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Ditopic Dithiophosphonates And Their Related Rotaxanes

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Ditopic Dithiophosphonates and Their Related Rotaxanes

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BY

Robert Ray Baum. Jr.

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Robert R. Baum, Jr.

ABSTRACT

Grafting dithiophosphonate groups onto a naphthalenediimide core yields anionic axles, which in conjunction with the 15DN38C10 crown ether and cationic metallic systems generate neutral bimetallic rotaxanes. The association constant for the rotaxane system was calculated by the single-point method using ^{1}H NMR spectroscopy. Metallic systems reacted with our anionic axles were $SnMe_3$, $SnPh_3$, $Cu(PPH_3)_2$, $SnMe_2$, and $SnPh_2$. The structures of several axle-metal complexes and one rotaxane were obtained by X-ray crystallography.

ACKNOWLEDGEMENTS

I would like to thank Dr. Radu Semeniuc for being an excellent mentor over the past 18 months. I would also like to thank Dr. Mark McGuire, Dr. Sean Peebles, and Dr. Kraig Wheeler for being on my committee. This research was funded in part by the American Chemical Society Petroleum Research Fund (48039-GB3). The author is grateful to the donors of the Sidney R. Steele Student Summer Award for assistance during the summer of 2009.

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Chapter 1: INTRODUCTION

The last decades witnessed an increased interest in the synthesis and characterization of molecular machines and devices.[1-6] Mechanically interlocked molecules, such as rotaxanes[7-12] and catenanes,[13-17] have become the representative class of active components in devices at the molecular level. These devices are held together *via* a mechanical bond. A mechanical bond can be described as an interaction in which two or more molecular components become mechanically interlocked in some way.

A catenane is a mechanically interlocked compound in which two or more molecular loops are joined together, while a rotaxane is a mechanically interlocked compound which consists of an axle, a rotor, and a cap or stopper on each end of the axle. The axle contains one or more recognition sites (guests) that can interact with the rotor (host). Typical guests include tetrathiafulvalenes[21], naphthalenediimides[10], and pyromelliticdiimides[10]. Typical rotors include neutral crown ethers such as 1,5-dinaphtho[38]crown-10 (1,5DN38C10)[10] and ionic compounds such as tetracationic cyclophane cyclobis(paraquat-*p*-phelylene)[21]. The rotor can also be referred to as the macrocycle. Stoppers can include organometallic complexes such as trialkyl tin compounds.

The synthetic methods leading to the formation of rotaxanes are summarized in Figure 1. The capping approach to rotaxane synthesis involves combining the axle and rotor and then adding the stoppers to the resulting pseudorotaxane. The clipping approach involves removing a piece of the rotor to allow for assembly with the capped axle follower by reassembling the rotor.

Rotaxanes can also be prepared by the slippage approach. In this method, the axle is first capped. A solution of the capped axle is then heated in the presence of the rotor to enable the rotor to slip onto the axle. This requires caps that are small enough to allow the rotor to move over them when heated yet large enough to prevent the rotor from slipping off when the system has cooled.

The active template approach to rotaxanes involves the use of a catalyst that complexes with the rotor. The two pieces of the stoppered axle are then assembled at the catalyst to form a rotaxane.

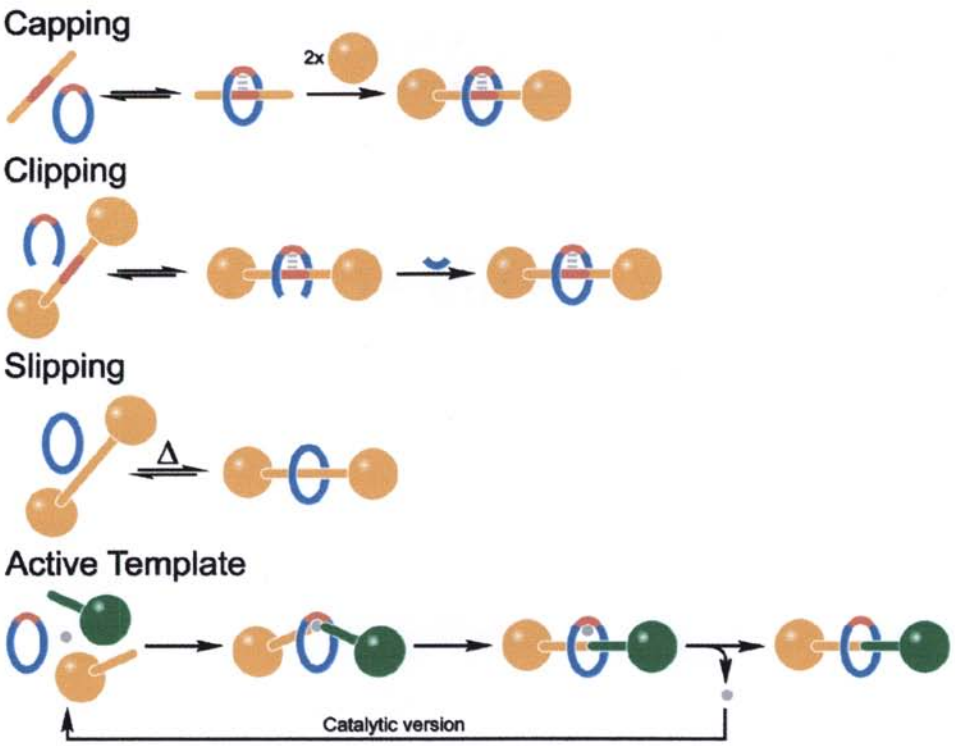


Figure 1: Illustration of the various methods for rotaxane synthesis. (From reference 18)

Multistation rotaxanes are particularly promising since their topology allows the macrocyclic component to undergo a reversible translational motion when subjected to appropriate stimuli, thus behaving as a molecular shuttle or switch.[1-6, 10] Another possible motion in rotaxanes is ring rotation,[19] which can also be present in catenanes. These are described in Figure 2.

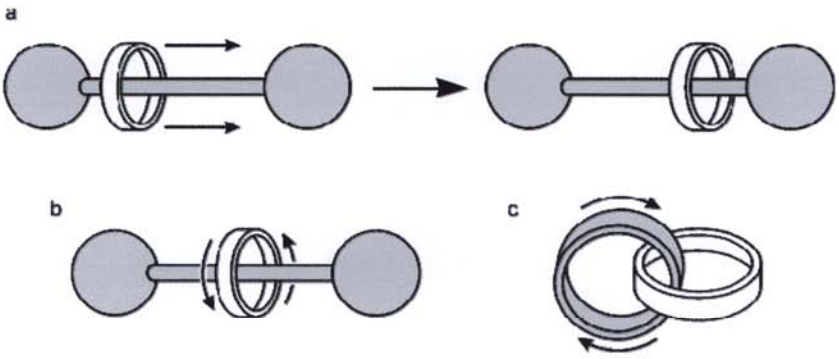


Figure 2: Examples of motion in rotaxanes and catenanes. a) ring shuttling in rotaxanes. b) ring rotation in rotaxanes. c) ring rotation in catenanes. (from reference 19)

There are several different kinds of molecular devices that can be made from rotaxanes, pseudorotaxanes, and catenanes. Pseudorotaxanes can be used as a molecular plug and socket device.[20, 21] A binapthocrown ether can be threaded onto a (9-anthracenyl)benzylammonium ion. Trifluoromethane-sulfonic acid is used to protonate the nitrogen on the "plug", forming a complex with the crown, as seen in figure 3. Transfer of light energy occurs from the binaphthyl group to the anthracenyl group. The pseudorotaxane can be unplugged by adding tributylamine. The plugging/unplugging action is reversible. Controlling the flow of electrons is essential for any electronic device.

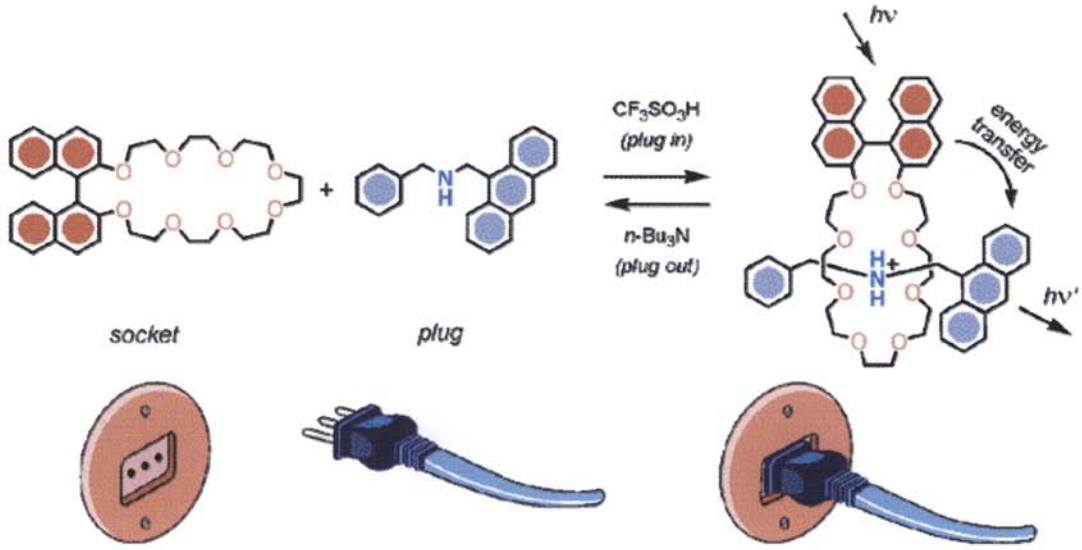


Figure 3: A molecular level plug/socket device (figure from reference 21).

