Electronic Supplementary Material (ESI) for RSC Advances.

Molecular Flattening Effect to Enhance the Conductivity of Fused Porphyrin Tapes Thin Films

Supporting information.

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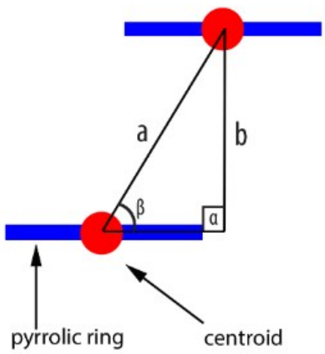
Experimental Section

Cyclic voltammetric measurements were carried out in a glovebox with a BioLogic SP-50 voltammetric analyzer in CH_2Cl_2 containing 0.1 M [^nBu4N]$^-$ [PF6] as supporting electrolyte at a platinum working electrode, a platinum wire as counter electrode, and a 0.01 M Ag/$AgNO_3$ electrode as the reference electrode. All cyclic voltammetric measurements were recorded at 100 mV s^{-1} scan rate. Ferrocene was employed as an internal reference redox system. The thin films thicknesses were measured using a KLA-Tencor P-17 Stylus profiler.The optical absorbance of the films was measured in the range of 250–2000 nm using a UV-Vis-NIR spectrophotometer (Perkin Elmer, Lambda 950) with a 150 mm diameter integrating sphere. The absorption spectra were recorded directly on the glass substrates.

A model composed of two identical porphyrin was geometrically optimized by density functional theory (BP86/def2-SVP/RIJCOSX/ZORA level of theory). A centroid was placed in every pyrrolic ring and the interplanar distance was than calculated considering the angle formed between the pyrrolic ring, and the two centroid (β) (See scheme S1) using the law of sines:

$$\frac{a}{\sin\alpha} = \frac{b}{\sin\beta}$$

Assuming $\alpha = 90°$



$$a\sin\beta = b$$

Scheme S1. Schematic of the method used to calculated the intramoleculra distance in the two porphyrins model.

The distances between all the four pyrrolic ring and the underlying one were calculated and the average assumed as intramolecular distance between the two porphyrins.

Images of the topography and conductivity of the samples were simultaneously acquired using the C-AFM mode of an Innova AFM (Bruker). Conductive AFM tips ElectriMulti75-G from BudgetSensors coated with a layer of 5 nm Chromium and 25nm of Platinum with nominal spring constants of 3 N/m and nominal radius <25 nm were used. Images of a 2x2 um^2 area with a resolution of 256x256 pixels were taken at a scan rate of 1Hz. Samples were deposited on monocrystalline silicon wafers and connected to the conductive stage via a colloidal carbon ink. The topography was obtained by maintaining the tip deflection constant via the feedback loop of the AFM acting on the piezo Z direction. A bias of 4V was applied to the back electrode of the samples while the grounded conductive tip was collecting electrons for the current measured by an amplifier (DLPCA-200, Femto). A 109 VA-1 amplification was used and the signal output was then transmitted to the AFM electronic and recorded. The reported average and standard deviation values of conductivity and roughness (Ra) consider at least 4 images in each sample for reliable results.

The Helium Ion Microscope images were recorded with an Orion Nanofab Instrument from Zeiss. The images were acquired from samples deposited on silicon wafers. Helium ions are generated using a gas field ionization source (GFIS). Within the GFIS a sharp needle having an apex radius of approximately 100 nm is set to a positive high voltage with respect to an extraction electrode accelerating the ions. For the HIM images within this manuscript we used a landing energy of 30 keV, impinging ion currents in between 0.1 and 1 pA and a tilt angle of the substrate holder stage of 20°. The helium ion beam scans the sample surface creating secondary electrons (SE). Contrast in the images is created mainly by composition and topography. Compared to the standard secondary electron microscope (SEM), the HIM allows to probe specimens with a better surface sensitivity and a higher depth of field which makes it very suitable for topographic imaging. [1,2]

Using a microprobe station (Cascade Microtech, PM8), 2-point current-voltage scans were recorded and the (lateral) thin-film conductivity was evaluated from a simple linear fit approximating all the samples to ohmic materials. The measurements were performed at room temperature and under ambient atmosphere and the geometry of the channel was 2.5 µm (length), 10 mm (total width), 40 nm (height). The data were recorded using a Keithley (2401) sourcemeter by sweeping the voltage from −4 V to 4 V and back (hysteresis scan) at a scan rate of 500 mV s−1. DFT calculation were performed by mean of ORCA program package (Version 4.0.1) program suite.[3] All the calculation were carried out using the BP86[4,5] functional in combination with D3[6-7] correction and RIJCOX[8] approximation. Relativistic effects were calculated at the zeroth order regular approximation (ZORA) level.[9] Geometry optimizations were performed by mean of Ahlrichs' split valence basis set def2-SVP[10] and Weigend's auxiliary basis set[11]. The optimized geometries were confirmed to be local minima on the respective potential energy surface by numerical frequency analysis that shows the absence negative frequencies.

Laser desorption/ionization high-resolution mass spectrometry (LDI-HRMS) measurements were performed on an AP-MALDI UHR ion source from MassTech, Inc. coupled to an LTQ/Orbitrap Elite from Thermo Scientific. oCVD coated Si wafers were directly placed on the sample holder, adjusting the working distance to optimum. In source fragmentation (E = 70 V) was used to prevent the formation of clusters. Gel permeation chromatography was performed using an Ultimate 3000 apparatus from Thermo Scientific, equipped with an ERC differential refractive index detector and a UV detector in serie. The GPC was coupled online to an LTQ/Orbitrap Elite mass spectrometer with an Ion Max source, equipped with an electrospray (ESI) probe from Thermo Scientific. Samples were dissolved in THF containing 1 vol% of pyridine, as described elsewhere[12] and filtered over a 0.45 µm pore size membrane prior to injection. A mesopore column 3 µm (300 x 7.5 mm) from Agilent Technologies was used at 30°C. Flow rate was set to 1 mL·min-1 and split post-column towards the RI and UV detection on one hand and the ESI-HRMS detection on another hand methanol was added post-split to promote ionization. The spray voltage was set to 3.2 kV. A tandem mass spectrometry method was included in the GPCxESI-HRMS measurements. MS/MS was performed by Collision Induced Dissociation (CID) using a normalized energy of 70. Parent ion selection and fragmentation was performed in the ion trap (LTQ) while analysis of the fragment ions was done by the high resolution Orbitrap.

Thermogravimetric analyses were performed under inert atmosphere (Ar) with a ramp of 10K per minute.

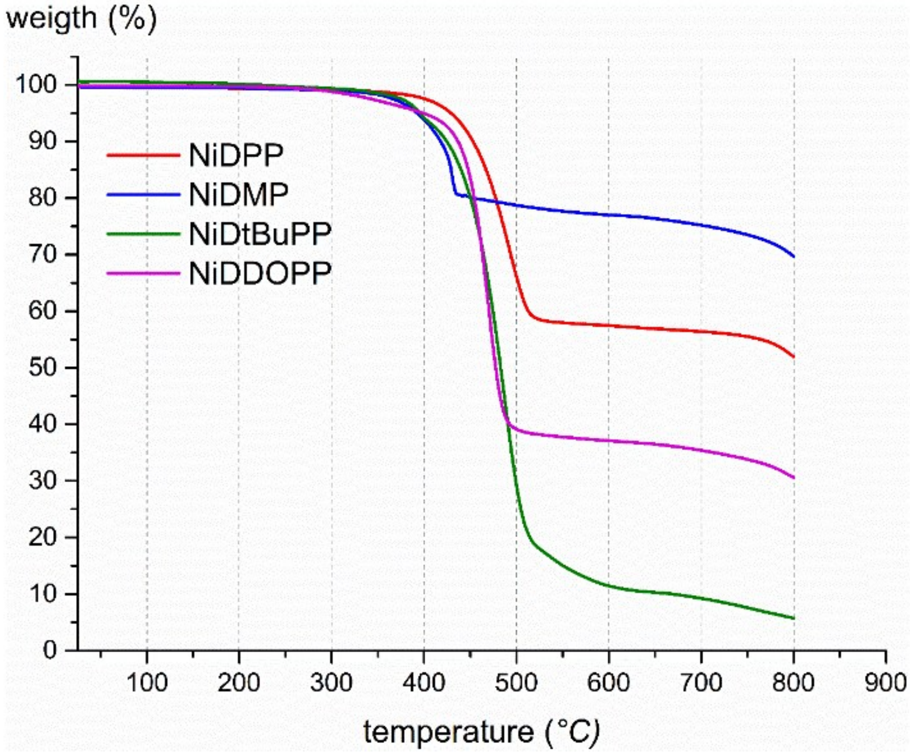


Figure S1. Thermo-gravimetric analysis of the monomer employed in the oCVD experiments. All the porphyrins exhibit a good thermal stability in the range of temperature used during the process.

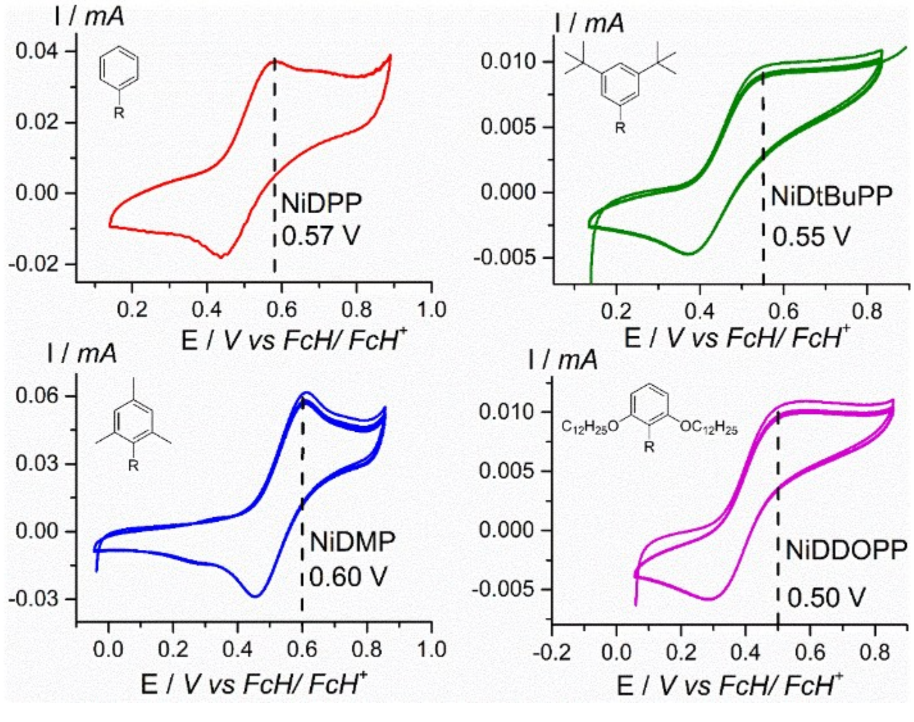


Figure S2. Cyclovoltammograms and respective oxidation potential obtained for of NiDPP (0.57 V), NiDtBuPP (0.55 V), NiDMP (0.60 V) and NiDDOPP (0.50 V) in CH_2Cl_2/[$^nBu_4N$][PF_6].

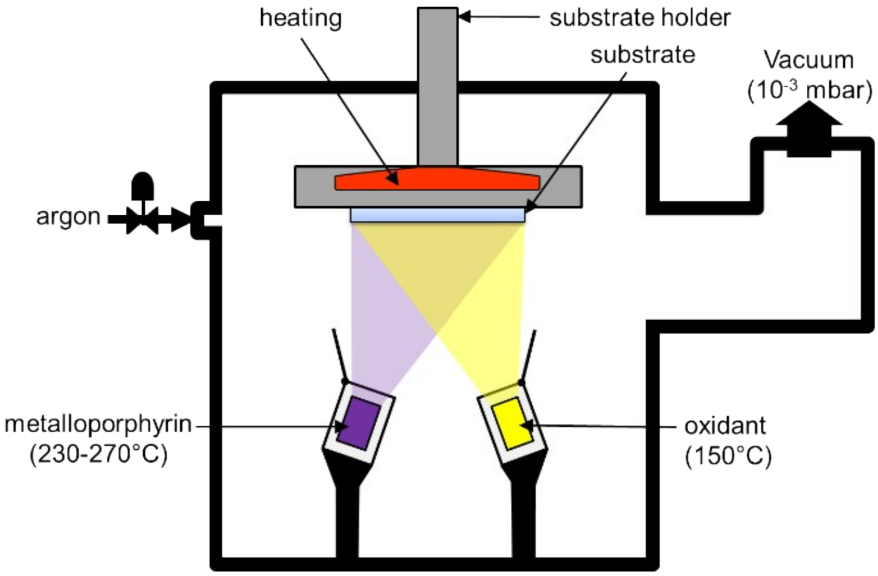


Figure S3. Schematic of the homemade built oCVD reactor used for the experiments. The porphyrins are sublimed under vacuum towards the substrate simultaneously to the oxidant ($FeCl_3$).

