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Supporting Information

Reactivity of Nickel(II) Porphyrins in oCVD Processes—Polymerisation, Intramolecular Cyclisation and Chlorination

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Author Contributions

G.B., K.B. and N.D.B. carried out the deposition experiments. G.B. performed the CV measurements and DFT calculations. G.B. and O.B. collected and analysed the EPR data. K.B. performed the UV/Vis/NIR measurements. G.F. performed the HRMS measurements. K.H. and N.D.B. designed the experiments and supervised the project. G.B., K.H. and N.D.B. wrote the manuscript with input from all authors. All authors discussed the experiments.

Supporting Information

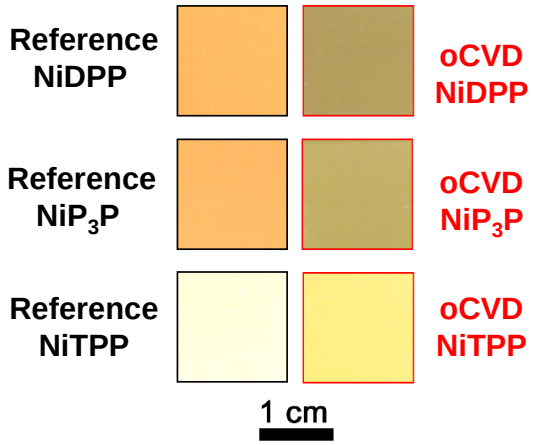

Figure S1. Optical images of reference and oCVD coatings of NiDPP, NiP_3P and NiTPP on glass.

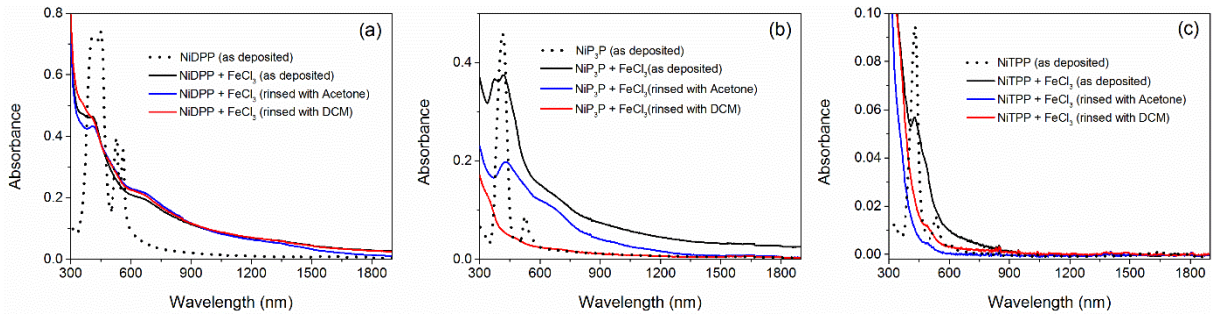

Figure S2. UV–Vis-NIR absorption spectra of the oCVD coatings on glass for (a) NiDPP, b) NiP_3P and (c) NiTPP before (black lines) and after rinsing with acetone (blue lines) or DCM (red lines). UV–Vis-NIR absorption spectra of the porphyrins sublimed in the absence of an oxidant are provided for comparison (dashed lines).