Rotaxanes can be used as molecular shuttles[22]. Figure 4 shows a molecular shuttle that contains two different stations on the axle of the rotaxane. The ring of the rotaxane is dibenzo-24-crown-8 (DB24C8). One station is a dialkylammonium center. The other station is a 4,4'-bipyridinium unit. The behavior of this system in an acetonitrile solution has been tested. The hydrogen bonding interactions between the macrocycle and the ammonium center are much stronger than the charge transfer interaction between the macrocycle and the bipyridimium station. When the ammonium station is deprotonated by a base such as tribuytlamine, the macrocycle moves to the bipyridinium station due to the loss of hydrogen bonding. Reprotonation allows for the macrocycle to return to the ammonium position. This is a reversible reaction that could be used in computer memory because of its binary logic behavior.

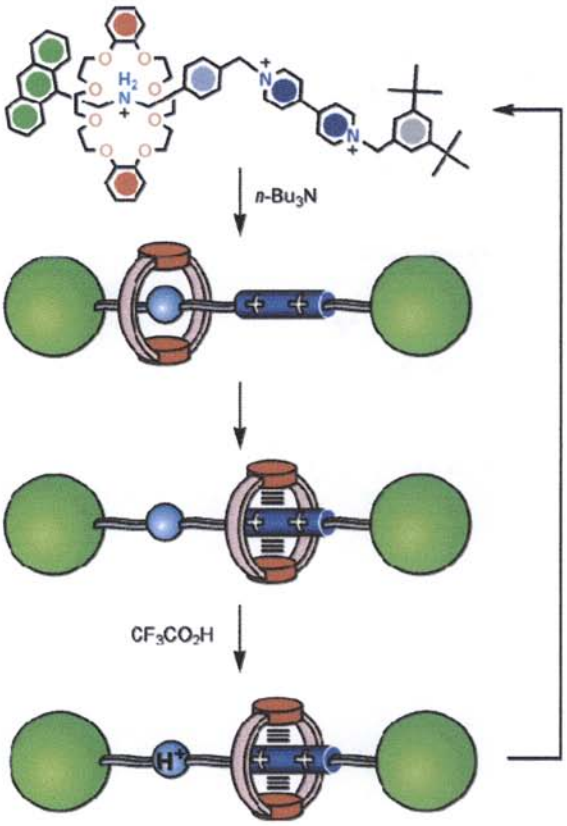


Figure 4: A molecular shuttle system (from reference 21)

Supramolecular systems can also be used as molecular switches.[23] Stoddart and colleagues have prepared a three-pole supramolecular switch with tetrathiafulvalene (TTF) as the guest and two host molecules: cyclophane cyclobis(paraquat-*p*-phenylene) ($CBPQT^{4+}$) and 1,5-dinaptho[38]crown-10 (1,5DN38C10). Neutral TTF forms a complex with $CBPQT^{4+}$. The TTF dication (TTF^{2+}) forms a complex with 1,5DN38C10. The radical monocation $TTF^{+\bullet}$ does not form complexes with either host molecule. Molecular shuttles such as the one seen in the previous paragraph can also be used as two-pole molecular switches. A scheme for a generic three-pole supramolecular switch is given in Figure 5.

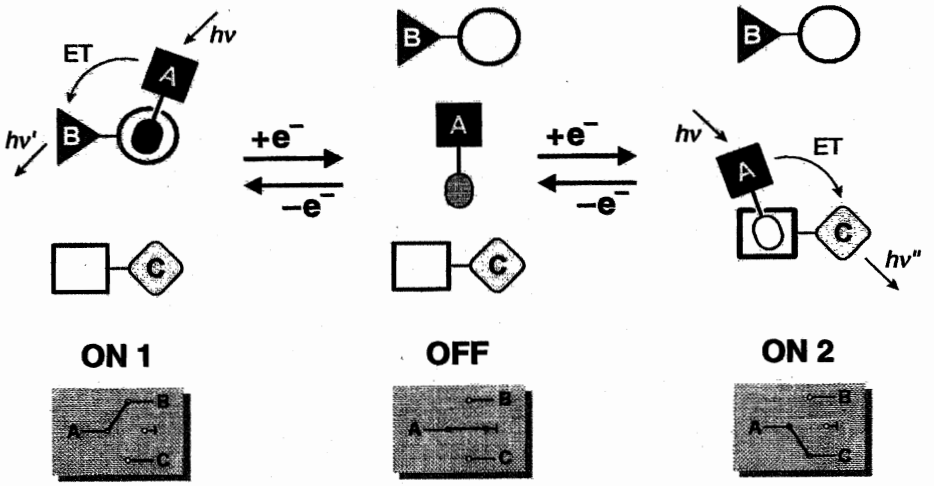


Figure 5: Schematic diagram for a generic three-pole supramolecular switch. (from reference 23)

An important research direction in this field is the use of rotaxanes as ligands,[24, 25] with the ultimate goal of synthesizing functional Metal-Organic-Rotaxane-Frameworks (MORFs).[26-30] MORFs are a particular class of Metal-Organic-Frameworks (MOFs) with rotaxanes acting as linkers between metal nodes, thus generating crystalline materials comprised of interlocked molecular components.

Metal-Organic-Frameworks (MOFs) consist of metal ions or clusters connected through bridging organic ligands into extended 1-, 2-, or 3-dimensional frameworks. Omar Yaghi, currently of the University of California at Los Angeles, prepared numerous examples of MOFs that are porous and can be used for gas storage.[31, 32]

MOFs can also be prepared from rotaxanes. These Metal-Organic-*Rotaxane*-frameworks (MO*R*Fs) are necessary to create ordered arrays of molecular machines.[27] However, many discrete rotaxane systems rely on counterions. These counterions make molecular motion more difficult, especially in MORFs.

While several examples of MORFs are known,[26-30, 33-36] they lack the necessary features to allow molecular motion. Ideally, such a MORF should be built on a two station rotaxane and should consist of a robust, porous, and overall neutral crystalline material, free of counter-ions and solvent molecules that would interfere with the translational movement of the wheel between the rotaxane stations.

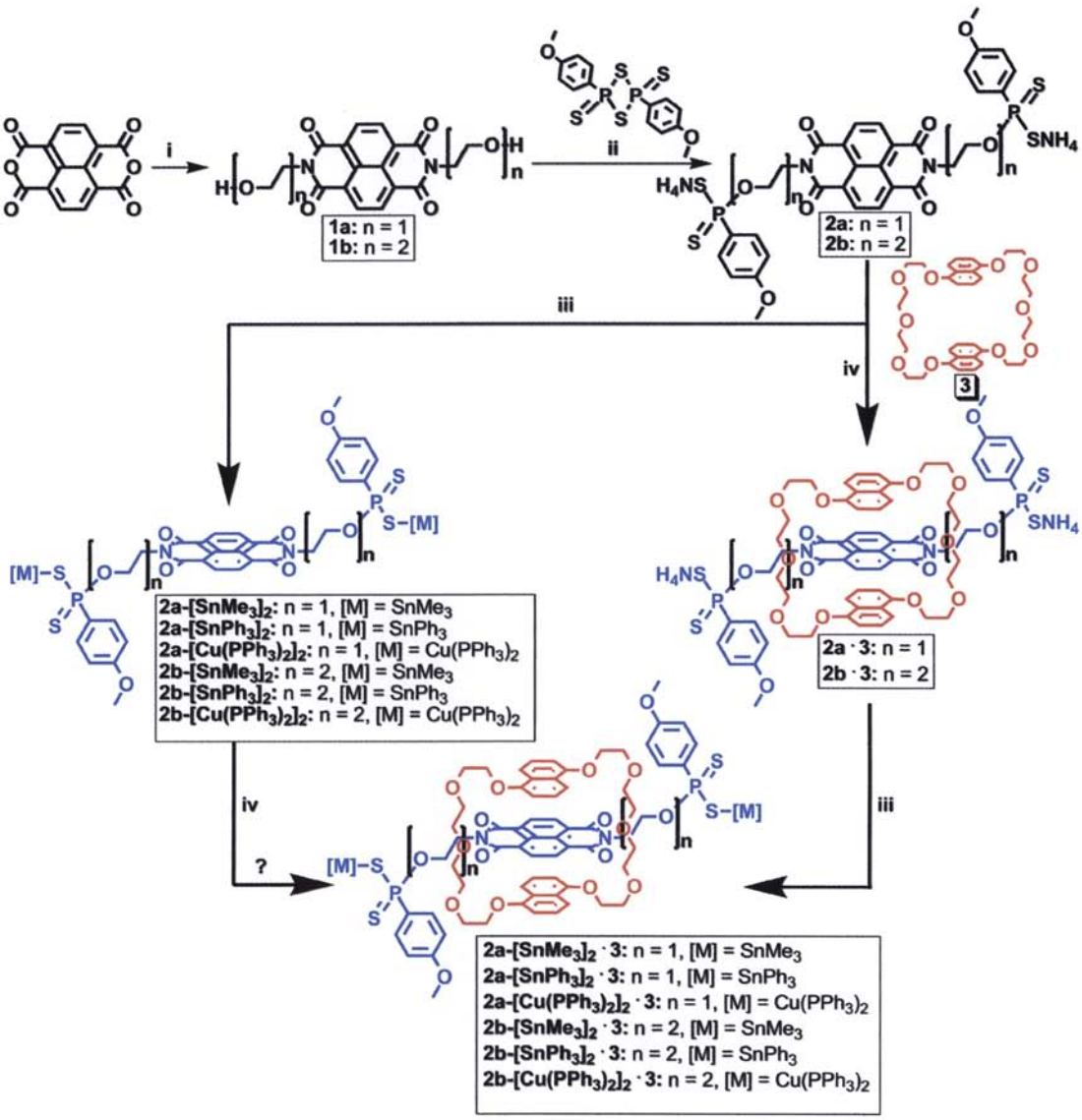
An elegant strategy toward this goal was recently suggested by Loeb,[26] employing zwitterionic rotaxanes[9, 12, 26] as ligands and connecting them to neutral metallic nodes.

