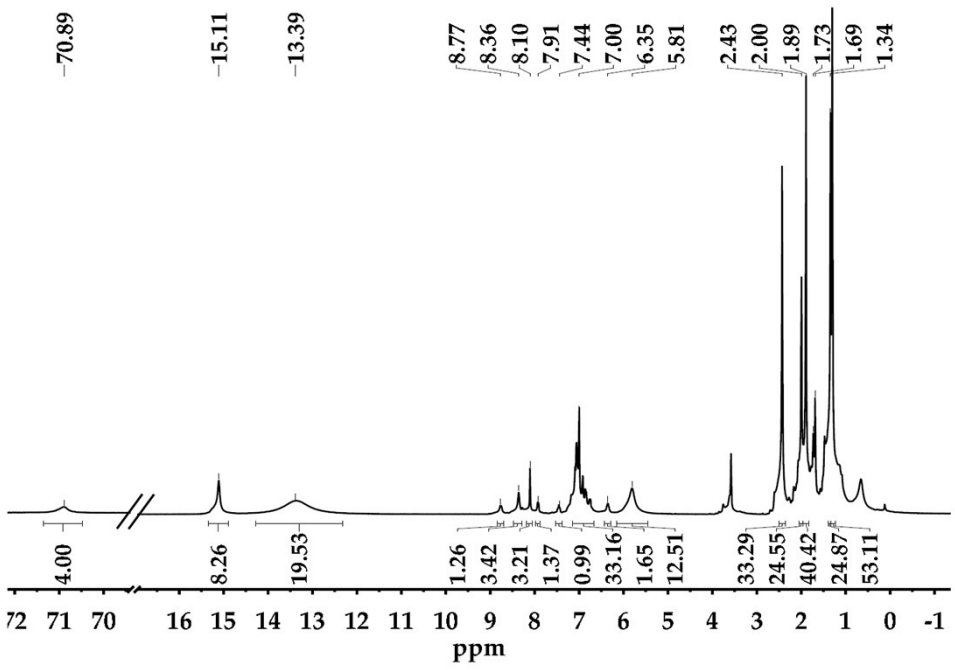


**Figure S15:** $^{1}$H-NMR spectrum of compound **9-$NiCl_2$** in THF-$d_8$, 300 MHz, RT.

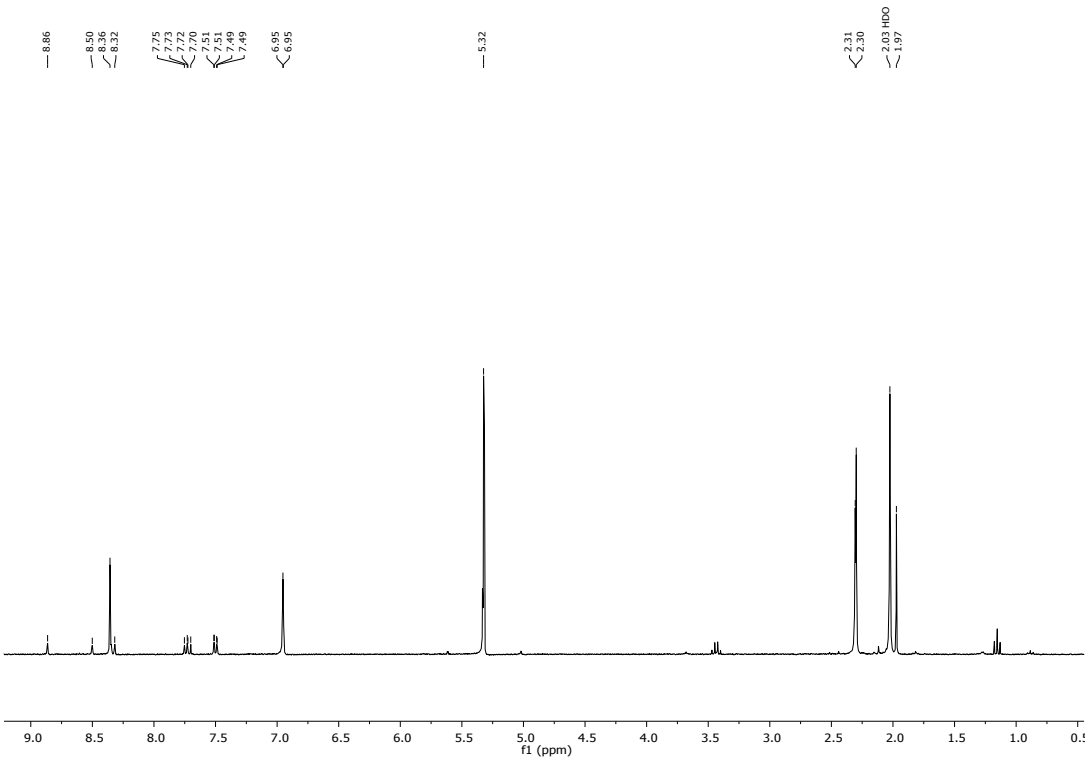


**Figure S16:** $^{1}$H-NMR spectrum of compound **10-Zn(OTf)$_2$** in $CD_2Cl_2$, 600 MHz.

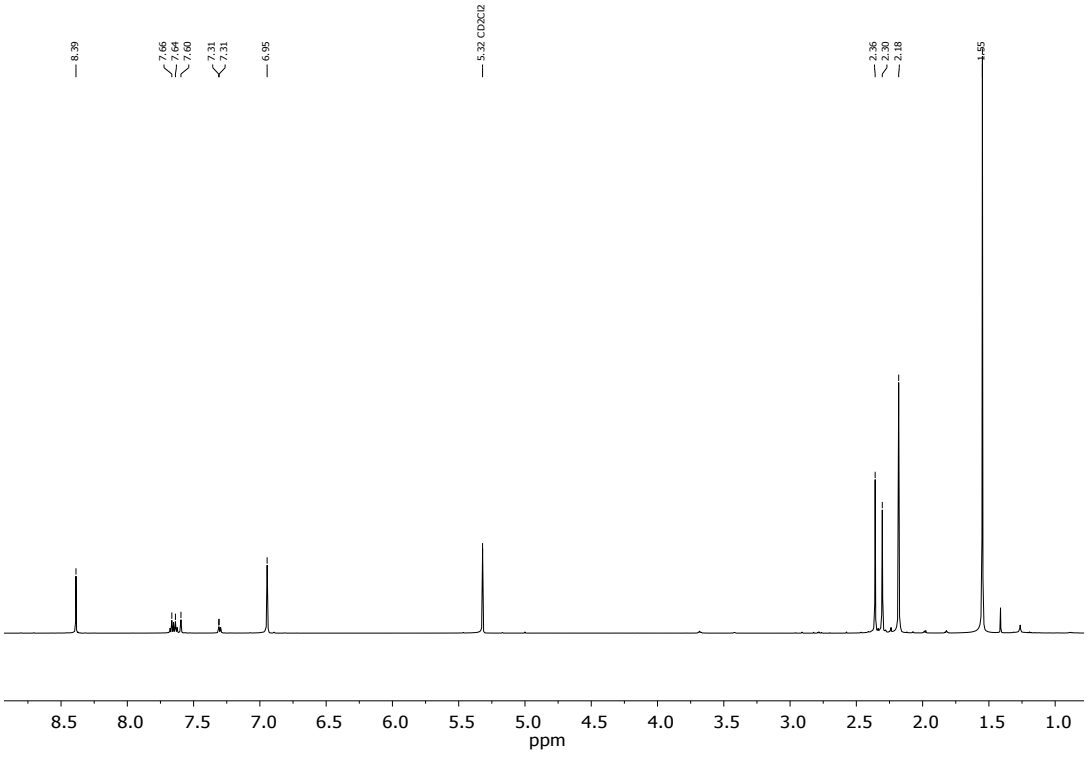