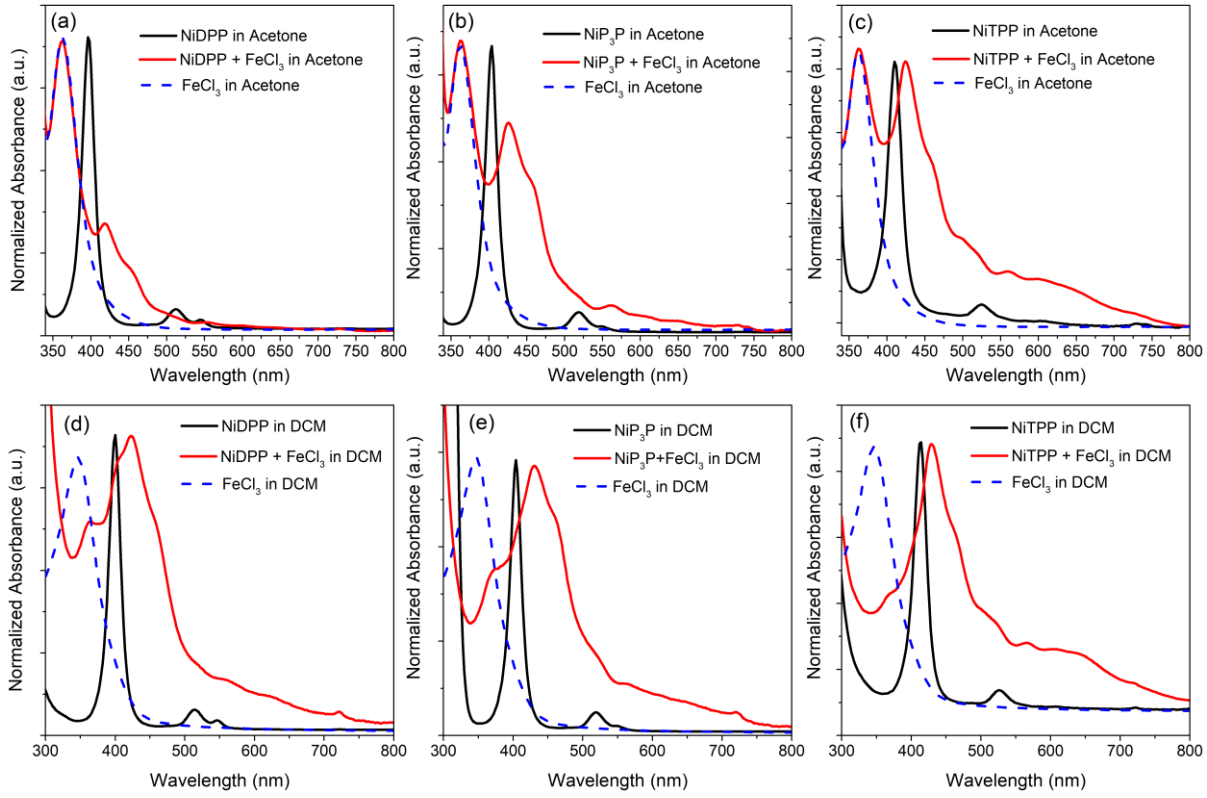

Figure S3. UV–Vis absorption spectra of the acetone and CH_2Cl_2 solutions of dissolved thin films formed by the oCVD reaction of (a, d) NiDPP, (b, e) NiP_3P and (c, f) NiTPP with $FeCl_3$ before and after rinsing with acetone or CH_2Cl_2. UV–vis absorption spectra of the dissolved sublimed porphyrins and $FeCl_3$ solutions are provided for comparison.

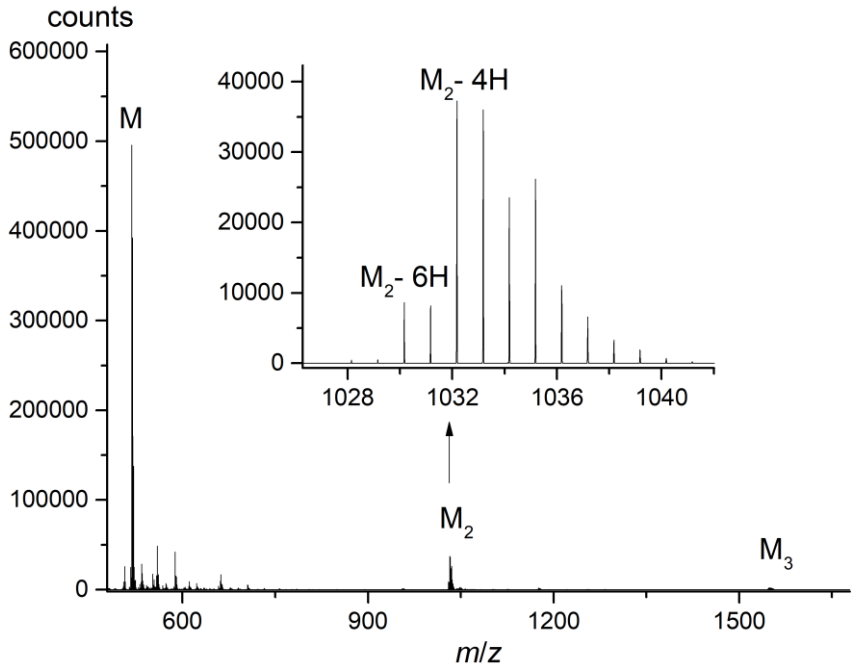

Figure S4. HR-MALDI mass spectrum of the NiDPP/WCl_6 mixture in CH_2Cl_2 solution at the end of the EPR measurements. Matrix α-cyano-4-hydroxycinnamic acid. The spectrum shows the formation of oligomers (M_2 – M_3). Inset: The dimer region (M_2) shows the sequential loss of 2H pairs.

film	**$\lambda(CH_2Cl_2)$ / nm**	**λ(acetone) / nm**
NiDPP	400	397
oCVD NiDPP	423	418
NiP_3P	404	404
oCVD NiP_3P	430	426
NiTPP	410	410
oCVD NiTPP	425	424

Table S1. Wavelength of the maximum absorption (Soret bands) of the washing solutions of reference and oCVD coatings (CH_2Cl_2 and acetone).