These zwitterionic rotaxanes consist of a 1,2-bis(4,4'-bipyridinium)ethane dication as the axle and negatively charged crown ethers as the rotor.

Loeb's one-dimensional MORFs use $Cu_2(BnO_4)$ paddlewheel units as the neutral linkages[26]. The lone pairs on the nitrogens of the terminal pyridine groups bind to the two open coordination sites of the Cu(II) paddlewheel.

We propose here an alternative method for the synthesis of counter-ion free MORFs, based on anionic axles with donor capabilities that would produce a neutral network upon threading and coordination to cationic metal-containing nodes. Such an approach raises two questions: is it possible to synthesize anionic axles with donor properties that would still maintain a strong recognition site for rotaxane formation and what would be the stability of such rotaxanes during the coordination process? To answer these questions we investigated the formation of *discrete* rotaxanes rather than MORFs, to avoid solubility problems that could arise from the latter species.

The synthetic path toward neutral bimetallic rotaxanes is described in Scheme 1.



Scheme 1. Reaction scheme for the synthesis of our axles, complexes, and rotaxanes.

The research described in this thesis involves anionic axles. Our axles consist of a naphthalenediimide (NDI) station joined to a phosphorus-1,1-ditholate (PS_2) anionic donor at each end by either one or two ethoxy linkages. Our rotor is 1,5DN38C10. The interaction between these two moieties has been successfully used in directing the formation of mechanically interlocked systems.[10,11,13] Initial research involved the reaction of the two axles with metallic centers containing one or two coordination sites to study the coordination behavior of the anionic axle. The next step was to prepare neutral rotaxanes.

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EXPERIMENTAL

2.1 Instrumentation

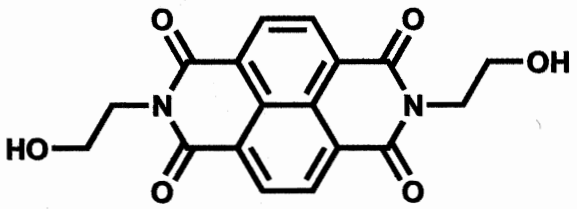
Operations requiring inert (nitrogen) atmosphere were carried out using standard Schlenk techniques and an MBraun LabStar dry-box. Elemental analyses were performed by Robertson Microlit Laboratories, NJ. NMR spectra were recorded by using a 400 MHz Bruker Avance FT-NMR Spectrometer and a Varian Mercury/VX 400 Spectrometer.

2.2 Materials

Dimethylformamide (DMF) was distilled before use and stored over molecular sieves. $(Ph_3P)_2CuNO_3$[1] and the 15DN38C10[2] crown ether were prepared according to published procedures. All other reagents were purchased from commercial suppliers and used as received.

2.3 Syntheses

2.3.1 Synthesis of NDI-$[CH_2CH_2OH]_2$



A 250-mL flask was charged with a stirring bar, 1,4,5,8-naphthalenetetracarboxylic dianhydride (2.682 g, 0.01 mol) and 75 mL dry DMF. To this mixture was added, under stirring, a solution of 2-aminoethanol (1.222 g, 0.02 mol) in 50 mL dry DMF. The mixture was stirred overnight at 120° C. After cooling at room temperature, the mixture was poured into 600 mL ice cold water and the resulting precipitate was filtered, washed with water (100 mL), ethanol (75 mL) and diethyl ether (75 mL), to afford the desired product (3.21 g, 90.6 %) as a pink powder. ^{1}H-NMR (400 MHz, DMSO-d_6): δ = 8.68 (s, 4H, *NDI*), 4.86 (t, J = 6.3 Hz, 2H, -O*H*), 4.18 (t, J = 6.2 Hz, 4H, -CH_2-), 3.66 (m, 4H, -CH_2-).

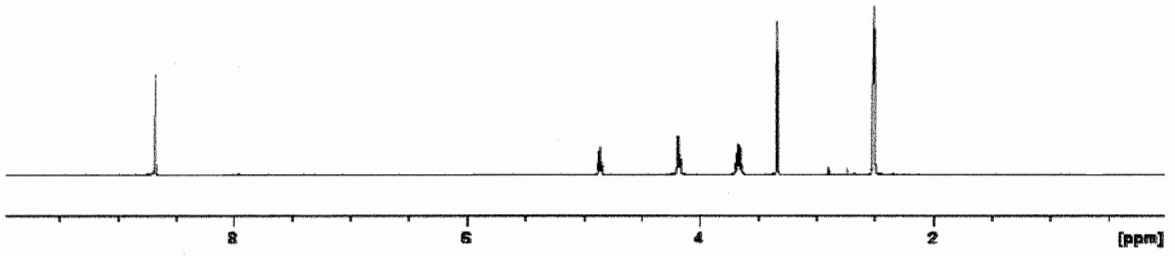
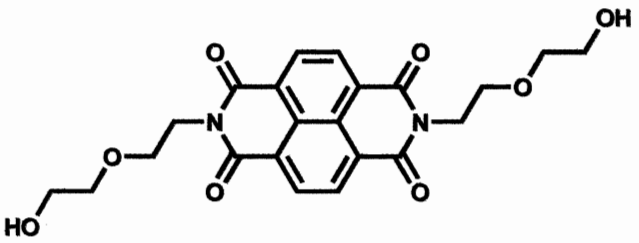


Figure 6: ^{1}H NMR spectrum of NDI-[CH_2CH_2OH]$_2$

2.3.2 Synthesis of NDI-[$CH_2CH_2OCH_2CH_2OH$]$_2$



This compound was prepared as described above for **NDI-[CH_2CH_2OH]$_2$**, using 1,4,5,8-naphthalene-tetracarboxylic dianhydride (2.682 g, 0.01 mol) in 75 mL dry DMF and a solution of 2-(2-aminoethoxy)-ethanol (2.103 g, 0.02 mol) in 50 mL dry DMF. The compound (3.94 g, 89.1 %) was isolated as a pale pink powder. ^{1}H-NMR (400 MHz, DMSO-d_6): δ = 8.66 (s, 4H, *NDI*), 4.57 (t, J = 5.3 Hz, 2H, -O*H*), 4.26 (m, 4H, -CH_2-), 3.69 (m, 4H, -CH_2-), 3.48 (m, 8H, -CH_2-).