NiDPP – Nickel(II) 5,15-(diphenyl)porphyrin	
Chemical formula:	$C_{32}H_{20}N_4Ni$
Molecular weight:	519.23 g·mol^{-1}
Sublimation temperature:	235°C
Sublimed amount (10^{-3} mbar & 235°C):	9.6 µmol

NiDMP – Nickel(II) 5,15-(dimesityl)porphyrin	
Chemical formula:	$C_{38}H_{32}N_4Ni$
Molecular weight:	603.40 g·mol^{-1}
Sublimation temperature:	230°C
Sublimed amount (10^{-3} mbar & 230°C):	13.1 µmol

NiDD*t*-BuPP – Nickel(II) 5,15-(di-3,5-di-tert-butylphenyl)porphyrin	
Chemical formula:	$C_{48}H_{52}N_4Ni$
Molecular weight:	743.67 g·mol^{-1}
Sublimation temperature:	260°C
Sublimed amount (10^{-3} mbar & 260°C):	9.7 µmol

NiDDOPP – Nickel(II) 5,15-(di-2,6-dodecyloxyphenyl)porphyrin	
Chemical formula:	$C_{80}H_{116}N_4NiO_4$
Molecular weight:	1256.53 g·mol^{-1}
Sublimation temperature:	270°C
Sublimed amount (10^{-3} mbar & 270°C):	8.8 µmol

$FeCl_3$ – Iron(III) Chloride	
Chemical formula:	Cl_3Fe
Molecular weight:	162.20 g·mol^{-1}
Sublimation temperature:	150°C
Sublimed amount (10^{-3} mbar & 150°C):	661.2 µmol

Table S1. Chemical formula, molecular weight, sublimation temperature and sublimed amount for the four porphyrins investigated and the oxidant. Substrate temperature was 150°C.

Porphyrin	**Film thickness**
NiDPP	169 nm
NiDMP	520 nm
NiDDt-BuPP	355 nm
NiDDOPP	560 nm

Table S2. Thickness of the oCVD coating measured by profilometry.

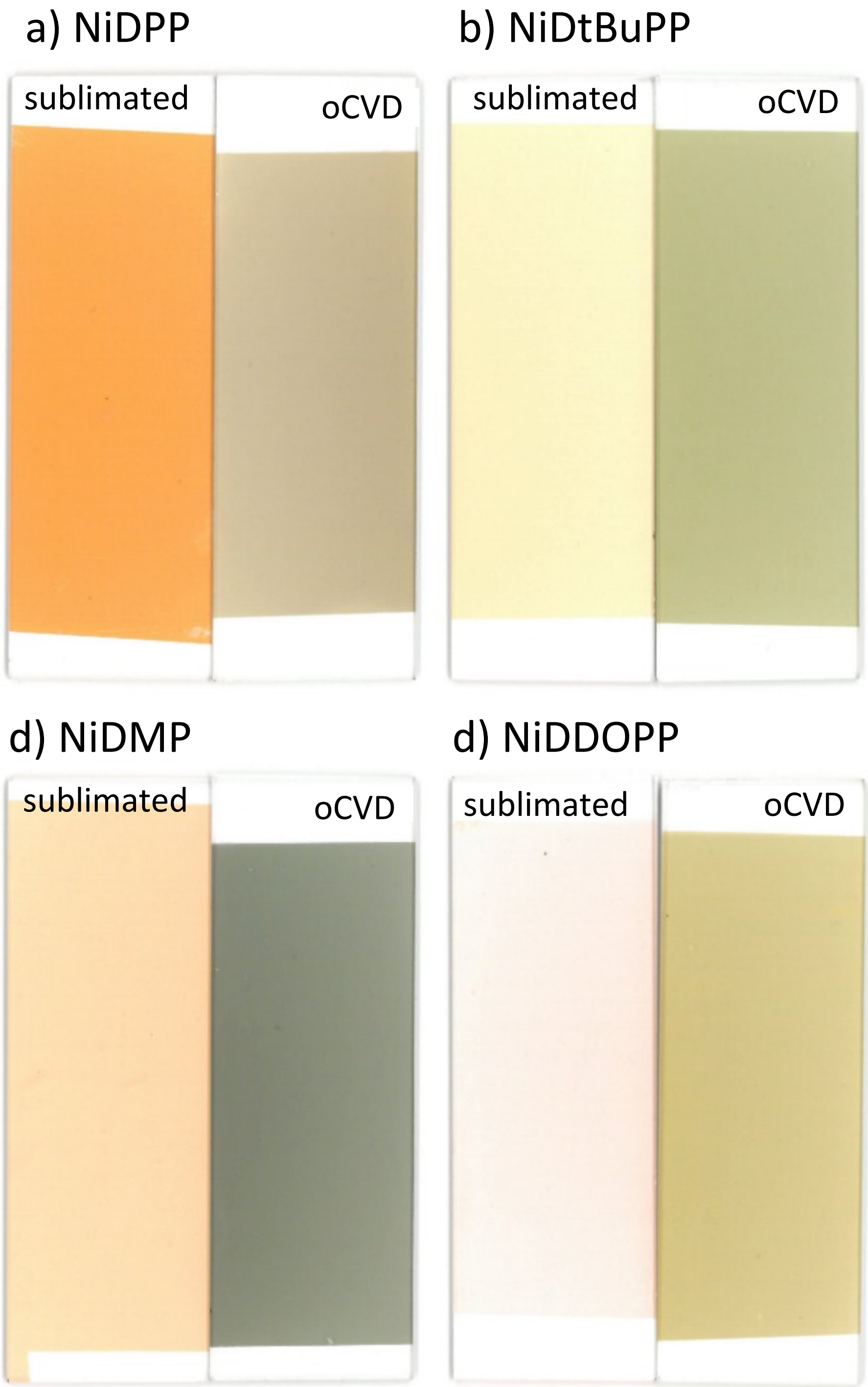


Figure S4. Optical image of the different coating obtained by simple sublimation (left) and oCVD (right) for each porphyrin on microscope glass. a) NiDPP, b) NiDtBuPP, c) NiDMP and d) NiDDOPP.

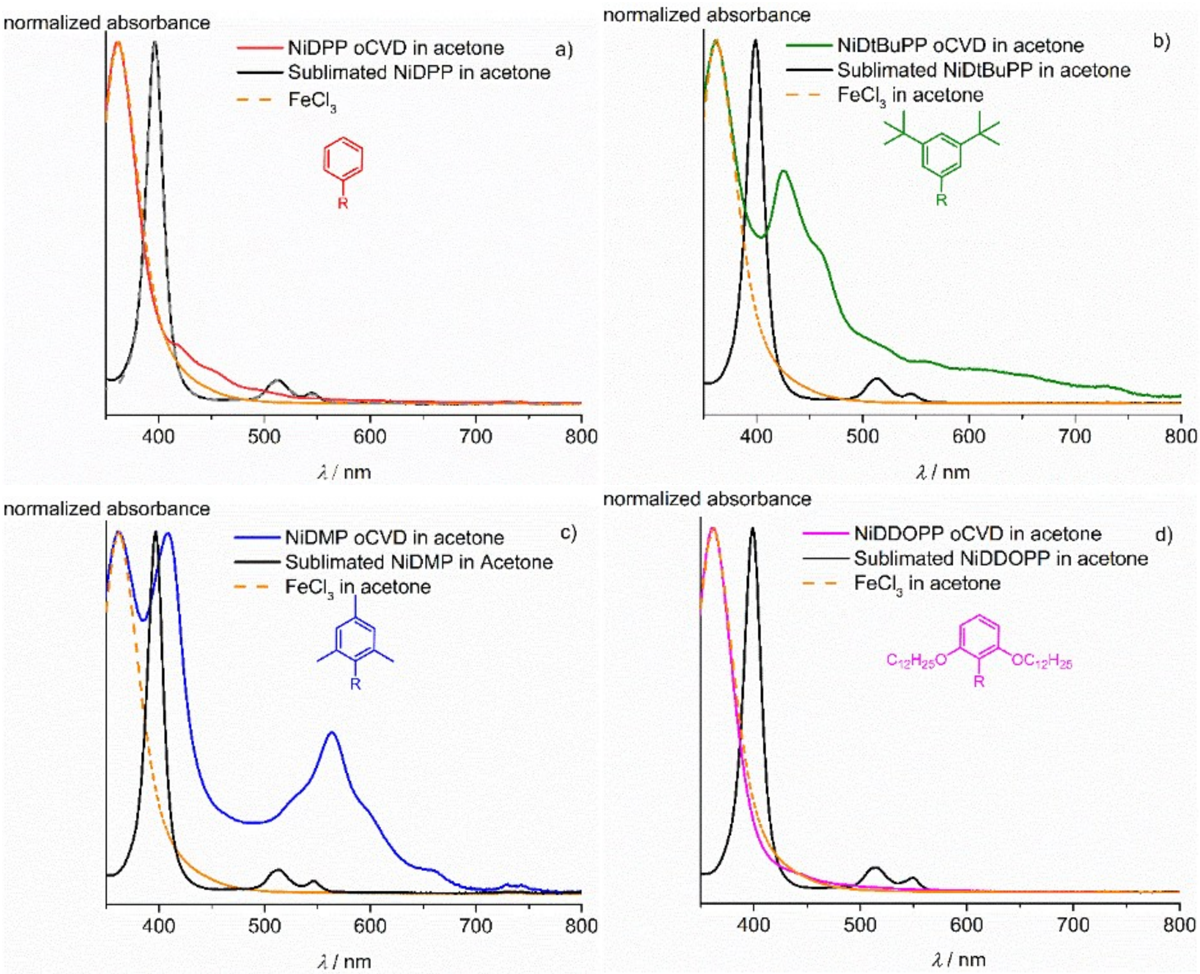
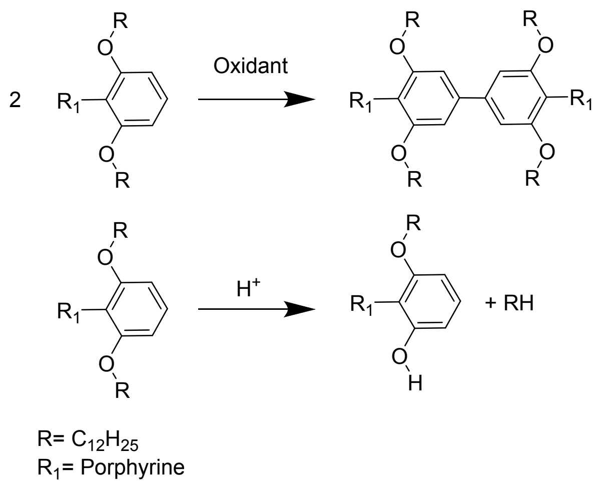


Figure S5. UV/Vis/ spectroscopy of the soluble fractions in acetone for the different oCVD coatings : a)NiDPP b) NiDtBuPP c) NiDMP d)NiDDOPP. For comparison the spectra of the sublimated porphyrin and of $FeCl_3$ solubilized in acetone are reported. All the samples exhibit residues of unreacted $FeCl_3$. The NiDPP and NiDDOPP coating are unsoluble and the only signal observed is related to the $FeCl_3$ residues.



Scheme S2. Schematic of the suggested dehydrogenative coupling occurring on the NiDDOPP phenyl rings. The position of the coupling is merely representative.

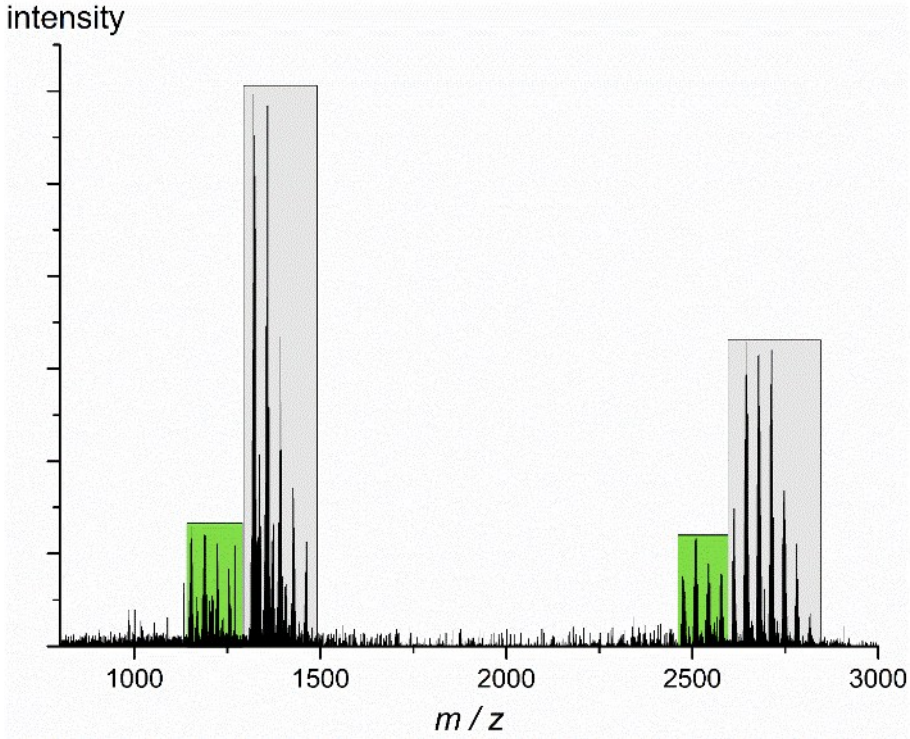


Figure S6. LDI-HRMS spectrum for the NiDDOPP oCVD coating synthesized in milder conditions (substrate temperature 50°C). The new spectrum evidence the presence of highly chlorinated monomer ($C_{80}H_{116}N_4NiO_4$)+nCl-nH (n= 2,3,4,5,6) and dimers ($C_{160}H_{232}N_8Ni_2O_8$)+ xCl –xH (x=3,4,5,6,7,8,9)-nH (n=2,4,6) (gray rectangles). The hydrolysis of the ether groups was observed both in the monomer ($C_{80}H_{116}N_4NiO_4$) + nCl – nH – $C_{12}H_{25}$ (n=2,3,4,5) and dimer region ($C_{160}H_{232}N_8Ni_2O_8$) + xCl – xH –nH – $C_{12}H_{25}$ (x=4,5,6,7,) (n=2,4,6) (green rectangles).