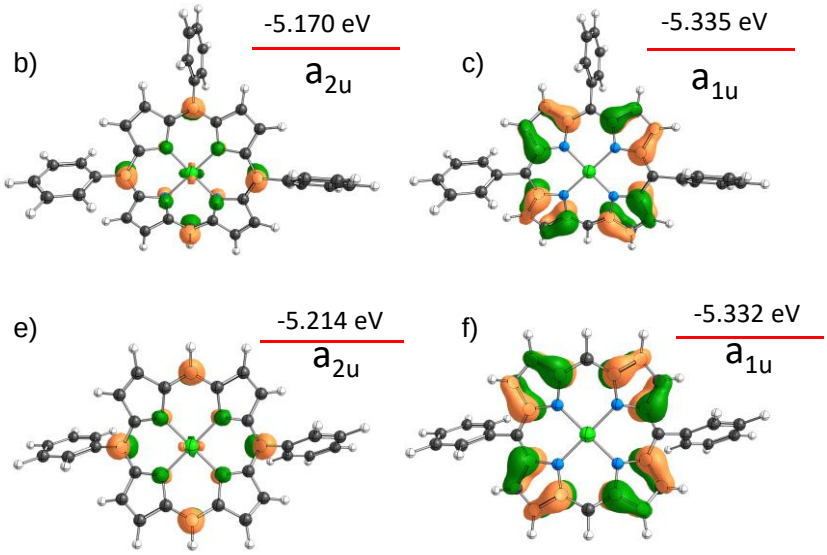

Figure S5. Illustration of a_{2u} and a_{1u} orbitals of NiP_3P and NiDPP and their respective energies (isosurface 0.006 and 0.004 a.u.) at the RIJCOSX-BP86-D3-ZORA/def2-TZVP/CPCM(CH_2Cl_2) level of theory.

Table S2. *DFT calculated Cartesian coordinates of* ***[NiDPP]***$^{\bullet+}$ *with and without solvent model.*

a) *[NiDPP]*$^{\bullet+}$ with solvent model

6	-1.346595000	-0.034744000	-3.072154000
6	-0.233812000	3.409784000	0.157009000
6	-1.347927000	0.108061000	3.534798000
6	-0.147391000	-3.306689000	0.305490000
7	-0.818594000	1.451635000	1.553986000
7	-0.795238000	1.402209000	-1.157976000
7	-0.782360000	-1.364164000	-1.091428000
7	-0.759832000	-1.314119000	1.620498000
6	-0.466560000	-2.691525000	-0.925127000
6	-1.168749000	-1.239060000	-2.418869000
6	-1.065532000	1.200682000	-2.493544000
6	-0.425097000	2.735692000	-1.053748000
6	-0.355355000	-2.637565000	1.516187000
6	-1.035020000	-1.119678000	2.956138000
6	-1.201396000	1.316572000	2.881483000
6	-0.536853000	2.786539000	1.387655000
6	-0.673856000	-3.417156000	-2.153427000
6	-1.142132000	-2.518786000	-3.071523000
6	-0.863606000	2.408376000	-3.242466000
6	-0.408451000	3.347420000	-2.358449000
6	-0.762562000	3.506659000	2.615943000
6	-1.207440000	2.596589000	3.534158000
6	-0.323037000	-3.248855000	2.820790000
6	-0.801641000	-2.321744000	3.705018000
1	-0.515692000	-4.482693000	-2.277509000
1	-1.416478000	-2.687316000	-4.108784000
1	-1.007560000	2.500081000	-4.315018000
1	-0.104605000	4.366619000	-2.566915000
1	-0.632147000	4.575952000	2.739831000
1	-1.485694000	2.758181000	4.571445000
1	0.006949000	-4.259993000	3.029169000
1	-0.942778000	-2.417243000	4.777607000
6	0.180373000	4.824743000	0.179214000
6	-0.546007000	5.818622000	-0.503986000
6	1.315764000	5.195633000	0.926268000
1	-1.454491000	5.547849000	-1.041433000
1	1.881723000	4.428892000	1.456158000
6	-0.137467000	7.150043000	-0.447873000
6	1.732007000	6.525055000	0.960215000
1	-0.718954000	7.914505000	-0.964044000
1	2.625050000	6.797051000	1.523612000
6	1.006143000	7.505848000	0.275210000
1	1.326858000	8.547487000	0.311408000
6	0.301379000	-4.711068000	0.283568000
6	1.445280000	-5.054700000	-0.463481000
6	-0.400766000	-5.721846000	0.967242000
1	1.993026000	-4.274740000	-0.993252000
1	-1.314994000	-5.472526000	1.505285000
6	1.892883000	-6.373893000	-0.497592000
6	0.039215000	-7.043226000	0.911019000
1	2.791916000	-6.624777000	-1.061266000
1	-0.523928000	-7.821189000	1.427359000
6	1.190624000	-7.371733000	0.187447000
1	1.535835000	-8.405495000	0.150522000
28	-0.763638000	0.044192000	0.231250000
1	-1.600607000	-0.057360000	-4.131331000
1	-1.602137000	0.124144000	4.594059000

b) *[NiDPP]*$^{\bullet+}$ without solvent model

6	-1.334166000	-0.032531000	-3.070161000
6	-0.227706000	3.412813000	0.158722000
6	-1.335204000	0.106325000	3.532886000
6	-0.142620000	-3.309947000	0.303748000
7	-0.806114000	1.451360000	1.554826000
7	-0.784304000	1.403905000	-1.157365000
7	-0.770628000	-1.363739000	-1.092239000
7	-0.749409000	-1.315692000	1.619967000
6	-0.456743000	-2.691820000	-0.926319000
6	-1.156124000	-1.238096000	-2.419286000
6	-1.054735000	1.202901000	-2.492965000
6	-0.417887000	2.737524000	-1.052235000