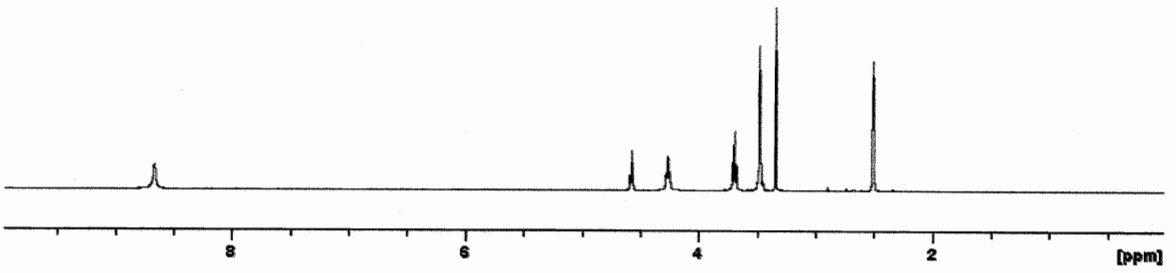
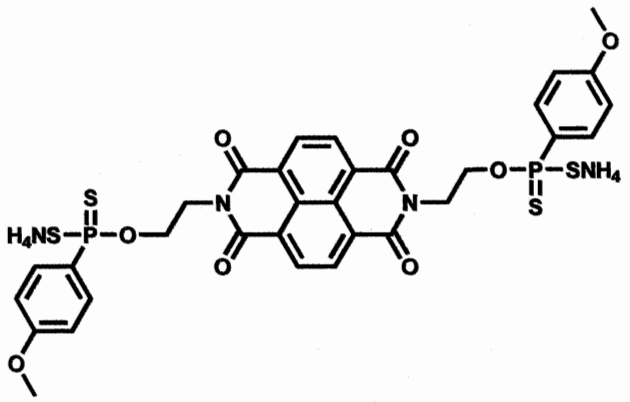


Figure 7: ^{1}H NMR spectrum of NDI-[$CH_2CH_2OCH_2CH_2OH$]$_2$

2.3.3. Synthesis of NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$



A 250 mL flask was charged with a stirring bar, NDI-$[CH_2CH_2OH]_2$ (1.771 g, 5.0 mmol), 1,3,2,4-dithiadiphosphetane-2,4-bis(4-methoxyphenyl)-2,4-disulfide (Lawesson's Reagent, L.R.) (2.022 g, 5.0 mmol) and 150 mL benzene. The mixture was stirred for 90 min. at 80° C, and allowed to cool at room temperature. Then dry NH_3 gas (prepared from NH_4OH dropped onto NaOH and dried by passing it through a tower filled with powdered NaOH) was bubbled through the cold solution. The resulting voluminous precipitate was filtered, washed with cold benzene (50 mL) and then ether (100 mL) to afford an orange product (3.08 g, 77.7 %), identified as NDI-$[CH_2CH_2O(An)PS_2NH_4]_2 \cdot 1/2\ C_6H_6$. ^{1}H-NMR (400 MHz, Acetone-d_6/D_2O 5:0.6 v/v): δ = 8.67 (s, 4H, *NDI*), 7.83 (m, 4H, MeO-C_6H_4-P), 7.33 (s, 3H, C_6H_6), 6.44 (m, 4H, MeO-C_6H_4-P), 4.39 (t, J = 6.9 Hz, 4H, -CH_2-), 4.15 (m, 4H, -CH_2-), 3.58 (s, 6H, -O-CH_3); Anal. Calcd. for $C_{32}H_{34}N_4O_8P_2S_4 \cdot 1/2\ C_6H_6$: C = 50.53, H = 4.48, N = 6.73; Found: C = 50.26, H = 4.46, N = 6.57.

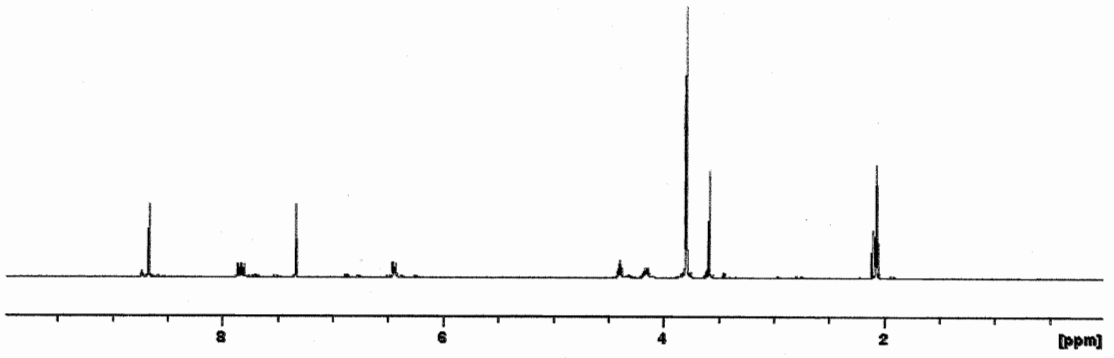
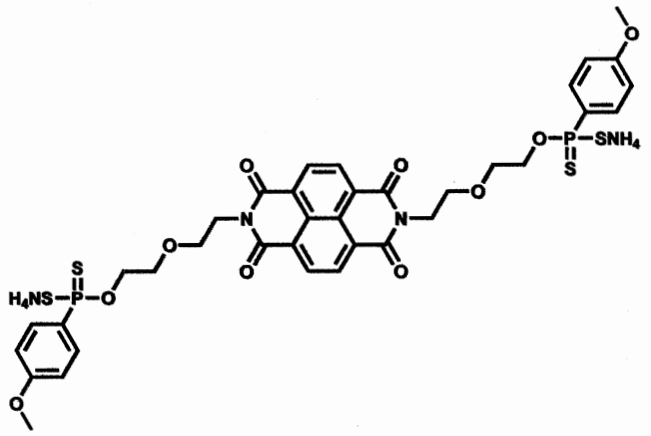


Figure 8: ^{1}H NMR spectrum of NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$

2.3.4 Synthesis of NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$



This compound was prepared as described above for NDI-[$CH_2CH_2O(An)PS_2NH_4]_2$, using NDI-[$CH_2CH_2OCH_2CH_2OH]_2$ (2.212 g, 5.0 mmol), L.R. (2.022 g, 5.0 mmol) and 150 mL benzene. The procedure afforded an orange product (3.28 g, 74.5 %), identified as NDI-[$CH_2CH_2OCH_2CH_2O$-$(An)PS_2NH_4]_2$. ^{1}H-NMR (400 MHz, Acetone-d_6/D_2O 5:0.6 v/v): δ = 8.72 (s, 4H, *NDI*), 7.96 (m, 4H, MeO-C_6H_4-P), 7.33 (s, 1H, C_6H_6), 6.75 (m, 4H, MeO-C_6H_4-P), 4.36 (t, J = 6.8 Hz, 4H, -CH_2-), 3.91 (m, 4H, -CH_2-), 3.74 (m, 10H, -CH_2- and -O-CH_3), 3.66 (m, 4H, -CH_2-); Anal. Calcd. for $C_{36}H_{42}N_4O_{10}P_2S_4$: C = 49.08, H = 4.81, N = 6.36; Found: C = 48.82, H = 5.00, N = 6.20.

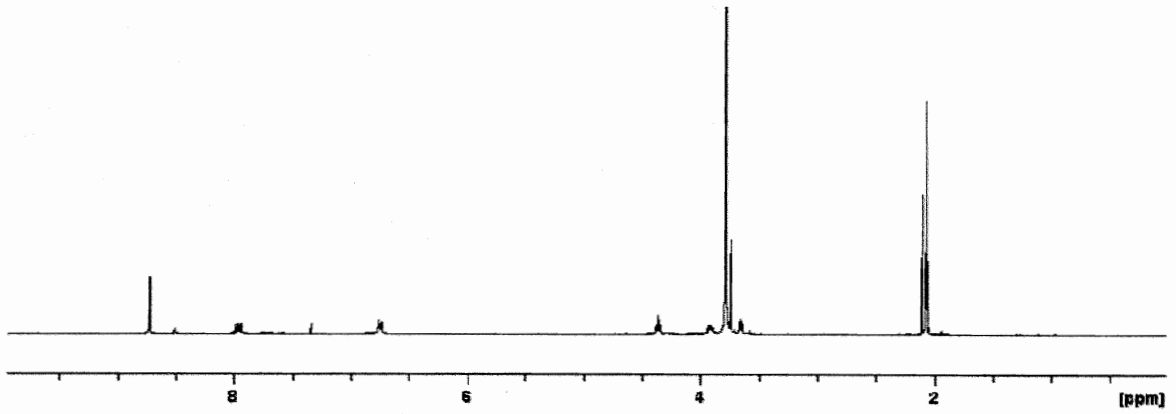
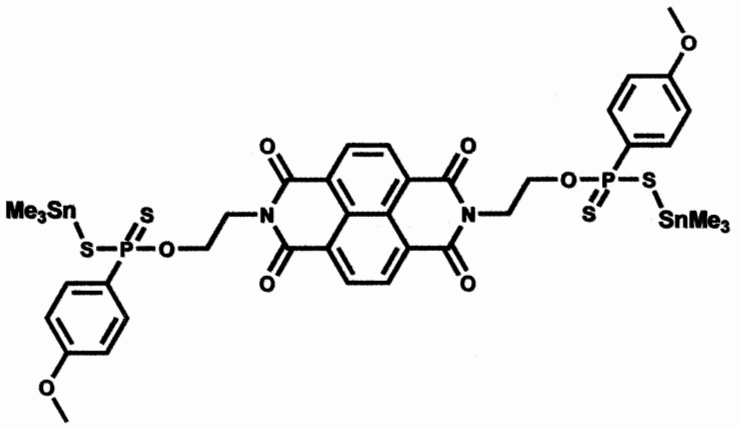


Figure 9: ^{1}H NMR spectrum of NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$

2.3.5 Synthesis of NDI-$[CH_2CH_2O(An)PS_2(SnMe_3)_2]_2$



A 250-mL flask was charged with a stirring bar and a solution of Me_3SnCl (0.0498 g, 0.25 mmol) in DCM (75 mL). To this colorless solution was added, under vigorous stirring, an orange aqueous solution of NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ (0.0991 g, 0.125 mmol) in 75 mL water, and the mixture was stirred for an additional 12 hours. The completion of the reaction was indicated by the loss of the color of the aqueous phase and the appearance of a pink color in the organic phase. The organic phase was separated, and the aqueous phase extracted with DCM (3 x 25 mL). The combined organic phases were dried over anhydrous Na_2SO_4 and removed under reduced pressure, to afford the desired compound as an orange solid (0.0722 g, 53.3 %). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.73 (s, 4H, *NDI*), 7.80 (m, 4H, MeO-C_6H_4-P), 6.82 (m, 4H, MeO-C_6H_4-P), 4.61 (m, 4H, -CH_2-), 4.46 (m, 4H, -CH_2-), 3.79 (s, 6H, -O-CH_3), 0.53 (s, J_{Sn-H} = 27.8 Hz, 18H, Sn(CH_3)$_3$). Anal. Calcd. for $C_{38}H_{44}N_2O_8P_2S_4Sn_2$: C = 42.09, H = 4.09, N = 2.58; Found: C = 42.21, H = 3.89, N = 2.77.