**Figure S17:** $^{1}$H-NMR spectrum of compound **11-ZnCl$_2$** in $CD_2Cl_2$, 600 MHz.

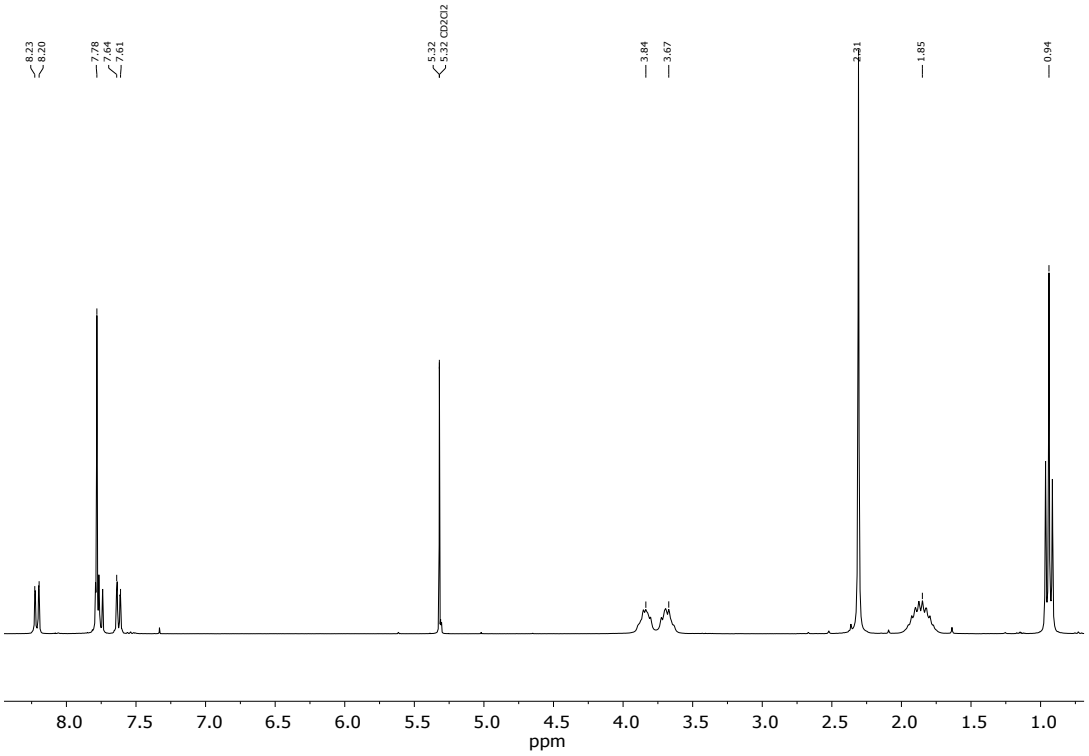


**Figure S18**: $^{1}$H-NMR spectrum of compound **12-$ZnCl_2$** in $CD_2Cl_2$, 300 MHz.

## Ortep plot of compound 8

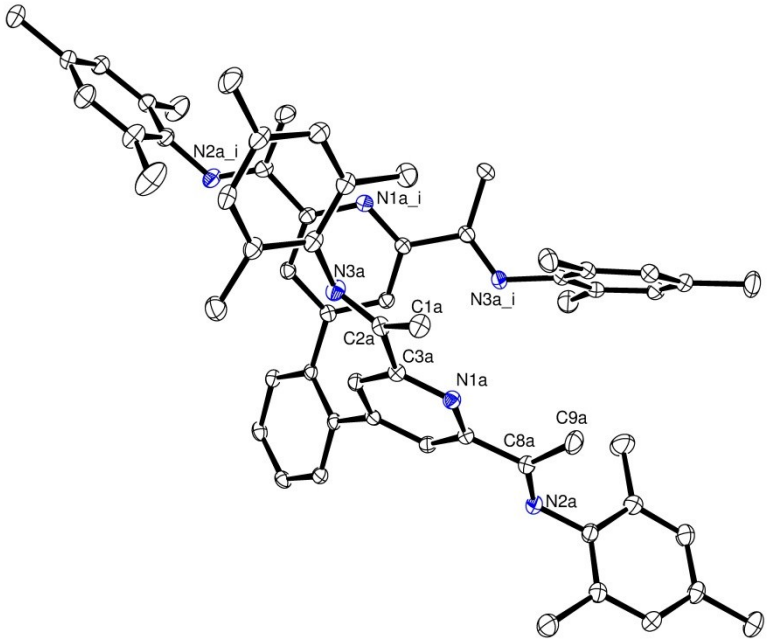


**Figure S19:** Ortep plot of **8** with anisotropic displacement parameters shown at the 50 % probability level. Hydrogen atoms are omitted for clarity. Selected bond lenght (Å): N3a-C2a, 1.281 (2); C2a-C3a, 1.500 (2); C3a-N1a, 1.345 (2); N1a-C7a, 1.349 (2); C7a-C8a, 1.503 (2).