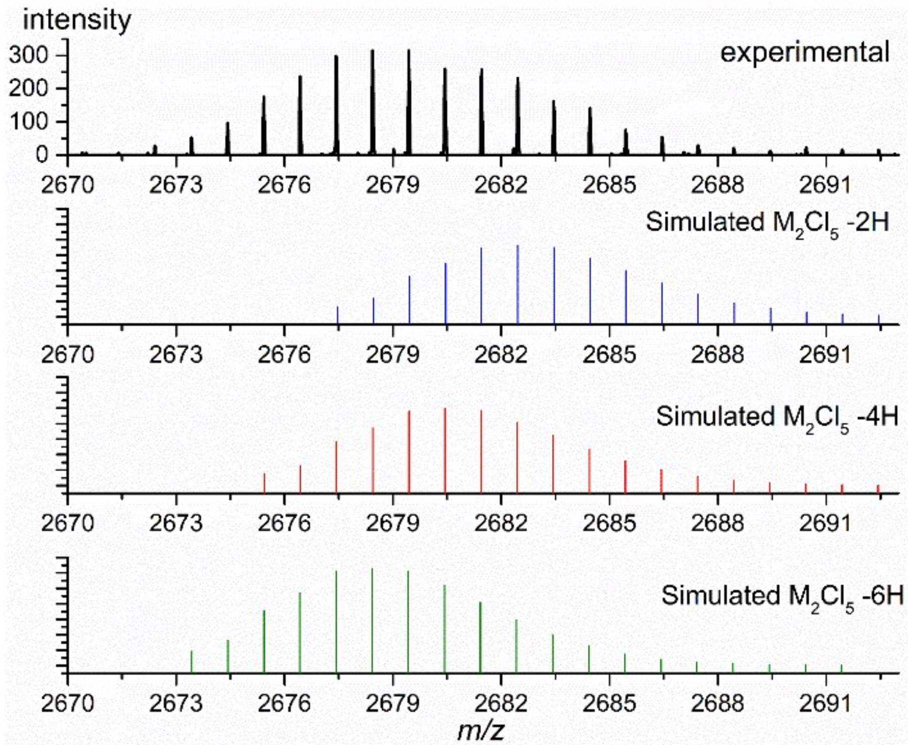


Figure S7. Experimental and simulated spectra for $(NiDDOPP)_2$+ 5Cl-xH. The spectra shows the existence of both triply, doubly and singly linked highly chlorinated dimers.

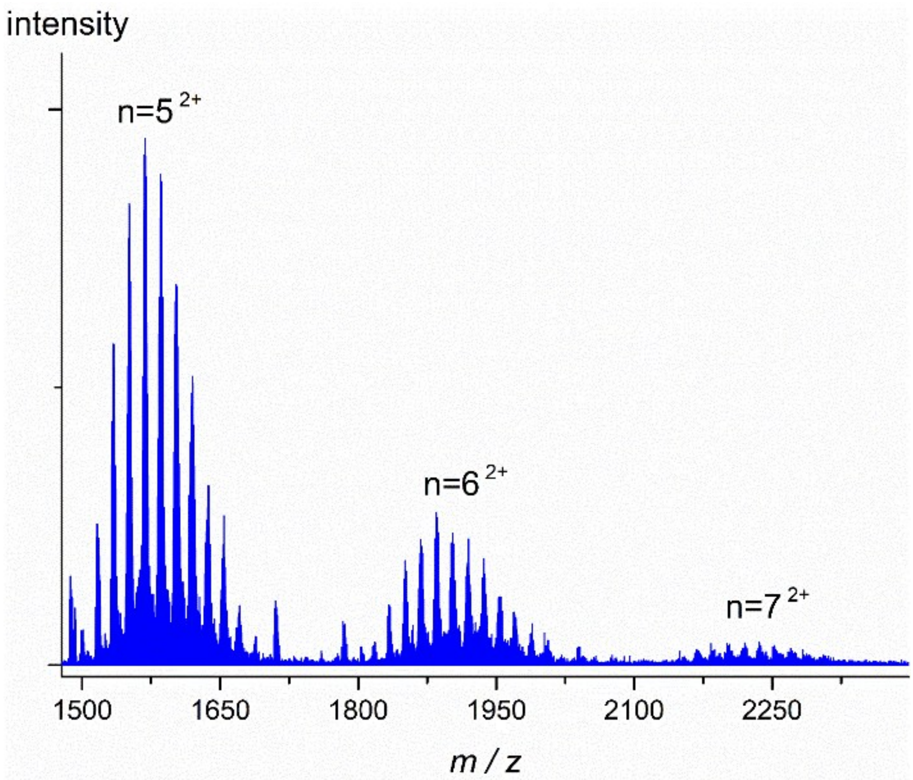


Figure S8. Sum of mass spectra recorded between 6.6 and 8.1 minutes of elution in GPCxESI-HRMS evidences the presence of doubly charged high oligomers (n= 5,6,7).

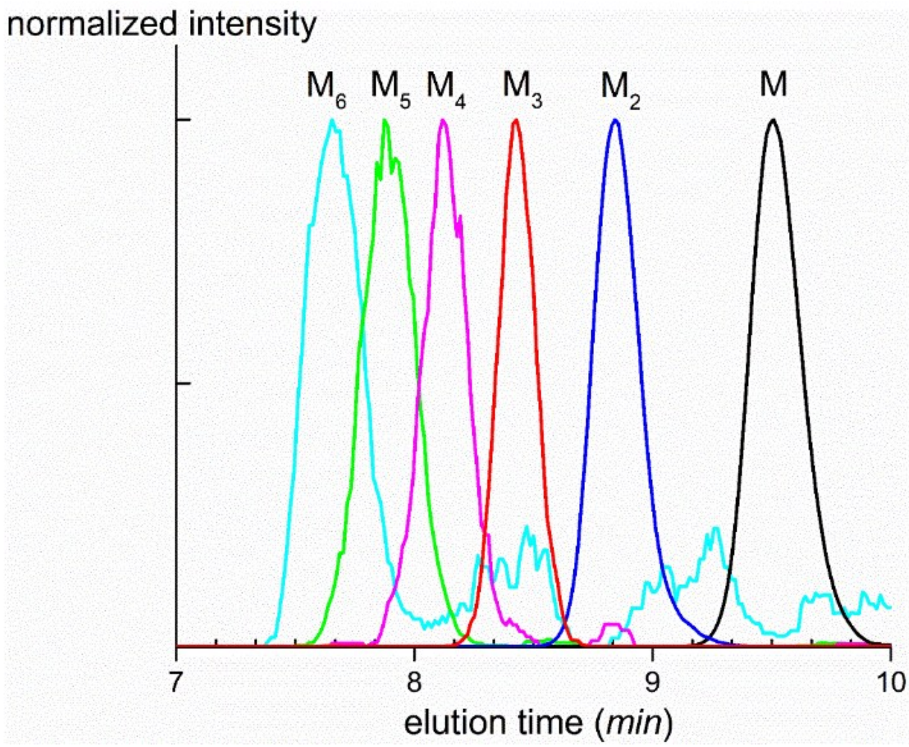


Figure S9. Extracted Ion Chromatogram (EIC) for the NiDMP oCVD coating different oligomers. The analysis clearly show different retention time for different *m/z* ratio going from hexamer (M_6) to monomer (M). The heptamer is omitted because of its low signal to noise ratio.

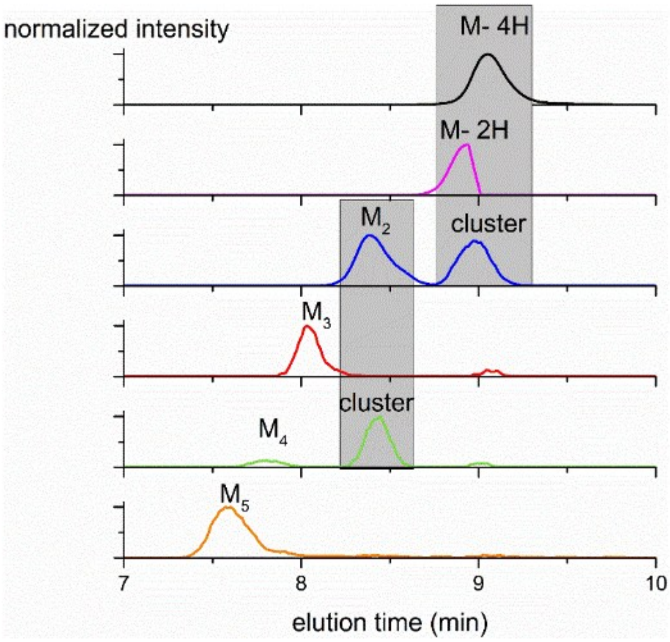


Figure S10. Extracted Ion Chromatograms (EIC) for the NiDtBuPP oCVD coating different oligomers. The analysis clearly show different retention time for different *m/z* going from pentamer (M_5) to the singly and doubly ring fused monomers (M-2H and M-4H). The signals around 8.5 minutes for M_4 and around 9 minutes for the M_2 (grey boxes) are attributed to the formation of clusters. Indeed, this signal is observed simultaneously to the elution of M_2 and M-2H/M-4H that forming dimeric clusters yield the same *m/z* ratio.

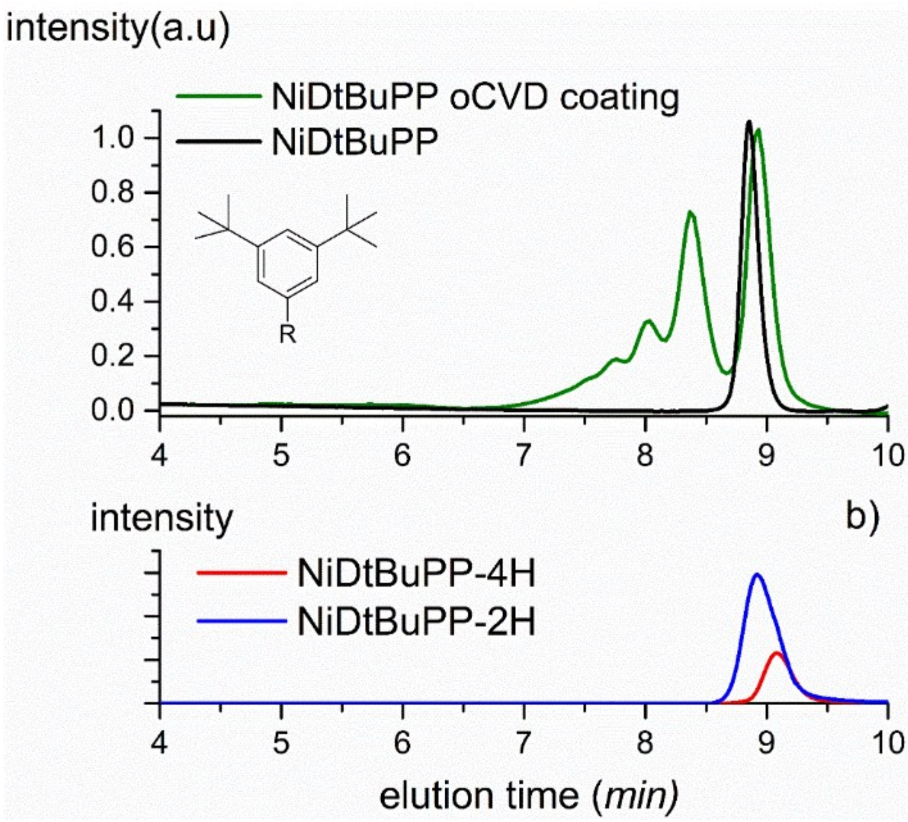


Figure S11. GPC analysis of the NiDtBUPP coating (a) and extracted ion chromatogram for *m/z = 741.35 (NiDtBuPP-2H)* and *739.33 (NiDtBuPP -4H).* The analysis shows that the cyclization reaction affect the geometry of the molecule causing smaller hydrodinamic volume.

Monomer	NiDtBuPP	NiDtBuPP–2H	NiDtBuPP–4H
Parent ion (m/z)	743.36	741.35	739.33
Fragment ion exact mass (Da) **[Loss]**	728.3135 **[CH_3]**	726.3191 **[CH_3]**	724.3033 **[CH_3]**
	687.2797 **[C_4H_8]**	685.2844 **[C_4H_8]**	683.2683 **[C_4H_8]**
	631.2161 **[$(C_4H_8)_2$]**	629.2217 **[$(C_4H_8)_2$]**	627.2057 **[$(C_4H_8)_2$]**
	575.1540 **[$(C_4H_8)_3$]**	573.1586 **[$(C_4H_8)_3$]**	571.1432 **[$(C_4H_8)_3$]**
	554.1975 **[$C_{14}H_{21}$]**	552.1821 **[$C_{14}H_{21}$]**	-
	-	517.0756 **[$(C_4H_8)_4$]**	515.0806 **[$(C_4H_8)_4$]**

Table S3. List of fragment ions and corresponding molecular formula loss from the MS-MS structural analysis of NiDtBuPP monomer and its fused derivatives. Parent ions are detected as protonated adducts $[M+H]^+$.