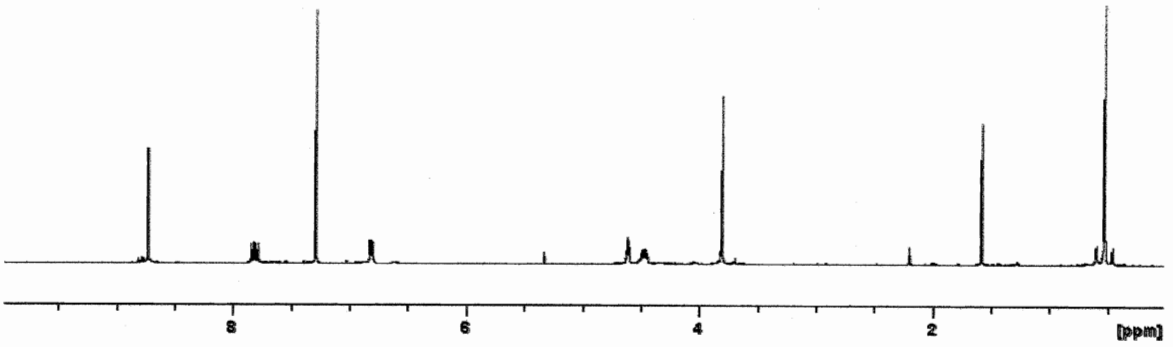
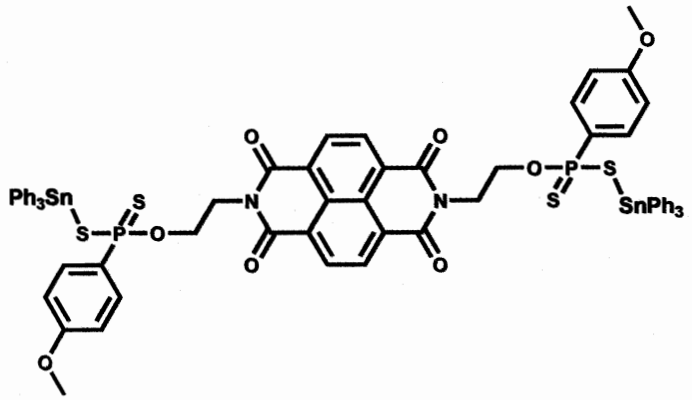


Figure 10: ^{1}H NMR spectrum of NDI-$[CH_2CH_2O(An)PS_2(SnMe_3)_2]_2$

2.3.6 Synthesis of NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$



This compound was prepared as described above for NDI-$[CH_2CH_2O(An)PS_2(SnMe_3)_2]_2$, using Ph_3SnCl (0.0964 g, 0.25 mmol) and NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ (0.0991 g, 0.125 mmol), to afford the desired compound as an orange solid (0.1192 g, 65.5 %). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.58 (s, 4H, *NDI*), 7.60-7.52 (m, 16H, 4H MeO-C_6H_4-P overlap with 12H, Sn-$(C_6H_5)_3$), 7.35 (m, 18H, Sn-$(C_6H_5)_3$), 6.67 (m, 4H, MeO-C_6H_4-P), 4.49 (m, 4H, -CH_2-), 4.31 (m, 4H, -CH_2-), 3.76 (s, 6H, -O-CH_3). Anal. Calcd. for $C_{68}H_{56}N_2O_8P_2S_4Sn_2$: C = 56.06, H = 3.87, N = 1.92; Found: C = 55.74, H = 3.69, N = 1.91.

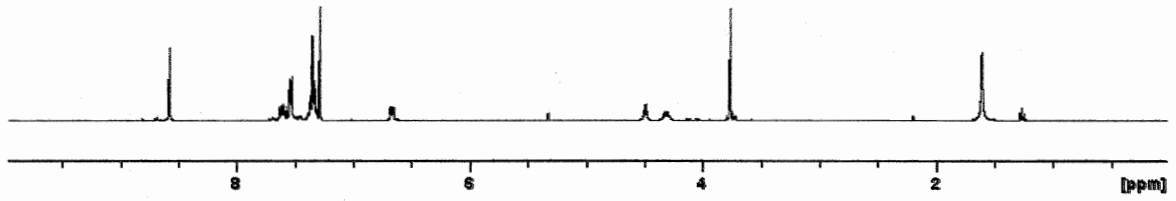
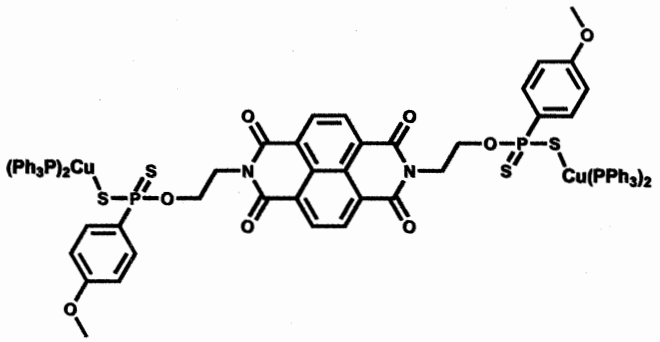


Figure 11: ^{1}H NMR spectrum of NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$

2.3.7 Synthesis of NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$



This compound was prepared as described above for NDI-$[CH_2CH_2O(An)PS_2(SnMe_3)_2]_2$, using $(Ph_3P)_2CuNO_3$ (0.1625 g, 0.25 mmol) and NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ (0.0991 g, 0.125 mmol), to afford the desired compound as a dark orange solid (0.1922 g, 79.5 %). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.59 (s, 4H, *NDI*), 7.76 (m, 4H, MeO-C_6H_4-P), 7.31 (m, 36H, -P(C_6H_5)$_3$), 7.17 (m, 24H, -P(C_6H_5)$_3$), 6.64 (m, 4H, MeO-C_6H_4-P), 4.46 (m, 4H, -CH_2-), 4.21 (m, 4H, -CH_2-), 3.73 (s, 6H, -O-CH_3). Anal. Calcd. for $C_{104}H_{86}Cu_2N_2O_8P_6S_4$: C = 64.62, H = 4.48, N = 1.45; Found: C = 64.38, H = 4.35, N = 1.57.

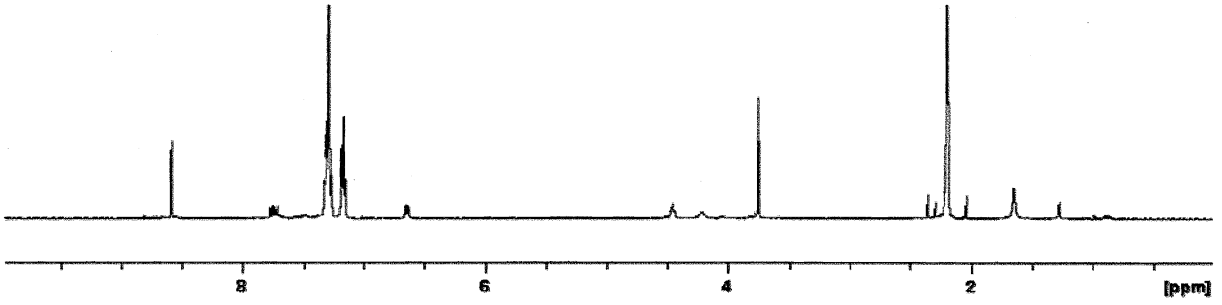
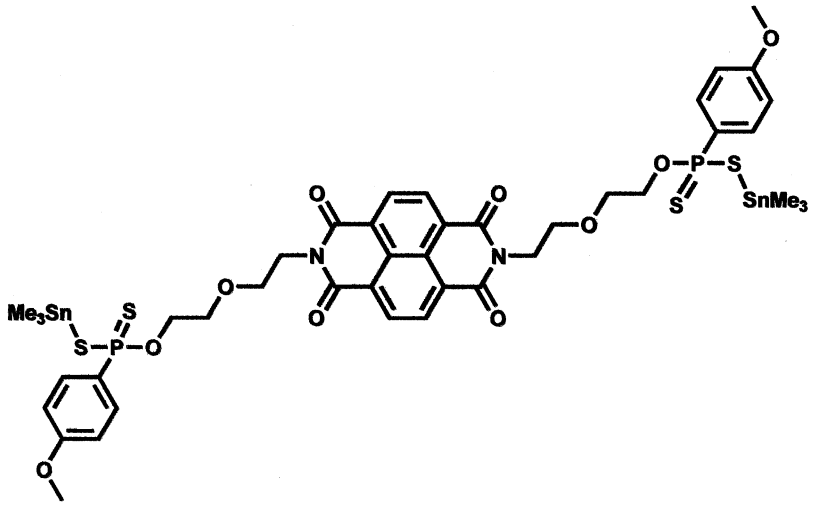