6	-0.349363000	-2.639599000	1.514742000
6	-1.024514000	-1.121597000	2.955642000
6	-1.188047000	1.316016000	2.881945000
6	-0.525950000	2.786938000	1.388837000
6	-0.664582000	-3.416851000	-2.154887000
6	-1.130493000	-2.517877000	-3.071917000
6	-0.854548000	2.412051000	-3.240442000
6	-0.400876000	3.350123000	-2.356213000
6	-0.751862000	3.506511000	2.617422000
6	-1.194703000	2.596044000	3.534556000
6	-0.316453000	-3.251549000	2.818725000
6	-0.793457000	-2.325245000	3.703083000
1	-0.510649000	-4.483037000	-2.276759000
1	-1.406264000	-2.689748000	-4.108124000
1	-0.995953000	2.507749000	-4.312871000
1	-0.092624000	4.368242000	-2.562545000
1	-0.624918000	4.576250000	2.739248000
1	-1.474544000	2.760923000	4.570803000
1	0.017537000	-4.261542000	3.024974000
1	-0.932043000	-2.424484000	4.775558000
6	0.176817000	4.830043000	0.179776000
6	-0.559775000	5.819219000	-0.499992000
6	1.311658000	5.211550000	0.922463000
1	-1.470086000	5.540979000	-1.030857000
1	1.887238000	4.449143000	1.448333000
6	-0.162998000	7.153148000	-0.444583000
6	1.717279000	6.543175000	0.953997000
1	-0.753926000	7.913856000	-0.955020000
1	2.611586000	6.822936000	1.511043000
6	0.980593000	7.517468000	0.272790000
1	1.292894000	8.561358000	0.307886000
6	0.296962000	-4.716703000	0.282771000
6	1.440916000	-5.070175000	-0.459793000
6	-0.415027000	-5.723670000	0.962647000
1	1.997615000	-4.293898000	-0.985708000
1	-1.331954000	-5.467883000	1.493413000
6	1.879218000	-6.391411000	-0.491169000
6	0.014509000	-7.047422000	0.907418000
1	2.780164000	-6.649131000	-1.048150000
1	-0.557529000	-7.822398000	1.417912000
6	1.166759000	-7.383503000	0.190130000
1	1.504729000	-8.419371000	0.155124000
28	-0.750071000	0.044278000	0.231280000
1	-1.589141000	-0.054714000	-4.129310000
1	-1.590434000	0.122037000	4.592089000

Table S3. *DFT calculated Cartesian coordinates of* ***[NiP$_3$P]$^{\bullet+}$*** *with and without solvent model.*