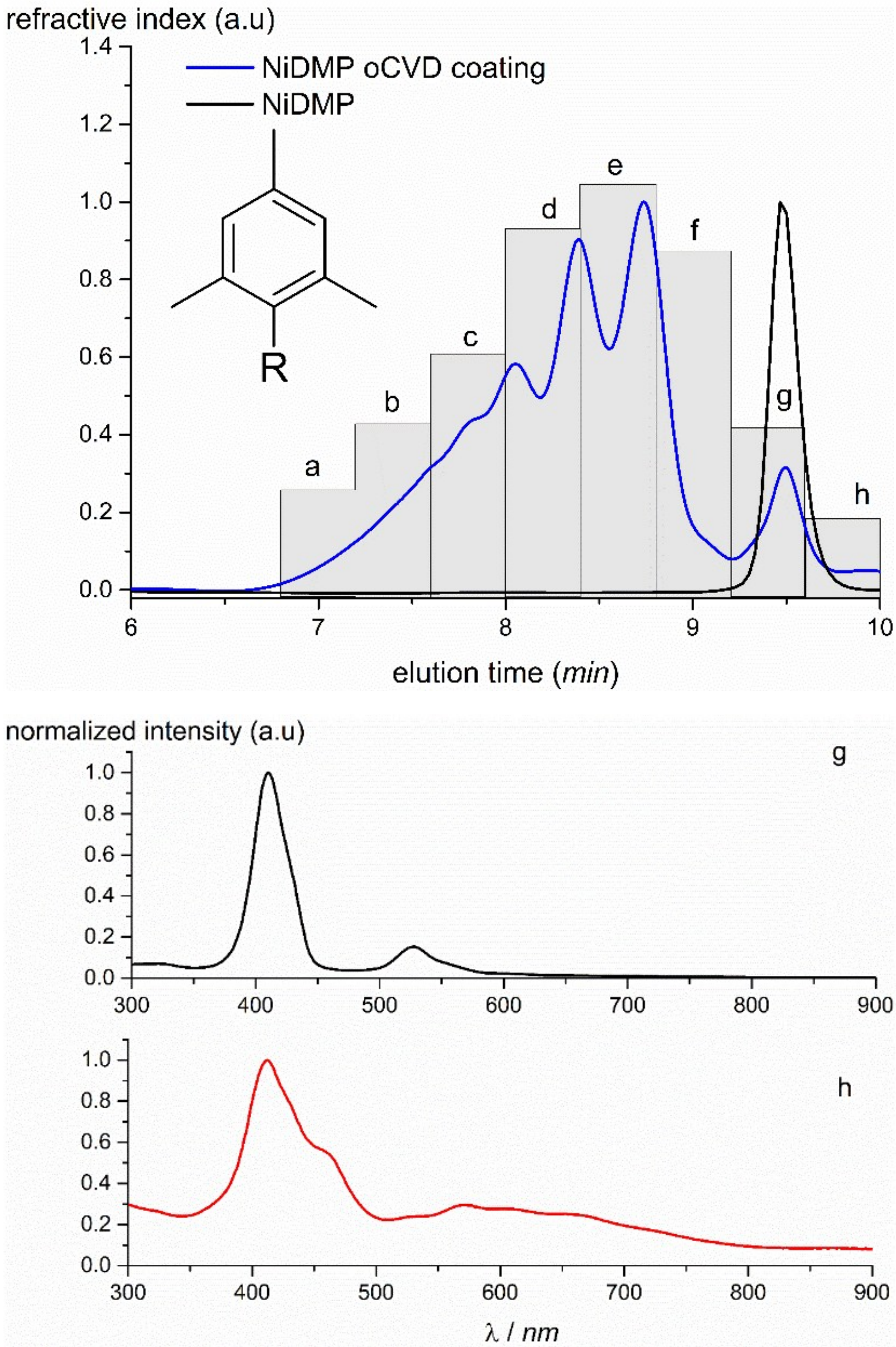


Figure S12. GPC of the NiDMP oCVD coating and UV-Vis spectra acquired along the GPC elution of monomeric species for NiDMP oCVD coating (indicated as fraction g and h).

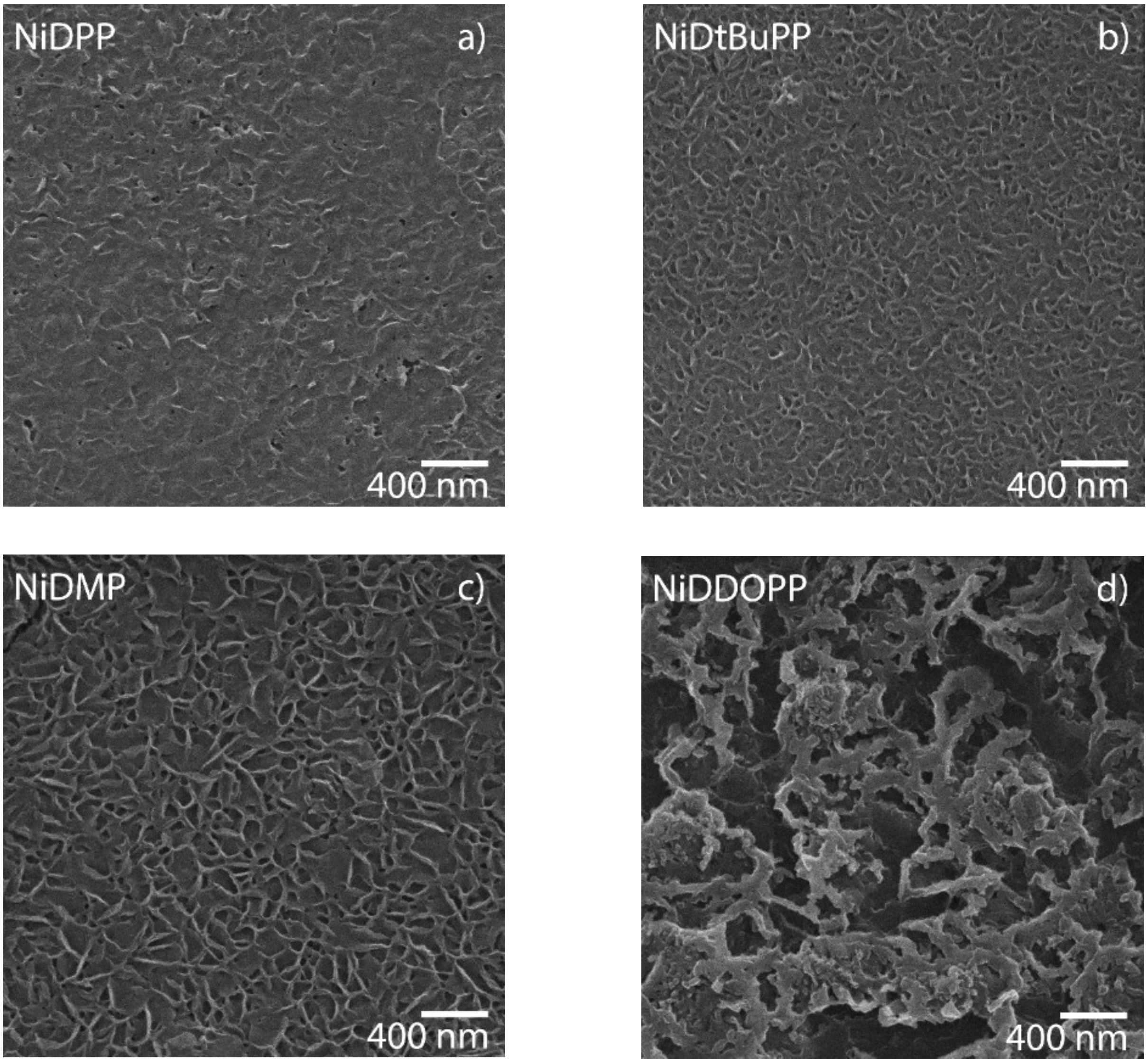


Figure S13. Helium ion microscope images of the a) NiDPP b) NiDtBuPP c) NiDMP d) NiDDOPP oCVD coatings deposited on silicon substrate. The images show the effect of the substituents on the morphology of the oCVD coatings. NiDPP (a) exhibit a smooth surface thanks to the intramolecular cyclization allowing more compact arrangements. Bigger substituents such as dimesity and di-tertbutyl cause a rugged surface (b,c). Finally, the long side chains of the NiDDOPP cause an even more rugged surface.

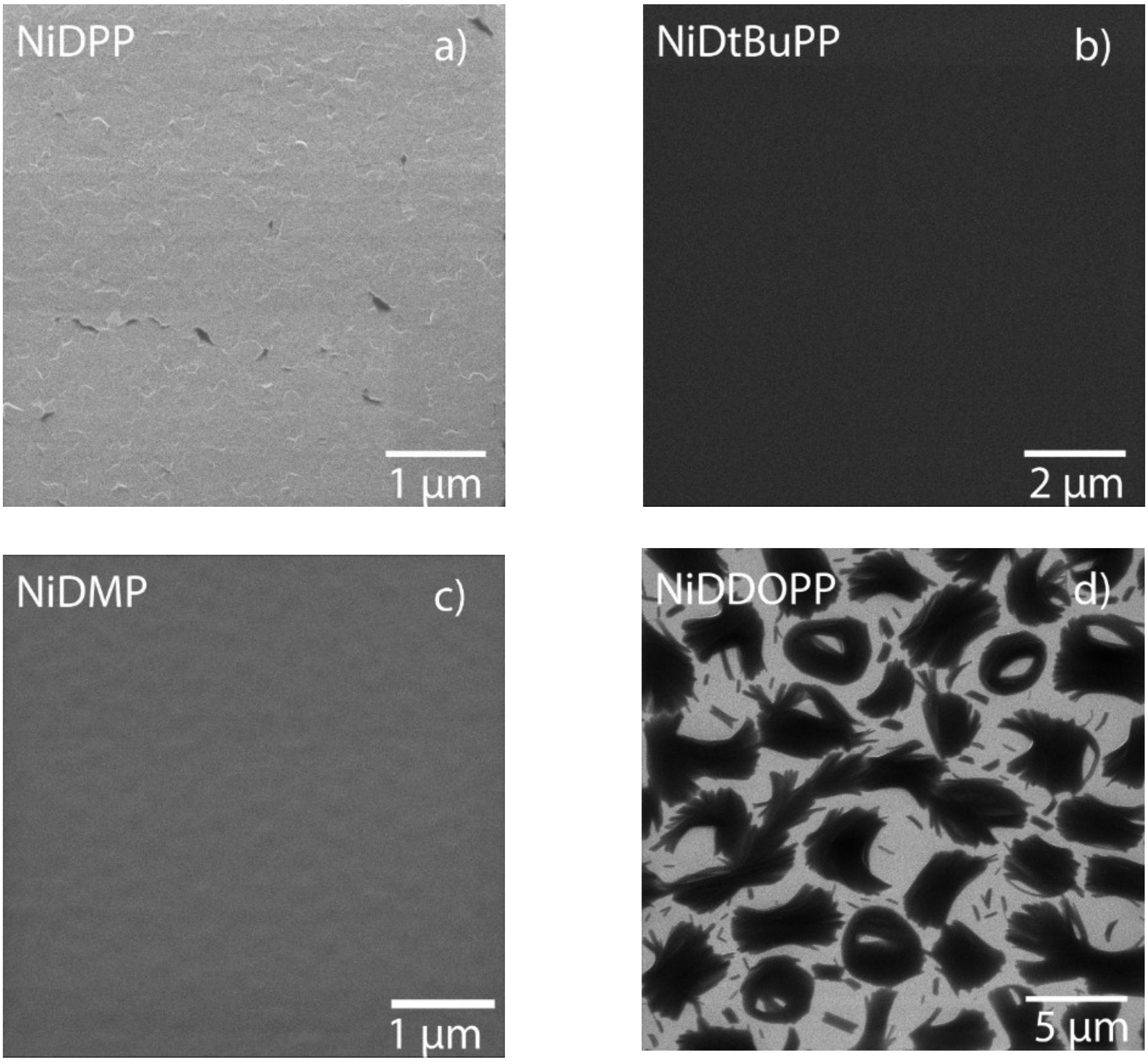


Figure S14. Helium ion microscope images of the sublimated porphyrins deposited on silicon substrate. All the porphyrins cover homogeneously and smoothly the surface. Only the NiDDOPP cover unomogenously the surface. This is probably related to the long chains inducing different interactions between the porphyrins.

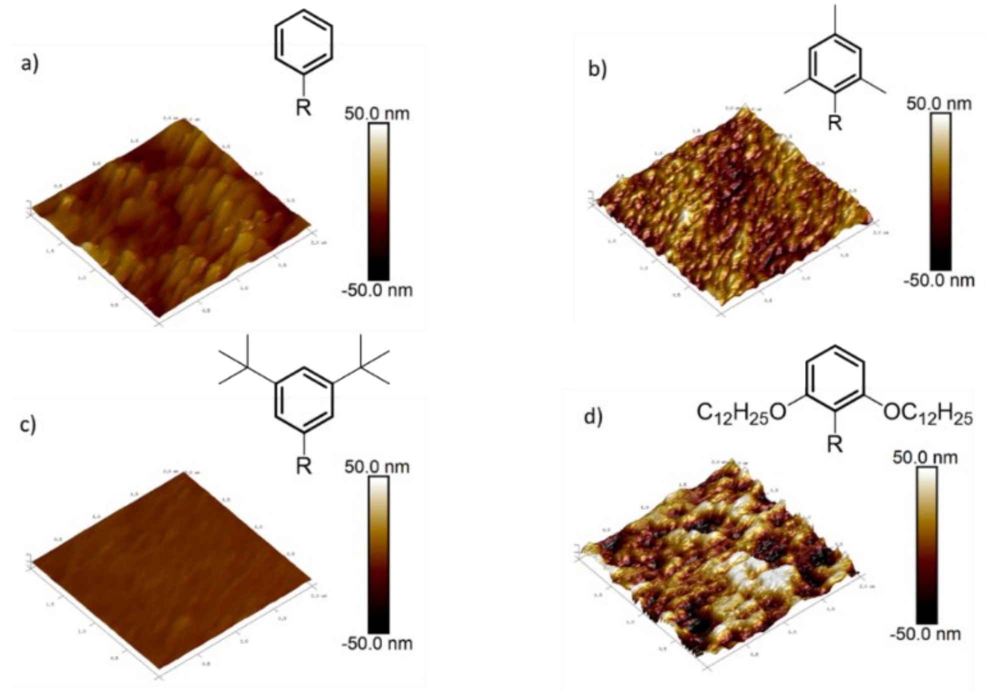


Figure S15. AFM Topography of the probed oCVD coatings on platinum substrate. The same scale used for the images to evidence differences in roughness between the coatings. a) NiDPP oCVD coating, b) NiDMP oCVD coating, c) NiDtBuPP oCVD coating, d) NiDDOPP oCVD coating.