Figure 12: ^{1}H NMR spectrum of NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$

2.3.8 Synthesis of NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnMe_3)_2]_2$



A 250-mL flask was charged with a stirring bar and a solution of Me_3SnCl (0.0498 g, 0.25 mmol) in DCM (75 mL). To this colorless solution was added, under vigorous stirring, an orange aqueous solution of NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$ (0.110 g, 0.125 mmol) in 75 mL water, and the mixture was stirred for an additional 12 hours. The completion of the reaction was indicated by the loss of the color of the aqueous phase and the appearance of a pink color in the organic phase. The organic phase was separated, and the

aqueous phase extracted with DCM (3 x 25 mL). The combined organic phases were dried over anhydrous Na_2SO_4 and removed under reduced pressure, to afford the desired compound as an orange solid (0.0952 g, 64.9 %). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.69 (s, 4H, *NDI*), 7.81 (m, 4H, MeO-C_6H_4-P), 6.84 (m, 4H, MeO-C_6H_4-P), 4.47 (m, 4H, -CH_2-), 4.14 (m, 4H, -CH_2-), 3.88-3.83 (m, 10H, 4H -CH_2- overlap with 6H -O-CH_3), 3.77 (m, 4H, -CH_2-), 0.59 (s, J_{Sn-H} = 28.2 Hz, 18H, Sn(CH_3)$_3$). Anal. Calcd. for $C_{42}H_{52}N_2O_{10}P_2S_4Sn_2$: C = 43.02, H = 4.47, N = 2.39; Found: C = 43.39, H = 4.38, N = 2.62.

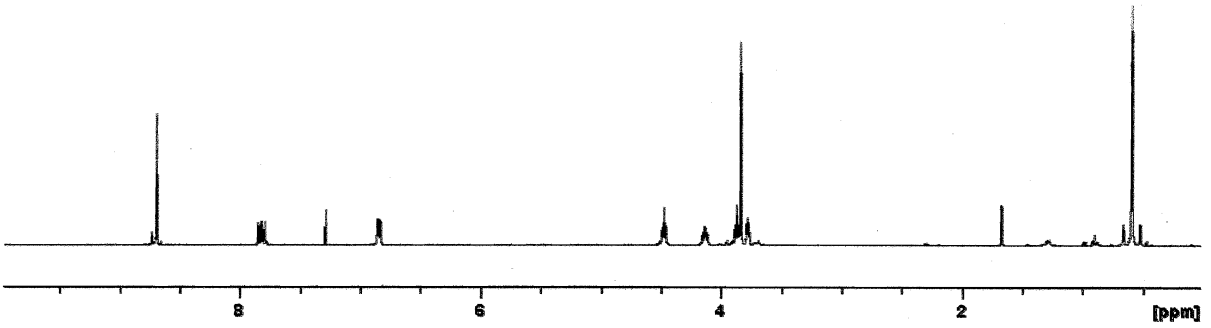
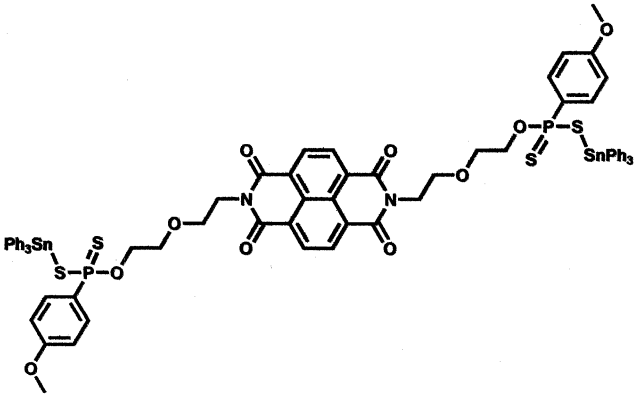


Figure 13: ^{1}H NMR spectrum of NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2(SnMe_3)_2]_2$

2.3.9 Synthesis of NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2(SnPh_3)_2]_2$



This compound was prepared as described above for NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2(SnMe_3)_2]_2$, using Ph_3SnCl (0.0964 g, 0.25 mmol) and NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2NH_4]_2$ (0.110 g, 0.125 mmol), to afford the desired compound as an orange solid (0.1427 g, 73.9 %). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.61 (s, 4H, *NDI*), 7.71-7.57 (m, 16H, 12H Sn-(C_6H_5)$_3$ overlap with 4H, MeO-C_6H_4-P), 7.41 (m, 18H, Sn-(C_6H_5)$_3$), 6.67 (m, 4H, MeO-C_6H_4-P), 4.42 (m, 4H, -CH_2-), 3.96 (m, 4H, -CH_2-), 3.82-3.76 (m, 10H, 6H, -

O-CH_3 overlap with 4H, -CH_2-), 3.56 (m, 4H, -CH_2-). Anal. Calcd. for $C_{72}H_{64}N_2O_{10}P_2S_4Sn_2$: C = 55.98, H = 4.18, N = 1.81; Found: C = 55.59, H = 3.90, N = 1.99.

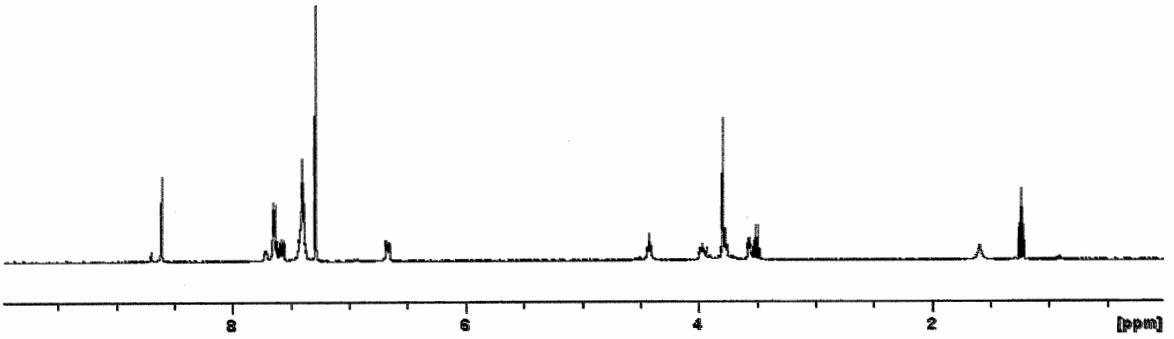
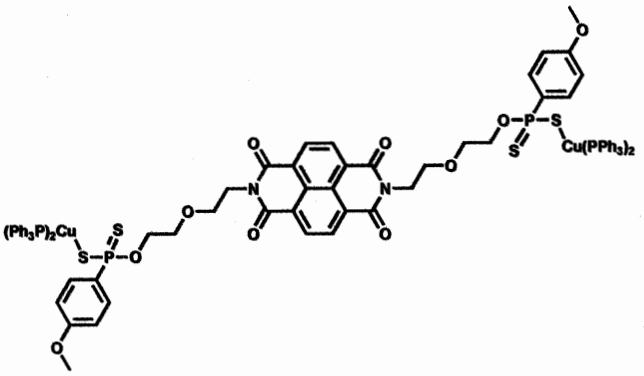


Figure 14: ^{1}H NMR spectrum of NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2(SnPh_3)_2]_2$

2.3.10 Synthesis of NDI-[$CH_2CH_2OCH_2CH_2O$(An)PS_2(Cu(PPh_3)$_2$]$_2$



This compound was prepared as described above for NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2(SnMe_3)_2]_2$, using $(Ph_3P)_2CuNO_3$ (0.1625 g, 0.25 mmol) and NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2NH_4]_2$ (0.110 g, 0.125 mmol), to afford the desired compound as a dark orange solid (0.2011 g, 79.6 %). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.57 (s, 4H, *NDI*), 7.65 (m, 4H, MeO-C_6H_4-P), 7.33 (m, 36H, -P(C_6H_5)$_3$), 7.23 (m, 24H, -P(C_6H_5)$_3$), 6.68 (m, 4H, MeO-C_6H_4-P), 4.46 (m, 4H, -CH_2-), 3.87-3.79 (m, 14H, 8H -CH_2- overlap with 6H -O-CH_3), 3.56 (m, 4H, -CH_2-). Anal. Calcd. for $C_{108}H_{94}Cu_2N_2O_{10}P_6S_4$: C = 64.18, H = 4.69, N = 1.39; Found: C = 63.85, H = 4.34, N = 1.62.