a) [NiP$_3$P]$^{\bullet+}$ with solvent model

6	0.691379072	0.163549108	-3.062418591
6	-1.186098415	3.496053946	-0.072535384
6	-0.914879200	0.130249042	3.435493844
6	-1.042922102	-3.245891223	-0.085369520
7	-0.984275504	1.499762938	1.377232475
7	-0.292848277	1.509350042	-1.264340976
7	-0.243241085	-1.239359576	-1.274477366
7	-0.913012791	-1.242905064	1.360443797
6	-0.561901570	-2.585845794	-1.213126672
6	0.337176926	-1.055348242	-2.517007772
6	0.323931090	1.366030322	-2.483806133
6	-0.634345406	2.862481668	-1.181297190
6	-1.108213049	-2.586676603	1.144359030
6	-0.929035749	-1.082961769	2.750671807
6	-1.035959188	1.337508726	2.752190017
6	-1.271747340	2.835329583	1.153943489
6	-0.211913263	-3.240081386	-2.460536093
6	0.389746452	-2.306384114	-3.242014470
6	0.408520603	2.645785172	-3.165833055
6	-0.215504260	3.558568301	-2.376522854
6	-1.550808433	3.508082674	2.412007364
6	-1.346254439	2.601865048	3.397880983
6	-1.258072871	-3.282444671	2.412940832
6	-1.114627736	-2.357261331	3.397988406
1	-0.397004118	-4.285707584	-2.679979548
1	0.801697711	-2.416057157	-4.240935484
1	0.877140924	2.789470554	-4.135271488
1	-0.359113969	4.619292454	-2.550067062
1	-1.833286953	4.550913229	2.502841697
1	-1.423220094	2.742328799	4.470240157
1	-1.424878007	-4.349839103	2.510241182
1	-1.158713492	-2.501537804	4.471712328
6	-1.564747491	4.930406872	-0.180128760
6	-2.672264673	5.298140609	-0.958827370
6	-0.815830448	5.925384457	0.466279770
1	-3.254796747	4.525430698	-1.462249562
1	0.059468410	5.644328894	1.053311968
6	-3.031757003	6.642569915	-1.079435332
6	-1.175865185	7.268603535	0.341110301
1	-3.898273636	6.917869087	-1.681579244
1	-0.583898410	8.035229495	0.842233747
6	-2.285440337	7.629504535	-0.429446388
1	-2.565849774	8.678966209	-0.525399982
6	-1.385452714	-4.690267295	-0.141588252
6	-0.407191839	-5.660054455	-0.411450128
6	-2.706065869	-5.097305672	0.106342931
1	0.625466870	-5.350859363	-0.577302216
1	-3.468409727	-4.345351680	0.315500768
6	-0.747594100	-7.014067690	-0.441244395
6	-3.044176264	-6.452057639	0.072597827
1	0.021894180	-7.759792736	-0.644727864
1	-4.074624071	-6.756251476	0.259647697
6	-2.066422340	-7.412745596	-0.202208152
1	-2.330433103	-8.470710620	-0.226011603
28	-0.608012488	0.131854037	0.050201458
1	1.161077327	0.179586354	-4.044024396
6	-0.895887557	0.112615269	4.923752468
6	-2.046817911	0.421011303	5.664023813
6	0.284191996	-0.237489987	5.596058933
6	-2.014067660	0.386806873	7.059889148
6	0.314199521	-0.268697686	6.992530705
6	-0.833671130	0.044039718	7.726398477
1	-2.971360945	0.673407154	5.142966260
1	1.178874616	-0.478681568	5.020371238
1	-2.915019973	0.623556011	7.627030631
1	1.237916510	-0.536159214	7.506902104
1	-0.809564460	0.018090983	8.816402537

***b) [NiP$_3$P]$^{\bullet+}$ without* solvent model**

6	-6.505044000	2.565616000	-1.316637000
6	-2.722732000	4.600981000	0.934035000

6	-2.377187000	0.414462000	3.406326000
6	-7.180790000	-0.060902000	2.700212000
7	-2.938170000	2.407195000	2.056271000
7	-4.624698000	3.269496000	0.087894000
7	-6.462389000	1.341371000	0.808382000
7	-4.759264000	0.473191000	2.741717000
6	-7.421285000	0.623766000	1.500396000
6	-7.057416000	1.695361000	-0.384598000
6	-5.390088000	3.346141000	-1.064231000
6	-3.788822000	4.361440000	0.046151000
6	-5.875668000	-0.190082000	3.211062000
6	-3.682305000	-0.096983000	3.396335000
6	-2.077725000	1.668072000	2.845097000
6	-2.293807000	3.615229000	1.832429000
6	-8.648255000	0.578510000	0.747264000
6	-8.400787000	1.192750000	-0.448719000
6	-4.995492000	4.478795000	-1.855239000
6	-4.024036000	5.131166000	-1.149859000
6	-1.039406000	3.642707000	2.534366000
6	-0.873099000	2.410060000	3.099307000
6	-5.493573000	-1.189409000	4.172194000
6	-4.130771000	-1.151159000	4.265843000
1	-9.572218000	0.126284000	1.087741000
1	-9.079354000	1.342585000	-1.283197000
1	-5.432955000	4.748805000	-2.811792000
1	-3.479949000	6.027941000	-1.424079000
1	-0.359695000	4.485840000	2.565230000
1	-0.020850000	2.043149000	3.658574000
1	-6.182233000	-1.856123000	4.678725000
1	-3.483895000	-1.750186000	4.896811000
6	-1.989761000	5.876761000	0.806794000
6	-2.682392000	7.087426000	0.996266000
6	-0.625344000	5.915482000	0.465215000
1	-3.740196000	7.062289000	1.260240000
1	-0.095114000	4.984333000	0.265215000
6	-2.016280000	8.305440000	0.879876000
6	0.030303000	7.137204000	0.327914000
1	-2.557586000	9.236013000	1.051325000
1	1.082032000	7.156199000	0.041591000
6	-0.659458000	8.333796000	0.544169000
1	-0.141919000	9.287885000	0.443011000
6	-8.275009000	-0.763762000	3.397685000
6	-9.042955000	-1.754432000	2.757792000
6	-8.540139000	-0.456599000	4.746013000
1	-8.810449000	-2.034456000	1.730402000
1	-7.949051000	0.311989000	5.244940000
6	-10.056418000	-2.413746000	3.449938000
6	-9.569862000	-1.103032000	5.425980000
1	-10.630478000	-3.195121000	2.951561000
1	-9.781343000	-0.840482000	6.462665000
6	-10.329111000	-2.083748000	4.780975000
1	-11.128203000	-2.595873000	5.317229000
28	-4.700662000	1.881169000	1.432415000
1	-7.052538000	2.738186000	-2.242812000
6	-1.335366000	-0.349684000	4.124311000
6	-0.687240000	0.169066000	5.259534000
6	-1.007193000	-1.643627000	3.679032000
6	0.273353000	-0.588244000	5.926891000
6	-0.030181000	-2.387833000	4.337475000
6	0.611263000	-1.863190000	5.462974000
1	-0.971183000	1.150688000	5.639286000
1	-1.508040000	-2.048958000	2.799206000
1	0.754468000	-0.185479000	6.818427000
1	0.231181000	-3.380670000	3.970916000
1	1.368875000	-2.449840000	5.982792000