## Compilation of the Crystallographic Data Collections and Refinements

**Tab. S1:** Summary of crystal data and structure refinement for the ligands **5**, **8** and **12**.

| | **5** | **8** | **12** |
|---|---|---|---|
| Chemical formula | $C_{33}H_{42}N_3O_2B$ | $C_{60}H_{64}N_6$ | $C_{40}H_{50}N_6$ |
| Formula Mass | 523.54 | 869.17 | 614.86 |
| Crystal system | Monoclinic | Monoclinic | Monoclinic |
| Space group | *P*21/*n* (No 14 ) | *C2/c* (No 15) | $P2_1/c$ (No 14) |
| *a* [Å] | 11.5588(4) | 10.6256(16) | 12.4198(2) |
| *b* [Å] | 10.1750(3) | 21.043(3) | 11.24410(10) |
| *c* [Å] | 26.5199(9) | 23.059(4) | 25.6150(3) |
| $\alpha$ [°] | 90.00 | 90.00 | 90.00 |
| $\beta$ [°] | 91.946(1) | 93.035(2) | 102.088(1) |
| $\gamma$ [°] | 90.00 | 90.00 | 90.00 |
| Unit cell volume [Å$^3$] | 3117.23(18) | 5148.7(14) | 3497.81(8) |
| Temperature [K] | 100.15 | 100 | 100 |
| *Z* | 4 | 4 | 4 |
| Radiation type | MoKα | MoKα | CuKα |
| Reflections measured | 35120 | 37410 | 70576 |
| Independent reflections | 6107 | 5905 | 7316 |
| Data/ restraints/ parameter | 6107/35/423 | 5905/ 0/ 306 | 7316/ 0/ 465 |
| $\theta_{max}$ [°]/ completeness | 26/99.8% | 27.5/ 99.7% | 76.51/ 99.5% |
| $R_{int}$ | 0.0605 | 0.0265 | 0.0473 |
| Final $R_1$ values ($I > 2\sigma(I)$) | 0.0846 | 0.0423 | 0.0377 |
| Final $wR(F^2)$ values ($I > 2\sigma(I)$) | 0.2306 | 0.1054 | 0.1003 |
| Final $R_1$ values (all data) | 0.0997 | 0.0480 | 0.0413 |
| Final $wR(F^2)$ values (all data) | 0.2396 | 0.1104 | 0.1038 |
| Goodness of fit on $F^2$ | 1.126 | 1.047 | 1.042 |
| Max/ min $\Delta\rho$ [e Å$^{-3}$] | 0.29/ -0.32 | 0.31/ -0.24 | 0.24/ -0.20 |
| | | - | |

**Tab. S2: Summary of crystal data and structure refinement for complexes 8-$ZnCl_2$, 9-$NiCl_2$, 10-$Zn(OTf)_2$ and 12-$ZnCl_2$.**

| | **8-$ZnCl_2$** | **9-$NiCl_2$** | **10-$Zn(OTf)_2$** | **12-$ZnCl_2$** |
|---|---|---|---|---|
| Chemical formula | $C_{60}H_{64}Cl_4N_6Zn_2$ | $C_{106}H_{147}Cl_4N_6Ni_2O_7C_{76}.5H79ClF_{12}N_6O_{13}S_4Zn_2$ | | $C_{44}H_{58}Cl_4N_6OZn_2$ |
| Formula Mass | 1141.77 | 1876.51 | 1816.37 | 959.50 |
| Crystal system | Monoclinic | Orthorhombic | Monoclinic | Monoclinic |
| Space group | $P2_1/c$ (No 14) | $P2_12_12_1$ (No 19) | *P*21/*n* (No 14) | $P2_1/c$ (No 14) |
| *a* [Å] | 21.4563(15) | 17.524(6) | 30.401(3) | 10.1202(11) |
| *b* [Å] | 12.4924(9) | 23.041(8) | 16.5325(15) | 13.9999(15) |
| *c* [Å] | 23.3307(17) | 24.556(8) | 36.065(3) | 31.600(3) |
| $\alpha$ [°] | 90.00 | 90 | 90 | 90 |
| $\beta$ [°] | 101.8830(10) | 90 | 103.5470(3) | 91.6246(14) |
| $\gamma$ [°] | 90.00 | 90 | 90 | 90 |
| Unit cell volume [Å$^3$] | 6121.2(8) | 9915(6) | 17622(3) | 4475.3(8) |
| Temperature [K] | 100 | 100 | 100 | 100 |
| *Z* | 4 | 4 | 8 | 4 |
| Radiation type | MoKα | MoKα | MoKα | MoKα |
| Reflections measured | 69742 | 59940 | 263207 | 66780 |
| Independent reflections | 14016 | 24266 | 40263 | 10236 |
| Data/ restraints/ parameter | 14016/ 0/ 685 | 24266/7/1133 | 40263/48/2130 | 10236/0/580 |
| $\theta_{max}$ [°]/ completeness | 27.5/ 99.6% | 29.143/ | 27.5/99.4% | 27.5/99.6% |
| $R_{int}$ | 0.0752 | 0.0628 | 0.0808 | 0.0228 |
| Final $R_1$ values ($I > 2\sigma(I)$) | 0.0437 | 0.0593 | 0.856 | 0.0309 |
| Final $wR(F^2)$ values ($I > 2\sigma(I)$) | 0.0826 | 0.1261 | 0.0586 | 0.0729 |
| Final $R_1$ values (all data) | 0.0784 | 0.1063 | 0.1142 | 0.0353 |
| Final $wR(F^2)$ values (all data) | 0.0943 | 0.1444 | 0.1945 | 0.0755 |
| Goodness of fit on $F^2$ | 1.016 | 0.995 | 1.085 | 1.050 |
| Max/ min $\Delta\rho$ [e Å$^{-3}$] | 0.37/ -0.49 | 0.95/-0.64 | 3.58/-1.39 | 1.20/-0.97 |
| Flack parameter | n/a | 0.044(5) | n/a | n/a |