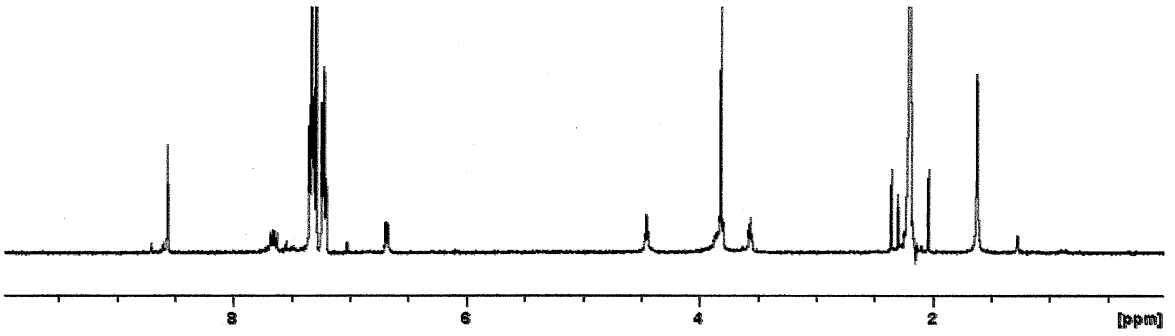
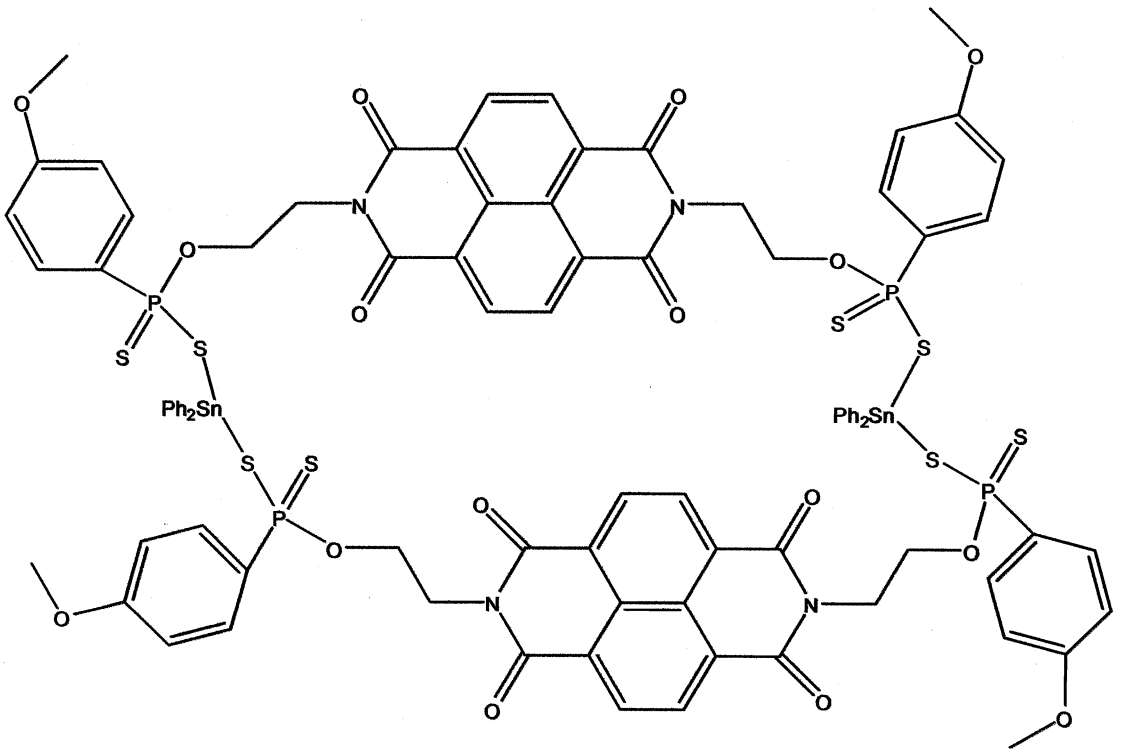


Figure 15: ^{1}H NMR spectrum of NDI-$[CH_2CH_2OCH_2CH_2OH]_2$-$[Cu(PPh_3)_2]_2$

2.3.11 Synthesis of $(NDI\text{-}[CH_2CH_2O(An)PS_2]_2)_2\text{-}[SnPh_2]_2$



A 250 mL flask was charged with a stirring bar and a solution of Ph_2SnCl_2 (0.0429 g, 0.125 mmol) in DCM (75 mL). To this colorless solution was added, under vigorous stirring, an orange aqueous solution of NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ (0.0991 g, 0.125 mmol) in 75 mL water, and the mixture was stirred for an additional 12 hours. The completion of the reaction was indicated by the loss of the color of the aqueous phase and the appearance of a pink color in the organic phase. The organic phase was separated, and the

aqueous phase extracted with DCM (3 x 25 mL). The combined organic phases were dried over anhydrous Na_2SO_4 and removed under reduced pressure, to afford the desired compound as a pale orange solid (0.0491 g, 38.1 %). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.57 (s, 8H, *NDI*), 7.70 (m, 8H, Sn-(C_6H_5)$_2$), 7.61 (m, 8H, MeO-C_6H_4-P), 7.50 (m, 8H, Sn-(C_6H_5)$_2$), 7.35 (m, 4H, Sn-(C_6H_5)$_2$), 6.66 (m, 8H, MeO-C_6H_4-P), 4.49 (m, 8H, -CH_2-), 4.31 (m, 8H, -CH_2-), 3.76 (s, 12H, -O-CH_3).

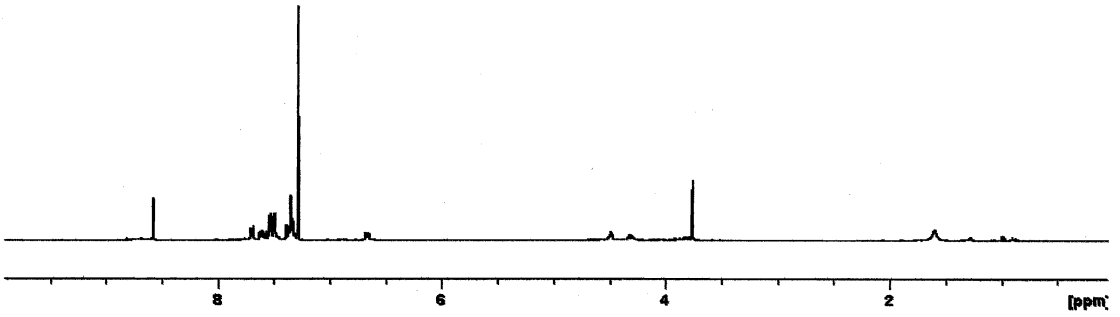
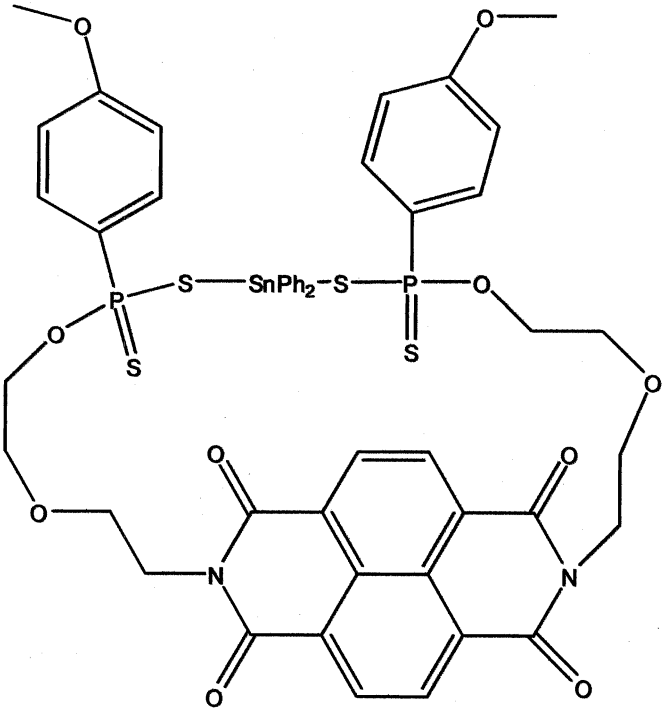


Figure 16: ^{1}H NMR spectrum of NDI-[CH_2CH_2O(An)PS_2]$_2$-[$SnPh_2$]$_2$

2.3.12 Synthesis of NDI-[$CH_2CH_2OCH_2CH_2O$(An)PS_2]$_2$-[$SnPh_2$]



The compound was prepared as described above for using NDI-[$CH_2CH_2OCH_2CH_2O$(An)-PS_2NH_4]$_2$ (0.1188 g, 0.134 mmol) to afford the desired compound as an orange solid (0.0237 g, 15.8%). ^{1}H-NMR (400 MHz, $CDCl_3$): δ = 8.59 (s, 4H, *NDI*), 7.60 (m, 4H, Sn-(C_6H_5)$_2$), 7.48 (m, 4H, MeO-C_6H_4-P), 7.32 (m, 6H, Sn-(C_6H_5)$_2$), 6.93 (m, 4H, MeO-C_6H_4-P), 4.53 (m, 4H, -CH_2-), 3.98 (m, 4H, -CH_2-), 3.93 (s, 6H, -O-CH_3), 3.64 (m, 4H, -CH_2-), 3.53 (m, 4H, -CH_2-).