Table S4. *DFT calculated Cartesian coordinates of* ***NiDPP*** *with and without solvent model.*

a) *NiDPP* with solvent model

6	-1.129697000	-0.013433000	-3.108884000
6	-0.224672000	3.439840000	0.176873000
6	-1.132554000	0.092367000	3.571466000
6	-0.140471000	-3.337211000	0.286132000
7	-0.686294000	1.447754000	1.569949000
7	-0.677622000	1.408261000	-1.154099000
7	-0.650336000	-1.357433000	-1.107315000
7	-0.644355000	-1.317633000	1.616860000
6	-0.377480000	-2.705811000	-0.933505000
6	-0.949312000	-1.217300000	-2.454406000
6	-0.921374000	1.212067000	-2.504055000
6	-0.393978000	2.762415000	-1.028378000
6	-0.326904000	-2.664201000	1.491311000
6	-0.893406000	-1.127527000	2.966713000
6	-0.982016000	1.300286000	2.916952000
6	-0.446333000	2.802771000	1.396397000
6	-0.507610000	-3.408386000	-2.186786000
6	-0.893127000	-2.490614000	-3.120313000
6	-0.792239000	2.448282000	-3.227339000
6	-0.421351000	3.399823000	-2.321988000
6	-0.594389000	3.501826000	2.649650000
6	-0.957626000	2.574721000	3.582908000
6	-0.338382000	-3.301950000	2.784991000
6	-0.733348000	-2.360015000	3.690169000
1	-0.350416000	-4.474536000	-2.312463000
1	-1.099472000	-2.639506000	-4.176772000
1	-0.932685000	2.548270000	-4.300222000
1	-0.203505000	4.447766000	-2.497918000
1	-0.463566000	4.571522000	2.775330000
1	-1.167822000	2.718412000	4.639319000
1	-0.094160000	-4.343998000	2.961213000
1	-0.871429000	-2.463433000	4.763022000
6	0.095237000	4.893203000	0.177329000
6	-0.824752000	5.839269000	-0.301612000
6	1.326417000	5.338106000	0.684239000
1	-1.790801000	5.501445000	-0.679176000
1	2.044081000	4.606763000	1.059141000
6	-0.516630000	7.201278000	-0.280144000
6	1.635412000	6.700195000	0.702904000
1	-1.243606000	7.925849000	-0.649766000
1	2.598466000	7.031043000	1.094283000
6	0.715011000	7.635357000	0.220049000
1	0.955431000	8.699216000	0.235923000
6	0.216125000	-4.781952000	0.285600000
6	1.456852000	-5.195752000	-0.224488000
6	-0.678176000	-5.750944000	0.767410000
1	2.154582000	-4.446673000	-0.602004000
1	-1.651542000	-5.437729000	1.147367000
6	1.800244000	-6.549534000	-0.243615000
6	-0.335582000	-7.104691000	0.745672000
1	2.770241000	-6.856008000	-0.637676000
1	-1.042780000	-7.847227000	1.118010000
6	0.905259000	-7.507584000	0.242157000
1	1.172478000	-8.565022000	0.225509000
28	-0.664660000	0.045329000	0.231387000
1	-1.333859000	-0.033005000	-4.178674000
1	-1.337470000	0.106910000	4.641206000

b) *NiDPP* without solvent model

6	-1.112116000	-0.012657000	-3.107197000
6	-0.221473000	3.439322000	0.176975000
6	-1.113042000	0.092083000	3.569912000
6	-0.136390000	-3.336478000	0.285640000
7	-0.676619000	1.447865000	1.570069000
7	-0.662649000	1.408832000	-1.155399000
7	-0.641463000	-1.357046000	-1.107412000
7	-0.628243000	-1.317684000	1.618045000
6	-0.374749000	-2.705500000	-0.933244000
6	-0.939342000	-1.216745000	-2.452727000
6	-0.900541000	1.212670000	-2.504555000
6	-0.381495000	2.761426000	-1.028476000