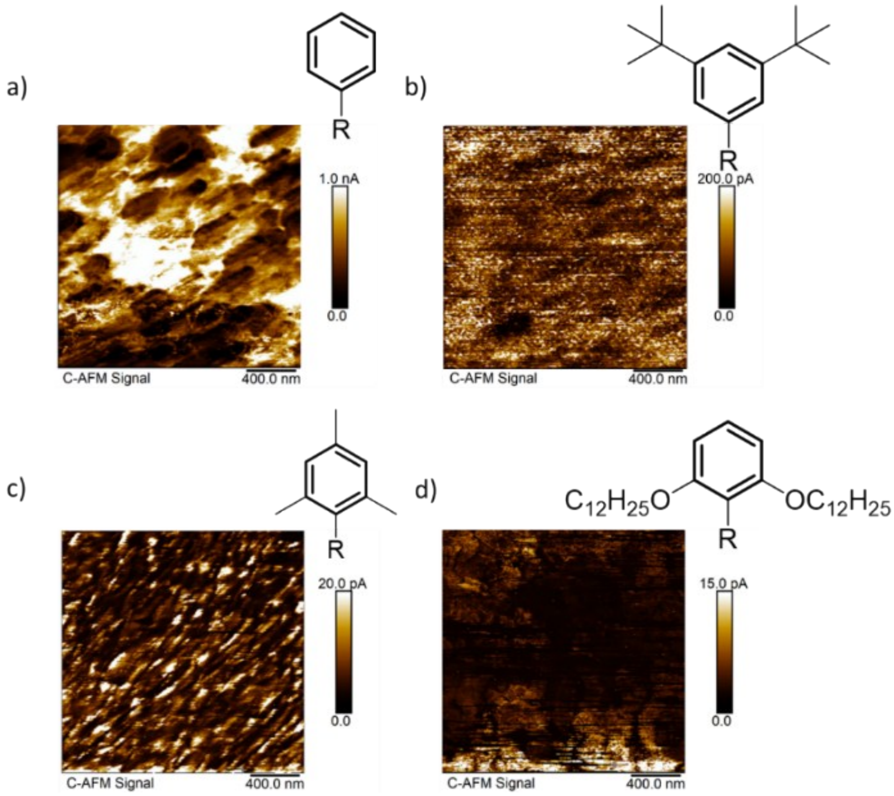


Figure S16. Conductivity AFM images of the probed oCVD coatings acquired simoultaneously to the topographic images. Due to their differences in conductivity, scales were adapted for contrast. a) NiDPP b) NiDMP c) NiDtBuPP and d) NiDDOPP oCVD coatings.

Porphyrin oCVD	Roughness (Ra / nm)	Current (pA)
NiDDOPP	21 ± 3	4.0 ± 1
NiDMP	10 ± 2	6.5 ± 0.6
NiDtBuPP	1.2 ± 0.2	77 ± 15
NiDPP	4.6 ± 0.7	440 ± 120

Table S4. Roughness and current of the different oCVD coatings obtained by C-AFM measurements.

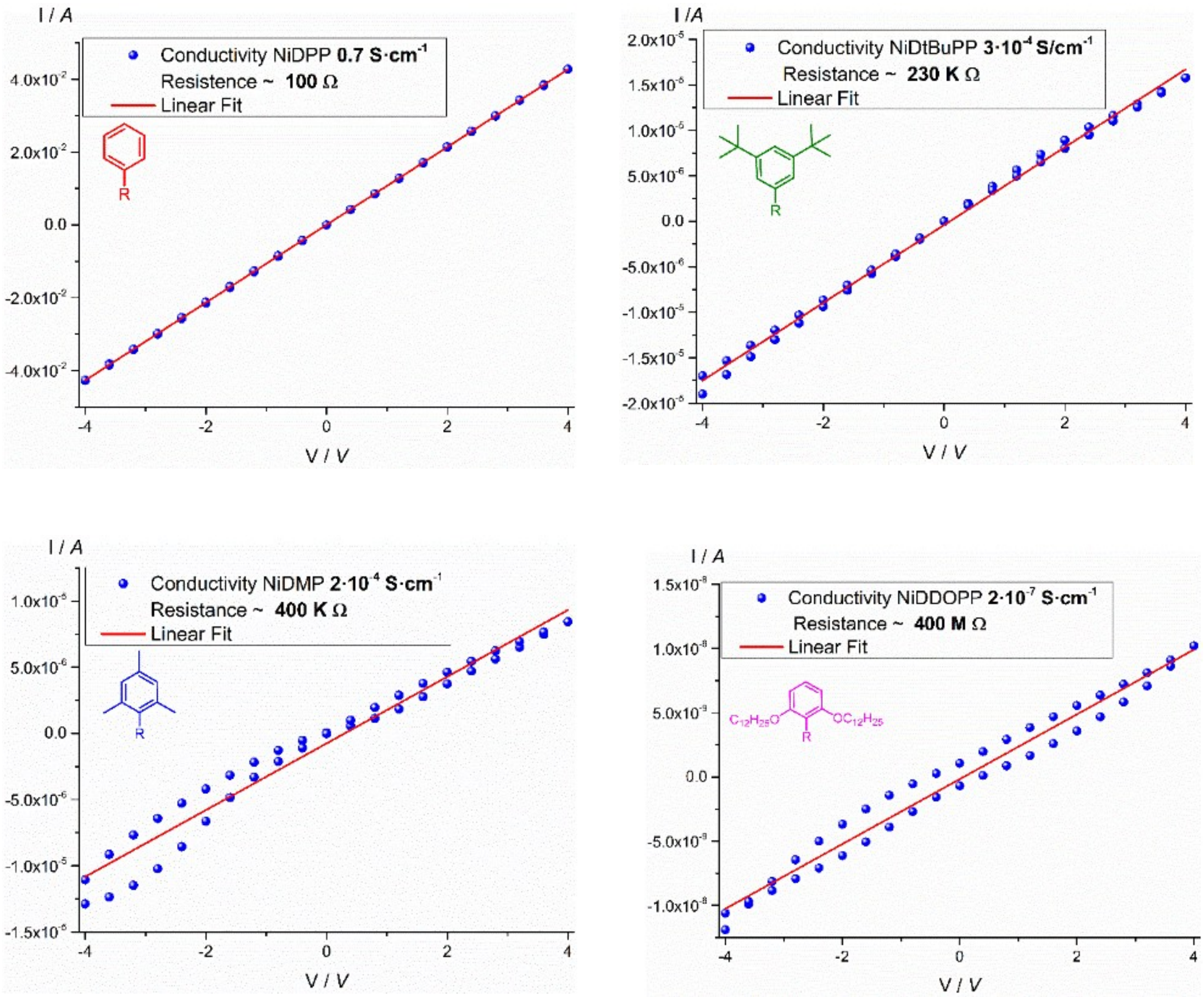


Figure S17. I-V curves obtained from 2-point-probes measurements. Only NiDPP present a perfectly ohmic behaviour. The conductivity is calculated assimilating the behaviour to ohmic also for the other compounds. The calculated conductivity is reported in each graph.

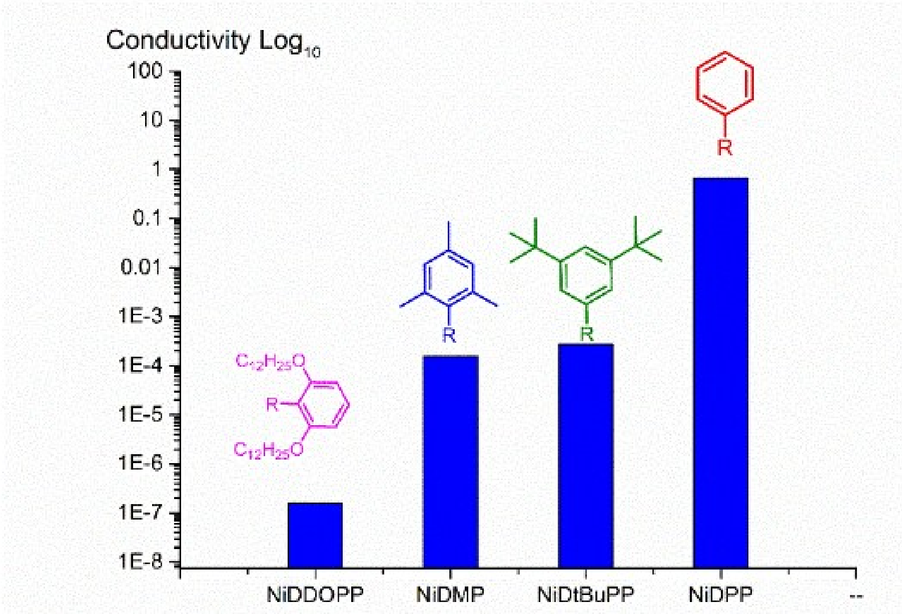


Figure S18. Conductivity calculated for the different oCVD coatings. The resulting conductivity is reported in logarithmic scale.

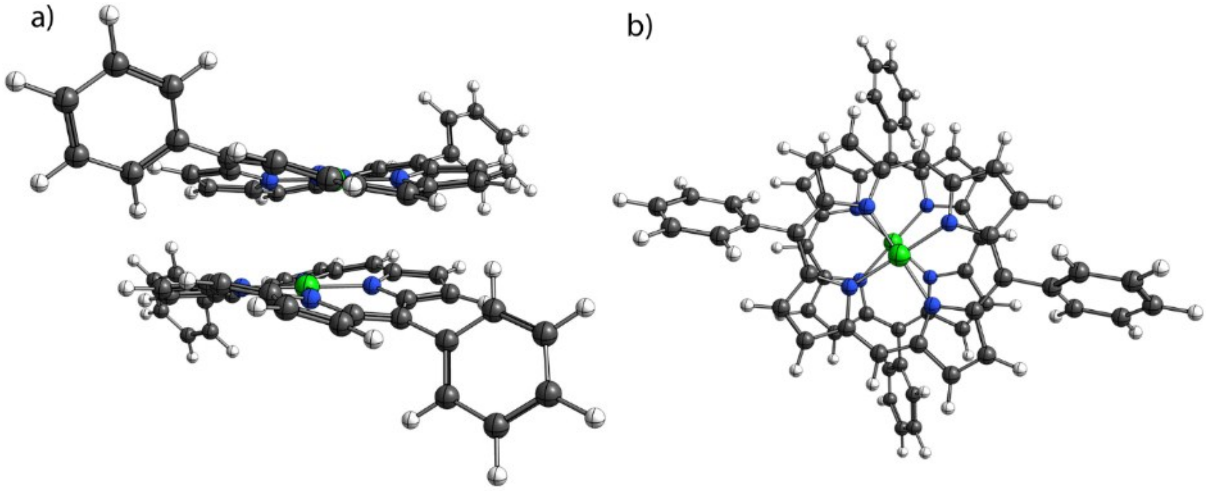


Figure S19. DFT calculated geometry for two NiDPP molecules. a) side view, b) top view. The NiDPP molecules present a saddle shape with the four substituents pointing to different direction to minimize the hindrance. RIJCOSX-BP86-D3BJ-ZORA/def2-SVP level of theory.

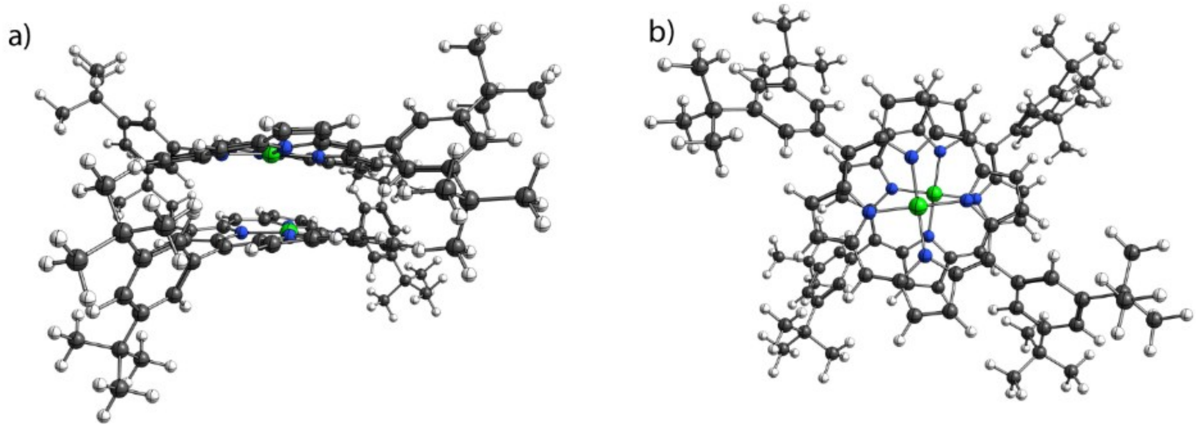


Figure S20. DFT calculated geometry for two NiDtBuPP molecules. a) side view, b) top view. The molecules adopt a saddled, staggered conformation with the *tertbutyl* groups pointing in different directions. RIJCOSX-BP86-D3BJ-ZORA/def2-SVP level of theory.