6	-0.313208000	-2.662792000	1.491107000
6	-0.870826000	-1.127536000	2.967232000
6	-0.970651000	1.300131000	2.915426000
6	-0.443788000	2.802578000	1.395884000
6	-0.509649000	-3.409747000	-2.184813000
6	-0.890306000	-2.490982000	-3.117759000
6	-0.766794000	2.448227000	-3.227511000
6	-0.401019000	3.399853000	-2.321730000
6	-0.596063000	3.503210000	2.647485000
6	-0.953439000	2.575189000	3.580476000
6	-0.316485000	-3.301467000	2.784385000
6	-0.705936000	-2.359318000	3.690198000
1	-0.359533000	-4.477148000	-2.306048000
1	-1.097997000	-2.641608000	-4.173426000
1	-0.899367000	2.549307000	-4.301058000
1	-0.178749000	4.447143000	-2.494198000
1	-0.472670000	4.574031000	2.768701000
1	-1.164628000	2.720538000	4.636190000
1	-0.067910000	-4.342822000	2.956879000
1	-0.835768000	-2.463668000	4.763768000
6	0.087820000	4.894519000	0.177723000
6	-0.837696000	5.833779000	-0.302719000
6	1.313519000	5.351141000	0.685634000
1	-1.800008000	5.485631000	-0.680009000
1	2.034655000	4.624201000	1.061674000
6	-0.540515000	7.197422000	-0.282738000
6	1.610964000	6.714889000	0.704698000
1	-1.272689000	7.916028000	-0.653666000
1	2.570686000	7.053914000	1.097072000
6	0.685359000	7.641704000	0.219237000
1	0.917157000	8.707363000	0.234810000
6	0.209230000	-4.783469000	0.284891000
6	1.445811000	-5.209297000	-0.223434000
6	-0.692277000	-5.745581000	0.765754000
1	2.148384000	-4.464572000	-0.599826000
1	-1.662900000	-5.421660000	1.143343000
6	1.777323000	-6.565162000	-0.242470000
6	-0.361030000	-7.101352000	0.745793000
1	2.745096000	-6.880081000	-0.635160000
1	-1.074832000	-7.838043000	1.117054000
6	0.875409000	-7.514829000	0.243416000
1	1.133828000	-8.574348000	0.227879000
28	-0.651601000	0.045495000	0.231326000
1	-1.314764000	-0.032617000	-4.177284000
1	-1.315974000	0.106950000	4.640027000

Table S5. *DFT calculated Cartesian coordinates for* ***NiP₃P*** *with and without solvent model.*

a) *NiP₃P* with solvent model

6	1.139151000	0.041590000	-2.861041000
6	-0.410280000	3.383470000	0.294563000
6	0.139993000	0.002204000	3.757118000
6	-0.347497000	-3.358217000	0.261399000
7	-0.095671000	1.383779000	1.719371000
7	0.327745000	1.400949000	-0.981766000
7	0.361771000	-1.356996000	-0.994419000
7	-0.053171000	-1.362505000	1.701744000
6	0.039927000	-2.704703000	-0.905498000
6	0.835132000	-1.178235000	-2.284148000
6	0.839008000	1.250729000	-2.261587000
6	0.007641000	2.745167000	-0.870712000
6	-0.307422000	-2.711222000	1.496867000
6	0.053201000	-1.210766000	3.077143000
6	-0.013723000	1.218796000	3.096014000
6	-0.384808000	2.728732000	1.525316000
6	0.281587000	-3.358543000	-2.168500000
6	0.818523000	-2.422983000	-3.005004000
6	0.865619000	2.516204000	-2.945876000
6	0.318354000	3.435992000	-2.098851000
6	-0.518164000	3.395989000	2.794599000
6	-0.234456000	2.476226000	3.761782000
6	-0.370613000	-3.402608000	2.759035000
6	-0.114869000	-2.481746000	3.733159000
1	0.082096000	-4.405486000	-2.370246000
1	1.141179000	-2.538479000	-4.036186000
1	1.234235000	2.657953000	-3.958206000
1	0.162561000	4.497094000	-2.263616000
1	-0.765299000	4.444648000	2.919626000
1	-0.205850000	2.620905000	4.836327000
1	-0.557494000	-4.465490000	2.870619000
1	-0.072741000	-2.631560000	4.806903000
6	-0.778349000	4.824269000	0.223677000
6	-1.955882000	5.210964000	-0.435059000
6	0.044902000	5.814231000	0.782817000
1	-2.597310000	4.445157000	-0.873868000
1	0.971324000	5.521926000	1.279104000
6	-2.308841000	6.559667000	-0.523882000
6	-0.307031000	7.162695000	0.691722000
1	-3.230031000	6.845067000	-1.033876000
1	0.345005000	7.921927000	1.125967000
6	-1.485875000	7.539023000	0.040290000
1	-1.760411000	8.592385000	-0.029995000
6	-0.706722000	-4.801770000	0.224904000
6	0.247913000	-5.781785000	-0.089680000
6	-2.016841000	-5.202477000	0.531524000
1	1.272742000	-5.479225000	-0.309024000
1	-2.761809000	-4.444777000	0.779186000
6	-0.102765000	-7.133579000	-0.104556000
6	-2.367751000	-6.554294000	0.514160000
1	0.650962000	-7.884703000	-0.345092000
1	-3.391100000	-6.850334000	0.749182000
6	-1.411840000	-7.523530000	0.195069000
1	-1.685071000	-8.579507000	0.183491000
28	0.134590000	0.016737000	0.361785000
1	1.518849000	0.050548000	-3.881941000
6	0.286105000	-0.023554000	5.239147000
6	-0.782605000	0.322038000	6.080661000
6	1.503359000	-0.421759000	5.812777000
6	-0.634041000	0.277243000	7.468709000
6	1.652239000	-0.464598000	7.201195000
6	0.584246000	-0.114298000	8.032679000
1	-1.736837000	0.615219000	5.640705000
1	2.335737000	-0.694437000	5.162207000
1	-1.474458000	0.543851000	8.111163000
1	2.605744000	-0.771077000	7.633650000
1	0.699717000	-0.149110000	9.116806000