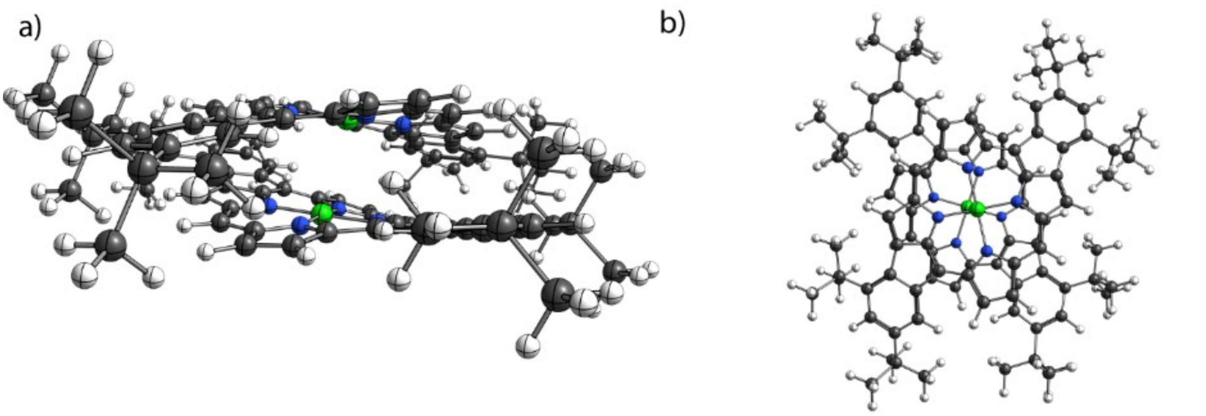


Figure S21. DFT calculated geometry for two NiDtBuPP molecules undergone to cyclization reaction between the phenyl and the porphyrin macrocycle (Fused NiDtBuPP).a) side view, b) top view. The porphyrin present an increase planarity if compared to NiDtBuPP. Only part of the *tert-butyl* group is pointing out of the plane. RIJCOSX-BP86-D3BJ-ZORA/def2-SVP level of theory.

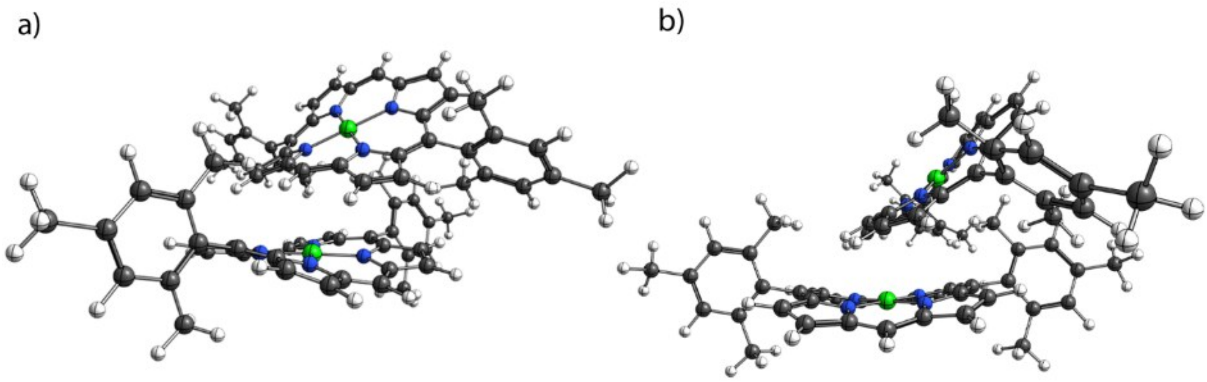


Figure S22. DFT calculated geometry for two NiDMP molecules. a),b) two different side view. Differently from NiDPP the molecules adopt a face to edge conformation. RIJCOSX-BP86-D3BJ-ZORA/def2-SVP level of theory.

Table S5. XYZ Coordinate calculated for two molecules of NiDPP.

	X	Y	Z
6	-0.556183000	-0.394667000	-3.256676000
6	0.199166000	3.395932000	-0.293014000
6	-0.818666000	0.380626000	3.399000000
6	0.351715000	-3.352484000	0.506012000
7	-0.273823000	1.541514000	1.293493000
7	-0.240932000	1.241712000	-1.438801000
7	-0.121520000	-1.525888000	-1.109518000
7	-0.310140000	-1.230184000	1.602419000
6	0.219272000	-2.832763000	-0.790575000
6	-0.338609000	-1.524615000	-2.479369000
6	-0.424844000	0.901801000	-2.769566000
6	0.031100000	2.604834000	-1.438211000
6	0.004181000	-2.583428000	1.626309000
6	-0.645730000	-0.905973000	2.908023000
6	-0.564554000	1.522188000	2.649059000
6	-0.006054000	2.871226000	0.991930000
6	0.238566000	-3.653505000	-1.986139000
6	-0.146063000	-2.847451000	-3.026373000
6	-0.274491000	2.063073000	-3.615903000
6	0.052194000	3.112630000	-2.794239000
6	-0.114509000	3.688426000	2.184455000
6	-0.485079000	2.851103000	3.206911000
6	-0.129315000	-3.105207000	2.971710000
6	-0.578938000	-2.072733000	3.754115000
1	0.464049000	-4.724315000	-1.999465000
1	-0.279338000	-3.105449000	-4.082969000
1	-0.343599000	2.050592000	-4.710129000
1	0.284242000	4.145737000	-3.070108000
1	0.041372000	4.771583000	2.210215000
1	-0.680990000	3.092073000	4.257768000
1	0.092433000	-4.133400000	3.269962000

1	-0.786092000	-2.068801000	4.829927000
6	0.520380000	4.845130000	-0.427381000
6	-0.367530000	5.738265000	-1.066551000
6	1.722189000	5.357212000	0.110340000
1	-1.311458000	5.349531000	-1.474807000
1	2.420072000	4.665979000	0.606406000
6	-0.061270000	7.103755000	-1.169713000
6	2.028590000	6.722574000	0.007678000
1	-0.768393000	7.785653000	-1.666602000
1	2.972490000	7.103006000	0.427407000
6	1.138381000	7.600607000	-0.633376000
1	1.378791000	8.671682000	-0.713741000
6	0.792907000	-4.766842000	0.662144000
6	2.058115000	-5.161735000	0.171469000
6	-0.027536000	-5.742894000	1.269986000
1	2.706112000	-4.406078000	-0.297486000
1	-1.016125000	-5.447528000	1.644705000
6	2.489490000	-6.491807000	0.285750000
6	0.404407000	-7.072853000	1.384716000
1	3.480701000	-6.778413000	-0.097969000
1	-0.252188000	-7.819808000	1.857110000
6	1.664223000	-7.453165000	0.892974000
1	2.002522000	-8.496685000	0.982816000
28	-0.267724000	0.007532000	0.086186000
1	-0.708120000	-0.534020000	-4.335188000
1	-1.069544000	0.502968000	4.460435000
6	-3.204531000	2.661225000	0.981529000
6	-3.898285000	-0.192921000	-2.897245000
6	-2.935035000	-3.971701000	0.021858000
6	-4.161529000	-1.182155000	3.821134000
7	-3.442765000	-1.826989000	-1.083022000
7	-3.465634000	0.881797000	-0.706144000
7	-3.674924000	0.489331000	2.047051000
7	-3.488060000	-2.229450000	1.676636000

6	-4.016307000	0.129527000	3.344919000
6	-3.485842000	1.862008000	2.082487000
6	-3.247837000	2.197227000	-0.325585000
6	-3.684404000	0.924822000	-2.077423000
6	-3.853187000	-2.287971000	3.016518000
6	-3.186161000	-3.533366000	1.318014000
6	-3.132305000	-3.178670000	-1.100684000
6	-3.714232000	-1.492700000	-2.402229000
6	-4.058215000	1.302136000	4.196542000
6	-3.705006000	2.373321000	3.414497000
6	-3.291137000	3.071392000	-1.472744000
6	-3.609316000	2.291279000	-2.554479000
6	-3.595653000	-2.662158000	-3.251942000
6	-3.196884000	-3.697912000	-2.447028000
6	-3.810823000	-3.656568000	3.488286000
6	-3.354580000	-4.422125000	2.444729000
1	-4.294927000	1.284349000	5.265082000
1	-3.606695000	3.428143000	3.694384000
1	-3.160880000	4.158179000	-1.426632000
1	-3.778075000	2.604159000	-3.588392000
1	-3.746007000	-2.658813000	-4.335940000
1	-2.974867000	-4.735352000	-2.721281000
1	-4.093462000	-3.978388000	4.495138000
1	-3.207550000	-5.508105000	2.409746000
6	-4.248268000	-0.023501000	-4.335526000
6	-3.404439000	0.665929000	-5.234375000
6	-5.447040000	-0.583369000	-4.832646000
1	-2.466518000	1.095899000	-4.859481000
1	-6.113251000	-1.116317000	-4.137678000
6	-3.749192000	0.792449000	-6.588527000
6	-5.791234000	-0.457246000	-6.186819000
1	-3.075374000	1.329059000	-7.274245000
1	-6.731999000	-0.895895000	-6.553447000
6	-4.943442000	0.231370000	-7.070651000

1	-5.213285000	0.330656000	-8.133088000
6	-4.573743000	-1.383027000	5.239396000
6	-5.844564000	-0.947237000	5.676301000
6	-3.707138000	-1.984893000	6.178184000
1	-6.526196000	-0.481135000	4.948960000
1	-2.711228000	-2.313663000	5.848401000
6	-6.238224000	-1.112497000	7.012884000
6	-4.100690000	-2.150746000	7.514781000
1	-7.234548000	-0.772077000	7.334291000
1	-3.409358000	-2.617139000	8.233427000
6	-5.368054000	-1.715488000	7.936740000
1	-5.676979000	-1.844986000	8.985194000
28	-3.485069000	-0.671180000	0.485295000
1	-3.040811000	3.733744000	1.147133000
1	-2.697601000	-5.032567000	-0.133114000

Table S6. XYZ Coordinate calculated for two molecules of fused NiDPP.

	X	Y	Z
6	6.041859000	-1.368733000	-2.177541000
6	8.397279000	0.970675000	1.364599000
6	5.878694000	-1.520056000	4.705722000
6	3.512151000	-3.848723000	1.160727000
7	6.863386000	-0.565688000	2.680057000
7	7.029467000	-0.415223000	-0.110165000
7	5.068534000	-2.331300000	-0.151989000
7	4.911033000	-2.494661000	2.637125000
6	4.095135000	-3.259977000	0.040179000
6	5.162694000	-2.226777000	-1.540551000
6	6.905002000	-0.516645000	-1.488911000
6	8.002458000	0.573770000	0.088939000
6	3.931010000	-3.470917000	2.438472000
6	5.031865000	-2.387705000	4.015716000
6	6.745184000	-0.645933000	4.070820000
6	7.808479000	0.387432000	2.488247000
6	3.537060000	-3.773425000	-1.187632000
6	4.215991000	-3.127166000	-2.198126000
6	7.794982000	0.404849000	-2.153584000
6	8.476162000	1.083367000	-1.172976000
6	8.317064000	0.952786000	3.714654000
6	7.643782000	0.299839000	4.727304000
6	3.446732000	-3.972855000	3.700038000
6	4.131260000	-3.298199000	4.681825000
1	4.122752000	-3.222645000	-3.286010000
1	7.880000000	0.507345000	-3.240838000
1	9.236888000	1.859009000	-1.292948000
1	7.715851000	0.419233000	5.815229000
1	4.040650000	-3.394445000	5.770346000
6	9.360410000	1.979587000	1.884839000
6	10.235303000	2.854971000	1.235744000

6	9.305416000	1.967464000	3.328755000
1	10.313133000	2.871524000	0.141085000
6	11.042111000	3.723465000	2.002620000
6	10.111924000	2.827059000	4.076647000
1	11.738700000	4.402596000	1.490470000
1	10.068795000	2.815239000	5.176103000
6	10.982284000	3.711863000	3.402783000
1	11.625976000	4.390131000	3.982645000
6	2.504740000	-4.813231000	0.640465000
6	1.629316000	-5.690865000	1.286358000
6	2.522965000	-4.761557000	-0.804933000
1	1.592975000	-5.753642000	2.382584000
6	0.776738000	-6.513132000	0.514583000
6	1.676351000	-5.576821000	-1.555142000
1	0.087861000	-7.203709000	1.024280000
1	1.701441000	-5.540743000	-2.653886000
6	0.797543000	-6.457321000	-0.885640000
1	0.128446000	-7.107144000	-1.469568000
28	5.994214000	-1.477439000	1.262767000
1	6.057583000	-1.344980000	-3.274658000
1	5.848746000	-1.531780000	5.803920000
1	2.675495000	-4.739679000	3.818094000
6	9.010380000	-2.800306000	-3.278690000
6	11.376114000	-0.469291000	0.265344000
6	8.847181000	-2.949170000	3.604276000
6	6.490467000	-5.288724000	0.063089000
7	9.820128000	-1.986828000	1.578492000
7	9.977773000	-1.824411000	-1.210350000
7	8.024535000	-3.752940000	-1.252917000
7	7.858999000	-3.903076000	1.537232000
6	7.079103000	-4.705638000	-1.060727000
6	8.143194000	-3.673678000	-2.643688000
6	9.857270000	-1.932577000	-2.588898000
6	10.957640000	-0.847907000	-1.012314000

6	6.885980000	-4.892112000	1.338630000
6	7.984169000	-3.801584000	2.915910000
6	9.725875000	-2.090777000	2.967103000
6	10.792909000	-1.057555000	1.386023000
6	6.570436000	-5.271367000	-2.286951000
6	7.244285000	-4.619347000	-3.299833000
6	10.758043000	-1.022590000	-3.255521000
6	11.442297000	-0.347058000	-2.274148000
6	11.350521000	-0.543244000	2.613704000
6	10.671869000	-1.189476000	3.624402000
6	6.413030000	-5.401854000	2.600763000
6	7.094550000	-4.723159000	3.581010000
1	7.172373000	-4.739332000	-4.387702000
1	10.848962000	-0.927284000	-4.344102000
1	12.213537000	0.419695000	-2.392649000
1	10.765043000	-1.093592000	4.712255000
1	7.010048000	-4.825686000	4.668307000
6	12.382812000	0.496065000	0.785321000
6	13.258048000	1.373656000	0.139131000
6	12.364246000	0.445171000	2.230754000
1	13.294649000	1.435778000	-0.957125000
6	14.110122000	2.196698000	0.910647000
6	13.210351000	1.261205000	2.980686000
1	14.798861000	2.887248000	0.400728000
1	13.184982000	1.225799000	4.079445000
6	14.088975000	2.141675000	2.310890000
1	14.757662000	2.792085000	2.894633000
6	5.527349000	-6.297797000	-0.456801000
6	4.652490000	-7.172946000	0.192643000
6	5.582062000	-6.285902000	-1.900725000
1	4.574972000	-7.189365000	1.287326000
6	3.845330000	-8.041400000	-0.573923000
6	4.775080000	-7.145324000	-2.648300000
1	3.148763000	-8.720356000	-0.061515000

1	4.817917000	-7.133675000	-3.747770000
6	3.904709000	-8.029872000	-1.974102000
1	3.260691000	-8.708018000	-2.553744000
28	8.894186000	-2.841094000	0.164064000
1	9.040898000	-2.789267000	-4.376882000
1	8.831581000	-2.972894000	4.701395000
1	5.652523000	-6.177651000	2.721131000

Table S7. XYZ Coordinate calculated for two molecules of NiDtBuPP.

	X	Y	Z
6	-4.065303000	0.280229000	-2.533904000
6	-2.922297000	2.653473000	1.553882000
6	-2.897160000	-1.616216000	3.861173000
6	-3.022146000	-3.963546000	-0.387767000
7	-2.870522000	0.288648000	2.298991000
7	-3.514353000	1.065336000	-0.261561000
7	-3.464490000	-1.614199000	-1.077198000
7	-3.155666000	-2.400094000	1.535378000
6	-3.244239000	-2.961097000	-1.340572000
6	-3.788353000	-1.058047000	-2.307477000
6	-3.929832000	1.266300000	-1.569665000
6	-3.363358000	2.344941000	0.263852000
6	-3.082524000	-3.675713000	0.983482000
6	-3.101619000	-2.601444000	2.909365000
6	-2.725636000	-0.275168000	3.556655000
6	-2.675668000	1.651382000	2.498646000
6	-3.415959000	-3.238421000	-2.753288000
6	-3.768693000	-2.056301000	-3.349189000
6	-4.078343000	2.672186000	-1.858112000
6	-3.704962000	3.347397000	-0.725047000
6	-2.350951000	1.925327000	3.883706000
6	-2.393081000	0.723946000	4.542421000
6	-3.017939000	-4.676988000	2.028478000
6	-3.068781000	-4.009034000	3.223142000
1	-3.330963000	-4.232044000	-3.201915000
1	-4.022141000	-1.865446000	-4.397770000
1	-4.394794000	3.072242000	-2.828192000
1	-3.643700000	4.427313000	-0.559075000
1	-2.163631000	2.923948000	4.289913000
1	-2.232975000	0.511788000	5.605986000
1	-2.927786000	-5.752634000	1.858663000

1	-3.026316000	-4.421716000	4.237277000
6	-2.830727000	4.079735000	1.976060000
6	-3.999270000	4.861627000	2.040569000
6	-1.603651000	4.655695000	2.351393000
1	-4.951899000	4.396492000	1.749841000
1	-0.697595000	4.034824000	2.290489000
6	-3.966467000	6.200807000	2.469053000
6	-1.528582000	5.990926000	2.794036000
6	-2.720376000	6.743343000	2.843207000
1	-2.676579000	7.783417000	3.184436000
6	-2.669088000	-5.334040000	-0.856347000
6	-1.537770000	-5.497707000	-1.689354000
6	-3.401525000	-6.471108000	-0.479976000
1	-0.966891000	-4.601053000	-1.961670000
1	-4.290678000	-6.329082000	0.144549000
6	-1.143426000	-6.765113000	-2.144284000
6	-3.020509000	-7.764739000	-0.892276000
6	-1.896195000	-7.886400000	-1.725784000
1	-1.585092000	-8.883156000	-2.065485000
28	-3.280947000	-0.666097000	0.627989000
1	-4.331006000	0.593388000	-3.551194000
1	-2.809161000	-1.916181000	4.912392000
6	-0.163976000	6.573762000	3.206713000
6	0.801691000	6.507686000	1.999317000
6	0.406903000	5.734378000	4.375194000
1	-0.271258000	5.767264000	5.252374000
1	0.539476000	4.671351000	4.091471000
1	1.396769000	6.126172000	4.689579000
1	0.949693000	5.467376000	1.647806000
1	1.796512000	6.916475000	2.273938000
1	0.408624000	7.098358000	1.146929000
6	-5.278169000	7.005581000	2.516134000
6	-6.273243000	6.297051000	3.466672000
6	-5.879203000	7.068040000	1.091157000

1	-5.181990000	7.570893000	0.390275000
1	-6.087819000	6.056038000	0.689668000
1	-6.834230000	7.633713000	1.094246000
1	-6.506662000	5.268347000	3.126278000
1	-7.229640000	6.857909000	3.518728000
1	-5.857649000	6.226084000	4.492390000
6	-3.840904000	-8.977949000	-0.415381000
6	-3.224192000	-10.312823000	-0.872517000
6	-5.274880000	-8.879014000	-0.986347000
1	-5.787315000	-7.961387000	-0.635949000
1	-5.260703000	-8.855895000	-2.095004000
1	-5.887193000	-9.747344000	-0.665472000
1	-3.195112000	-10.396751000	-1.977768000
1	-3.830333000	-11.159383000	-0.490980000
1	-2.191143000	-10.439741000	-0.490062000
6	0.073431000	-6.969392000	-3.065689000
6	-0.397902000	-7.636628000	-4.380120000
6	1.100941000	-7.884839000	-2.358272000
1	1.447957000	-7.428177000	-1.409160000
1	0.670060000	-8.877184000	-2.117175000
1	1.986597000	-8.050169000	-3.006775000
1	-0.872657000	-8.620858000	-4.194661000
1	0.461161000	-7.799718000	-5.064021000
1	-1.138852000	-6.998102000	-4.903014000
6	-0.270567000	8.039714000	3.666410000
1	-0.654725000	8.697978000	2.860917000
1	-0.935015000	8.148961000	4.547501000
1	0.731317000	8.416713000	3.955666000
6	-5.060750000	8.444386000	3.019700000
1	-4.370952000	9.011342000	2.362150000
1	-6.027227000	8.987658000	3.037204000
1	-4.648538000	8.462591000	4.048945000
6	-3.903469000	-8.969895000	1.131040000
1	-4.381334000	-8.047554000	1.518473000

1	-4.491799000	-9.834604000	1.502723000
1	-2.886115000	-9.030918000	1.568277000
6	0.763974000	-5.638187000	-3.416199000
1	1.150223000	-5.123827000	-2.513198000
1	1.625905000	-5.826542000	-4.088005000
1	0.076806000	-4.942675000	-3.939211000
6	-6.381071000	1.626015000	0.872762000
6	-6.123035000	-1.875120000	4.226403000
6	-6.375769000	-5.170813000	0.667302000
6	-7.109466000	-1.679640000	-2.609550000
7	-6.344005000	-3.194277000	2.137733000
7	-6.187415000	-0.442623000	2.198314000
7	-6.757915000	-0.357414000	-0.540478000
7	-6.545986000	-3.100627000	-0.653834000
6	-7.156014000	-0.493606000	-1.866431000
6	-6.782687000	1.009186000	-0.302371000
6	-6.066213000	0.932980000	2.029076000
6	-5.984059000	-0.652024000	3.557523000
6	-6.732876000	-2.889132000	-2.015111000
6	-6.371549000	-4.473533000	-0.530969000
6	-6.426729000	-4.560411000	1.910215000
6	-6.340146000	-3.065191000	3.521611000
6	-7.516338000	0.792820000	-2.425797000
6	-7.254352000	1.729803000	-1.459217000
6	-5.707687000	1.577714000	3.268623000
6	-5.653857000	0.594854000	4.220833000
6	-6.503698000	-4.358661000	4.155498000
6	-6.536551000	-5.289401000	3.149785000
6	-6.565978000	-4.126249000	-2.751034000
6	-6.345348000	-5.111680000	-1.825635000
1	-7.904021000	0.942905000	-3.437779000
1	-7.369831000	2.818610000	-1.502589000
1	-5.519039000	2.650953000	3.380023000
1	-5.399007000	0.688529000	5.279498000

1	-6.580156000	-4.516421000	5.235372000
1	-6.633967000	-6.379107000	3.221479000
1	-6.608335000	-4.208151000	-3.840957000
1	-6.176788000	-6.181585000	-1.987318000
6	-5.991377000	-1.907535000	5.708392000
6	-6.801966000	-1.093836000	6.523577000
6	-5.030760000	-2.734219000	6.322909000
1	-7.565088000	-0.468914000	6.037410000
1	-4.406759000	-3.367362000	5.679768000
6	-6.651553000	-1.073538000	7.922825000
6	-4.856469000	-2.752879000	7.717807000
6	-5.672553000	-1.909404000	8.498578000
1	-5.543863000	-1.904252000	9.586534000
6	-7.435004000	-1.658640000	-4.062257000
6	-6.710278000	-0.832490000	-4.943745000
6	-8.459654000	-2.478496000	-4.577293000
1	-5.918302000	-0.206065000	-4.522229000
1	-9.023282000	-3.102542000	-3.872389000
6	-6.982216000	-0.814654000	-6.322405000
6	-8.759636000	-2.492522000	-5.951966000
6	-8.007842000	-1.654407000	-6.800599000
1	-8.232236000	-1.655202000	-7.878156000
28	-6.418994000	-1.772282000	0.780378000
1	-6.341180000	2.722492000	0.894268000
1	-6.389074000	-6.268069000	0.631886000
6	-3.789222000	-3.681589000	8.325789000
6	-2.403635000	-3.316587000	7.741219000
6	-4.133366000	-5.145420000	7.959491000
1	-5.123410000	-5.432353000	8.368797000
1	-4.168029000	-5.294991000	6.861473000
1	-3.373451000	-5.841379000	8.372194000
1	-2.373487000	-3.448111000	6.640987000
1	-1.613185000	-3.964306000	8.173932000
1	-2.144967000	-2.261148000	7.962619000

6	-7.549063000	-0.145609000	8.762632000
6	-9.029683000	-0.538913000	8.544681000
6	-7.326254000	1.315802000	8.303329000
1	-6.268980000	1.618035000	8.449503000
1	-7.569768000	1.451858000	7.230812000
1	-7.967082000	2.009938000	8.886172000
1	-9.324774000	-0.454336000	7.479984000
1	-9.698783000	0.121847000	9.134506000
1	-9.210426000	-1.586089000	8.862026000
6	-9.866667000	-3.383662000	-6.545614000
6	-9.239091000	-4.340580000	-7.587335000
6	-10.925733000	-2.488996000	-7.232627000
1	-11.384836000	-1.790739000	-6.503598000
1	-10.484807000	-1.881965000	-8.048500000
1	-11.733871000	-3.109847000	-7.672689000
1	-8.749989000	-3.787113000	-8.413727000
1	-10.017300000	-4.994485000	-8.033360000
1	-8.472429000	-4.988860000	-7.116046000
6	-6.198143000	0.079078000	-7.300369000
6	-7.181232000	1.051802000	-7.994225000
6	-5.508607000	-0.810314000	-8.362022000
1	-4.803290000	-1.520368000	-7.884028000
1	-6.244104000	-1.404853000	-8.939874000
1	-4.937392000	-0.187730000	-9.081862000
1	-7.966423000	0.508658000	-8.557019000
1	-6.642787000	1.706345000	-8.711023000
1	-7.687999000	1.698508000	-7.249231000
6	-3.718939000	-3.561857000	9.859257000
1	-3.454484000	-2.533839000	10.180152000
1	-4.680847000	-3.835354000	10.338154000
1	-2.942037000	-4.246243000	10.256213000
6	-7.235625000	-0.236878000	10.267574000
1	-6.188709000	0.053942000	10.489359000
1	-7.899144000	0.449075000	10.832188000

1	-7.400445000	-1.259905000	10.662480000
6	-10.567214000	-4.230839000	-5.466866000
1	-11.061081000	-3.598075000	-4.702164000
1	-11.349639000	-4.862862000	-5.933772000
1	-9.857366000	-4.905614000	-4.947121000
6	-5.116029000	0.908711000	-6.582689000
1	-4.359661000	0.262988000	-6.091755000
1	-4.581182000	1.546732000	-7.314793000
1	-5.551799000	1.576642000	-5.811977000

Table S8. XYZ Coordinate calculated for two molecules of fused NiDtBuPP.