b) *NiP₃P* no solvent model

6	1.099828000	0.040061000	-2.871735000
6	-0.409437000	3.383704000	0.294678000

6	0.134336000	0.002285000	3.751866000
6	-0.348069000	-3.358967000	0.262900000
7	-0.099780000	1.384040000	1.716699000
7	0.309477000	1.400733000	-0.988183000
7	0.341549000	-1.358101000	-1.000826000
7	-0.057294000	-1.363139000	1.699554000
6	0.026304000	-2.705117000	-0.907244000
6	0.801891000	-1.179655000	-2.293369000
6	0.808020000	1.249667000	-2.270952000
6	-0.003577000	2.744632000	-0.873673000
6	-0.306491000	-2.711573000	1.496963000
6	0.049444000	-1.210678000	3.073187000
6	-0.016858000	1.218703000	3.091413000
6	-0.382965000	2.728703000	1.524274000
6	0.257645000	-3.361169000	-2.170927000
6	0.782168000	-2.425055000	-3.012785000
6	0.833348000	2.515296000	-2.954730000
6	0.298809000	3.436555000	-2.103231000
6	-0.511696000	3.397197000	2.793703000
6	-0.231046000	2.476454000	3.759312000
6	-0.365717000	-3.403410000	2.759429000
6	-0.113634000	-2.481442000	3.731692000
1	0.055921000	-4.408517000	-2.366853000
1	1.092657000	-2.541773000	-4.047337000
1	1.192680000	2.657880000	-3.970047000
1	0.146485000	4.498736000	-2.262166000
1	-0.756186000	4.446571000	2.915835000
1	-0.197016000	2.617381000	4.833988000
1	-0.546880000	-4.467300000	2.868317000
1	-0.070234000	-2.626610000	4.805756000
6	-0.763924000	4.827704000	0.228265000
6	-1.942307000	5.229747000	-0.418223000
6	0.074213000	5.808943000	0.779463000
1	-2.594532000	4.469889000	-0.850860000
1	1.001614000	5.503114000	1.265366000
6	-2.280411000	6.581521000	-0.503440000
6	-0.263368000	7.160535000	0.693694000
1	-3.202975000	6.877977000	-1.004396000
1	0.401222000	7.912226000	1.121870000
6	-1.442659000	7.550629000	0.053732000
1	-1.705982000	8.606921000	-0.013333000
6	-0.693059000	-4.805755000	0.229198000
6	0.272144000	-5.776807000	-0.078647000
6	-1.998674000	-5.221724000	0.531169000
1	1.293661000	-5.460553000	-0.293592000
1	-2.751036000	-4.469950000	0.773466000
6	-0.063047000	-7.131657000	-0.092321000
6	-2.334145000	-6.576568000	0.516663000
1	0.699846000	-7.875239000	-0.327145000
1	-3.354980000	-6.883698000	0.747994000
6	-1.367594000	-7.535393000	0.203373000
1	-1.629028000	-8.594227000	0.193113000
28	0.123065000	0.016258000	0.357544000
1	1.469593000	0.048716000	-3.896300000
6	0.273497000	-0.022590000	5.234158000
6	-0.800505000	0.317866000	6.070242000
6	1.487622000	-0.414779000	5.816792000
6	-0.660411000	0.274829000	7.458357000
6	1.627975000	-0.457524000	7.205158000
6	0.554783000	-0.111462000	8.029736000
1	-1.752117000	0.605764000	5.621516000
1	2.323555000	-0.683414000	5.169490000
1	-1.505937000	0.537087000	8.095820000
1	2.579963000	-0.759800000	7.643685000
1	0.663786000	-0.145660000	9.114418000