	X	Y	Z
6	5.977339000	-1.085407000	-2.422983000
6	9.659072000	0.457704000	0.332783000
6	7.419111000	-1.285100000	4.272475000
6	4.475992000	-3.777770000	1.336607000
7	8.176507000	-0.672887000	2.029113000
7	7.643784000	-0.436183000	-0.705210000
7	5.603995000	-2.192662000	-0.278567000
7	6.037941000	-2.303419000	2.484759000
6	4.790942000	-3.205678000	0.105813000
6	5.320339000	-2.016075000	-1.632357000
6	7.072218000	-0.347478000	-1.969065000
6	8.808486000	0.328025000	-0.770379000
6	5.030153000	-3.268826000	2.512951000
6	6.343365000	-2.050565000	3.814204000
6	8.328471000	-0.686722000	3.413860000
6	9.280870000	-0.029469000	1.579606000
6	3.994610000	-3.753393000	-0.968172000
6	4.308345000	-2.972360000	-2.069851000
6	7.855633000	0.519306000	-2.815948000
6	8.937542000	0.931783000	-2.074564000
6	10.204245000	0.365639000	2.626763000
6	9.571457000	-0.026123000	3.795977000
6	4.674165000	-3.582766000	3.876258000
6	5.477438000	-2.812301000	4.684018000
1	3.926133000	-3.008749000	-3.096308000
1	7.625562000	0.734788000	-3.865796000
1	9.754064000	1.586357000	-2.391738000
1	9.866534000	0.086193000	4.841708000
1	5.515496000	-2.777935000	5.777898000
6	10.973702000	1.100983000	0.538562000
6	11.821353000	1.629954000	-0.429846000

6	11.345007000	1.035377000	1.942275000
1	11.509028000	1.622055000	-1.478178000
6	13.097547000	2.106047000	-0.067185000
6	12.620980000	1.516236000	2.319080000
6	13.451712000	2.032820000	1.287599000
1	14.447956000	2.396763000	1.577047000
6	3.510881000	-4.862812000	1.035913000
6	2.983379000	-5.835245000	1.879147000
6	3.219128000	-4.867829000	-0.382726000
1	3.248877000	-5.834191000	2.944198000
6	2.150960000	-6.854226000	1.355794000
6	2.390524000	-5.872635000	-0.921720000
6	1.875514000	-6.843473000	-0.021304000
1	1.235443000	-7.632453000	-0.428458000
28	6.881924000	-1.420441000	0.877841000
1	5.680079000	-0.972348000	-3.473767000
1	7.594139000	-1.231713000	5.355352000
1	3.890717000	-4.285622000	4.175692000
6	12.170969000	-2.218790000	1.808376000
6	9.886496000	-2.313300000	-2.471723000
6	6.770209000	-5.590816000	-0.705770000
6	8.358585000	-4.531686000	3.749711000
7	8.483259000	-3.888217000	-1.090962000
7	10.761899000	-2.535477000	-0.207864000
7	10.071403000	-3.370973000	2.293653000
7	7.885886000	-4.870245000	1.384951000
6	9.468602000	-3.742925000	3.448902000
6	11.259834000	-2.763898000	2.701726000
6	11.922400000	-2.124864000	0.437956000
6	10.888995000	-2.084952000	-1.522127000
6	7.640804000	-5.158268000	2.728479000
6	7.004108000	-5.668274000	0.670174000
6	7.435112000	-4.693859000	-1.527660000
6	8.823604000	-3.163053000	-2.184419000

6	10.206115000	-3.370922000	4.635822000
6	11.362553000	-2.773572000	4.156614000
6	12.805933000	-1.463647000	-0.490737000
6	12.160809000	-1.429536000	-1.705401000
6	7.999227000	-3.424082000	-3.348355000
6	7.140218000	-4.428676000	-2.931698000
6	6.628283000	-6.180937000	2.845298000
6	6.245777000	-6.510717000	1.565856000
1	12.225451000	-2.367986000	4.696650000
1	13.779903000	-1.040671000	-0.220183000
1	12.523021000	-1.006027000	-2.646931000
1	6.359578000	-4.972174000	-3.469355000
1	5.487480000	-7.232550000	1.243838000
6	9.674939000	-1.868895000	-3.865923000
6	10.382912000	-0.894845000	-4.564690000
6	8.498017000	-2.518006000	-4.419477000
1	11.238793000	-0.407306000	-4.087040000
6	9.951923000	-0.492791000	-5.845587000
6	8.059555000	-2.126889000	-5.706037000
6	8.812997000	-1.121207000	-6.370595000
1	8.468137000	-0.805986000	-7.365673000
6	8.285234000	-4.568801000	5.230651000
6	7.309848000	-5.122681000	6.053380000
6	9.410382000	-3.846528000	5.787379000
1	6.450433000	-5.637378000	5.605716000
6	7.403273000	-4.983939000	7.459075000
6	9.520798000	-3.699453000	7.185828000
6	8.499886000	-4.280573000	7.984088000
1	8.573147000	-4.169726000	9.070427000
28	9.284721000	-3.637051000	0.598349000
1	13.104796000	-1.790001000	2.194355000
1	5.980255000	-6.221919000	-1.134195000
1	6.269269000	-6.605485000	3.787437000
6	13.613386000	2.981194000	4.115343000

1	14.051428000	3.009237000	5.134843000
1	14.353575000	3.423315000	3.419872000
1	12.714554000	3.630494000	4.108436000
1	12.806179000	1.016828000	5.803483000
6	12.299519000	0.987201000	4.817586000
1	11.379665000	1.597074000	4.893364000
1	12.013955000	-0.060853000	4.616075000
6	13.239639000	1.527039000	3.734405000
6	14.513258000	0.645550000	3.735070000
1	15.270355000	0.997130000	3.006839000
1	14.983494000	0.647402000	4.740424000
1	14.263265000	-0.404406000	3.478788000
6	14.095179000	2.655645000	-1.101556000
6	13.512271000	2.633343000	-2.527545000
1	14.254612000	3.032357000	-3.247807000
1	12.598396000	3.255851000	-2.609480000
1	13.256523000	1.603657000	-2.849848000
6	14.456508000	4.115409000	-0.738684000
1	15.177733000	4.533599000	-1.471714000
1	14.918568000	4.184477000	0.266360000
1	13.552014000	4.756882000	-0.737705000
6	15.374012000	1.784314000	-1.086395000
1	16.116921000	2.166997000	-1.817064000
1	15.854660000	1.777888000	-0.087861000
1	15.138857000	0.734336000	-1.355555000
6	1.614689000	-7.939756000	2.304674000
6	2.815132000	-8.689246000	2.933461000
1	2.462613000	-9.474678000	3.634183000
1	3.476063000	-8.003779000	3.500987000
1	3.429923000	-9.177554000	2.149916000
6	0.778962000	-7.271579000	3.422778000
1	0.392141000	-8.035293000	4.129417000
1	-0.086271000	-6.725224000	2.995628000
1	1.378880000	-6.545651000	4.007235000

6 0.725907000 -8.965527000 1.577498000

1 0.360155000 -9.725317000 2.297555000

1 -0.161654000 -8.486713000 1.116516000

1 1.281347000 -9.500945000 0.781105000

6 2.067820000 -5.941812000 -2.426756000

6 1.151636000 -7.129907000 -2.781188000

1 0.949009000 -7.127281000 -3.871386000

1 0.174230000 -7.070581000 -2.261179000

1 1.618258000 -8.104570000 -2.532543000

6 1.336207000 -4.644596000 -2.846841000

1 1.158695000 -4.635052000 -3.942656000

1 1.904737000 -3.734866000 -2.580823000

1 0.352646000 -4.576619000 -2.339466000

6 3.386017000 -6.117312000 -3.220079000

1 3.187321000 -6.118647000 -4.312039000

1 4.111765000 -5.311611000 -3.006405000

1 3.867264000 -7.082173000 -2.959557000

6 10.691036000 -2.938061000 7.837103000

6 10.584976000 -2.890356000 9.374294000

1 11.449879000 -2.331875000 9.786221000

1 10.599070000 -3.903384000 9.824646000

1 9.663965000 -2.373327000 9.711930000

6 12.016602000 -3.652484000 7.480142000

1 12.884491000 -3.082898000 7.873561000

1 12.148482000 -3.773772000 6.389445000

1 12.039644000 -4.666406000 7.928307000

6 10.694605000 -1.478273000 7.324617000

1 11.560277000 -0.920430000 7.738171000

1 10.750829000 -1.425516000 6.222804000

1 9.768625000 -0.955251000 7.639937000

6 6.301827000 -5.591945000 8.344590000

6 4.942646000 -4.952999000 7.968905000

1 4.124579000 -5.385335000 8.581994000

1 4.689250000 -5.121932000 6.903192000

1	4.959364000	-3.857650000	8.143357000
6	6.239504000	-7.118570000	8.097116000
1	5.444341000	-7.582078000	8.717723000
1	7.204752000	-7.599641000	8.354763000
1	6.019954000	-7.354346000	7.036600000
6	6.556221000	-5.350185000	9.843815000
1	5.741428000	-5.804935000	10.442849000
1	7.510639000	-5.805286000	10.177461000
1	6.586304000	-4.268869000	10.087528000
6	6.824569000	-2.645982000	-6.475860000
6	5.851855000	-1.465134000	-6.718821000
1	4.957086000	-1.809876000	-7.277823000
1	6.319714000	-0.646913000	-7.300547000
1	5.507372000	-1.035652000	-5.755644000
6	7.282454000	-3.231368000	-7.834945000
1	6.407824000	-3.612288000	-8.402419000
1	7.986761000	-4.073731000	-7.680440000
1	7.791564000	-2.478682000	-8.468306000
6	6.050358000	-3.742497000	-5.734208000
1	5.185039000	-4.068265000	-6.346585000
1	6.685354000	-4.629441000	-5.550213000
1	5.660872000	-3.379734000	-4.765608000
6	10.658035000	0.617916000	-6.642653000
6	11.876216000	1.181370000	-5.886458000
1	12.363292000	1.974021000	-6.489467000
1	12.635941000	0.398861000	-5.686391000
1	11.585716000	1.633960000	-4.916745000
6	11.139201000	0.049945000	-7.998787000
1	11.647422000	0.837224000	-8.593928000
1	10.294716000	-0.337321000	-8.603191000
1	11.853668000	-0.784237000	-7.845997000
6	9.659167000	1.774785000	-6.886752000
1	10.141348000	2.593860000	-7.460281000
1	8.772881000	1.437183000	-7.460109000

1	9.298758000	2.193398000	-5.924774000

Table S9. XYZ Coordinate calculated for two molecules of NiDMP.

	X	Y	Z
6	-0.668769000	-0.511084000	-3.517404000
6	-2.275878000	2.262464000	0.153887000
6	-0.852718000	-1.316061000	3.133479000
6	-1.089150000	-4.401674000	-0.622848000
7	-1.535612000	0.191596000	1.302672000
7	-1.466097000	0.517584000	-1.419966000
7	-0.909259000	-2.185607000	-1.727260000
7	-1.001026000	-2.514817000	0.986421000
6	-0.952491000	-3.574073000	-1.743771000
6	-0.629605000	-1.813328000	-3.033493000
6	-1.116253000	0.565401000	-2.763167000
6	-1.932026000	1.789445000	-1.118584000
6	-1.048578000	-3.867507000	0.669866000
6	-0.789377000	-2.467492000	2.356302000
6	-1.284166000	-0.092517000	2.637094000
6	-2.061142000	1.478029000	1.294047000
6	-0.710879000	-4.073933000	-3.080829000
6	-0.469967000	-2.977729000	-3.873786000
6	-1.359951000	1.881504000	-3.307812000
6	-1.885305000	2.638287000	-2.291053000
6	-2.183727000	1.980413000	2.647993000
6	-1.665597000	1.020521000	3.477495000
6	-0.894587000	-4.673617000	1.862404000
6	-0.690081000	-3.801843000	2.904210000
1	-0.701541000	-5.136513000	-3.347107000
1	-0.239771000	-2.942928000	-4.945209000
1	-1.166758000	2.166480000	-4.348545000
1	-2.197436000	3.687956000	-2.300176000
1	-2.589242000	2.961849000	2.906468000
1	-1.579639000	1.035477000	4.570166000
1	-0.908392000	-5.768999000	1.869009000

1	-0.520460000	-4.026741000	3.963905000
6	-2.706068000	3.687736000	0.307248000
6	-4.019381000	4.079335000	-0.054235000
6	-1.782107000	4.650948000	0.794023000
6	-4.409898000	5.417540000	0.136589000
6	-2.216069000	5.978060000	0.968471000
1	-5.438882000	5.709627000	-0.129616000
1	-1.497971000	6.724658000	1.345942000
6	-3.530107000	6.380482000	0.661782000
6	-1.111308000	-5.886271000	-0.806639000
6	0.112173000	-6.602738000	-0.851626000
6	-2.346636000	-6.566046000	-0.945407000
6	0.074838000	-7.997483000	-1.034544000
6	-2.337227000	-7.961408000	-1.127063000
1	1.026163000	-8.553216000	-1.073507000
1	-3.299108000	-8.488281000	-1.238844000
6	-1.138493000	-8.697542000	-1.172347000
28	-1.250853000	-0.995819000	-0.216096000
1	-0.432395000	-0.340553000	-4.576374000
1	-0.679415000	-1.406335000	4.214391000
6	-3.986947000	7.798581000	0.908644000
1	-4.770394000	8.106683000	0.187889000
1	-4.421453000	7.904650000	1.926635000
1	-3.146994000	8.517931000	0.836431000
6	-0.348140000	4.276340000	1.088008000
1	-0.261192000	3.663880000	2.009650000
1	0.082144000	3.665396000	0.268653000
1	0.279522000	5.178972000	1.218889000
6	-4.982728000	3.082874000	-0.637700000
1	-4.800300000	2.923302000	-1.721391000
1	-4.875233000	2.086580000	-0.163573000
1	-6.033277000	3.407887000	-0.523264000
6	-3.648959000	-5.804487000	-0.901790000
1	-3.696773000	-5.033310000	-1.697735000

1	-4.517318000	-6.478850000	-1.027915000
1	-3.769922000	-5.267537000	0.061476000
6	1.428684000	-5.876933000	-0.711729000
1	1.487755000	-5.333135000	0.253740000
1	2.283362000	-6.578058000	-0.768007000
1	1.553365000	-5.111879000	-1.505798000
6	-1.155750000	-10.199309000	-1.333158000
1	-0.229149000	-10.569409000	-1.815185000
1	-1.235556000	-10.705029000	-0.346186000
1	-2.019775000	-10.535072000	-1.940632000
6	-9.394645000	2.069561000	-0.916503000
6	-6.252809000	0.984694000	2.643960000
6	-4.202392000	-2.118515000	-0.498635000
6	-5.939044000	0.703305000	-4.068460000
7	-5.460487000	-0.411184000	0.755433000
7	-7.608123000	1.284730000	0.588087000
7	-7.464018000	1.191982000	-2.175028000
7	-5.315867000	-0.508384000	-1.996736000
6	-7.077568000	1.293895000	-3.502711000
6	-8.707063000	1.804064000	-2.098531000
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