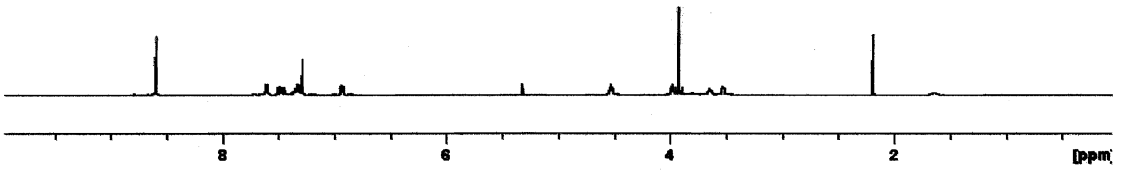


Figure 17: ^{1}H NMR spectrum of NDI-[$CH_2CH_2OCH_2CH_2OH$]-[$SnPh_2$]

General procedure for rotaxane synthesis and crystal growing procedure.

Acetone-water solutions of the axle and crown (0.1 mmol each) were stirred for 2 hours in an ice-water bath. To the red solutions, solid R_3SnCl (R = Me, Ph) or $(Ph_3P)_2CuNO_3$ was added, and the stirring was continued overnight. The resulting red solutions were transfered in vials which were subsequentely placed in larger vials already filled with ca. 10 mL of diethyl ether. The large vials were tightly closed and kept at 0 °C for several days, during which time red crystals formed and used for single crystal X-ray diffraction analysis.

Crystallographic studies.

The X-ray data were collected at 100 K on a Bruker SMART APEXII CCD diffractomer equipped with Cu Kα radiation. Intensities were collected using phi and omega scans and were corrected for Lorentz polarization and absorption effects. The *X-SEED* software platform,[3] equipped with *SHELXS* and *SHELXL* modules on a PC computer,[4] was used for all structure solution and refinement calculations and molecular graphics. The structure was solved by direct methods, and refined by anisotropic full-matrix least-squares for all non-hydrogen atoms. All hydrogen atoms were placed in calculated positions and refined using a riding model with fixed thermal parameters.

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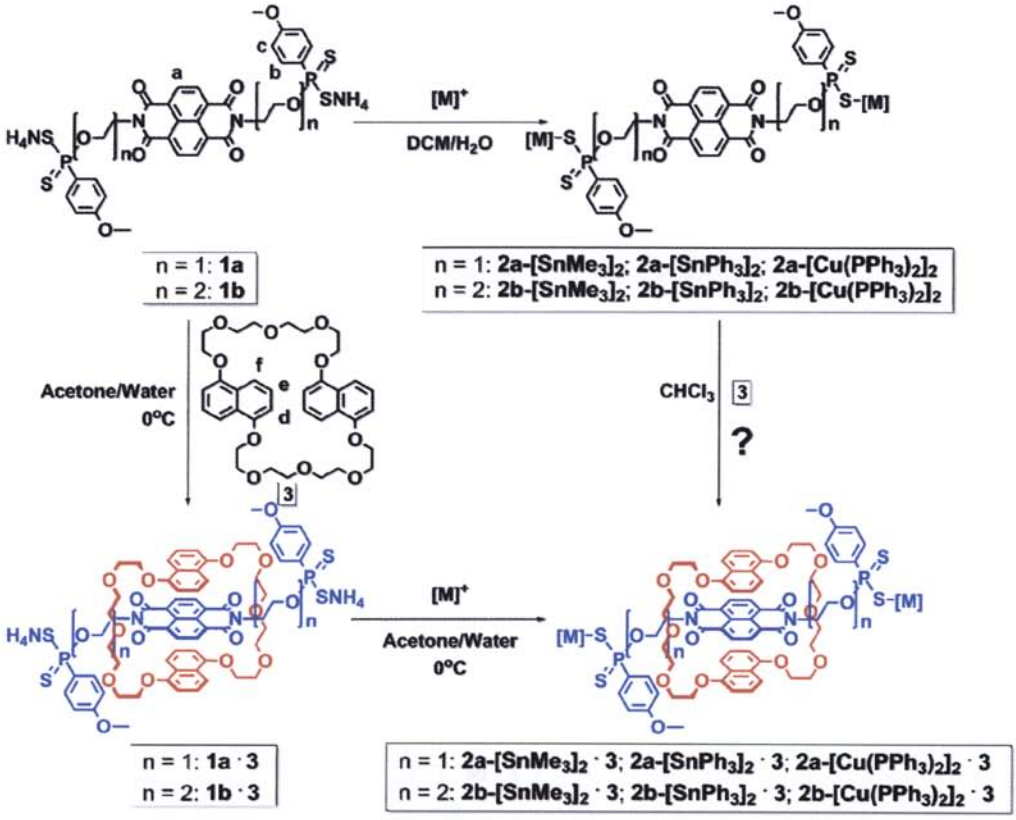
1. Cotton, F.A.; Goodgame, D. M. L., *J. Chem. Soc.*, **1960**, 5267.
2. Hamilton, D. J.; Davies, J. E.; Prodi, L.; Sanders, J. K. M. *Chem Eur. J.*, **1998**, 608
3. Barbour, L. J. *Supramol. Chem.*, **2001**, *1*, 189
4. Sheldrick, G. M. *Acta Crystalogr.*, **2008**, *A64*, 112

RESULTS AND DISCUSSION

Section 3.1: Synthesis and Characterization

In our design of an anionic rotaxane ligand, we have selected a dithiophosphonate group as the donor set towards metallic centers,[1] and the 1,4,5,8-naphthalenetetracarboxylic diimide (NDI) / 1,5-dinaphtho-38crown10 (15DN38C10) pair as complementary recognition sites, since the interaction between these moieties has been successfully used in directing the formation of mechanically interlocked systems.[1-3] The general approach is presented in Scheme 2.



Scheme 2. Two possible synthetic pathways toward neutral bimetallic rotaxanes starting from our anionic axles.

The ditopic dithiophosphonate axles were synthesized by the reaction of 1,4,5,8-naphthalene-tetracarboxylic dianhydride with two equivalents of either 2-aminoethanol or 2-(2-aminoethoxy)ethanol in DMF, followed by the reaction of the resulting diols with Lawesson's Reagent in benzene. The ammonium salts NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ and NDI-$[CH_2CH_2O\text{-}CH_2CH_2O(An)PS_2NH_4]_2$ (An = anisole) were

then precipitated by passing a stream of dry gaseous NH_3 through the cold benzene solution of the dithiophosphonic acids.

Characterization of the intermediate NDI-$[CH_2CH_2OH]_2$ was carried out by ^1H NMR (Figure 6) in DMSO-D_6. The singlet at 8.68 ppm was assigned to the four hydrogens on the NDI central piece. The triplet at 4.86 ppm was assigned to the two hydroxyl groups. The triplet at 4.18 ppm was assigned to the hydrogens on the carbon adjacent to the nitrogen on the NDI. The multiplet at 3.66 ppm was assigned to the hydrogens on the carbon adjacent to the hydroxyl group. The ^1H NMR spectrum of NDI-$[CH_2CH_2OCH_2CH_2OH]_2$ (Figure 7) is similar to that of NDI-$[CH_2CH_2OH]_2$, with two additional resonances corresponding to the additional CH_2-O-CH_2 hydrogens.

The ^1H NMR spectrum for NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ (Figure 8) as well as the elemental analysis indicate one-half equivalent solvated benzene. A sample of this axle was also prepared in acetonitrile. The axle prepared in acetonitrile did not contain the solvated benzene according to elemental analysis and NMR.

The reaction of these ditopic ligands with R_3SnCl (R = Me, Ph) or $(Ph_3P)_2CuNO_3$ (Scheme 2) yielded the bimetallic compounds NDI-$[CH_2CH_2O(An)PS_2(SnMe_3)_2]_2$; NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$; NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$; NDI-$[CH_2CH_2OCH_2$-$CH_2O(An)PS_2(SnMe_3)_2]_2$; NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$ and NDI-$[CH_2CH_2O$-$CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$. The structure of these bimetallic compounds was confirmed by ^1H NMR spectroscopy and elemental analysis.

3.2 Solution NMR studies

Both routes toward bimetallic rotaxanes were investigated (Scheme 2): a) pseudorotaxane formation followed by stoppering with metallic centers and b) slippage of the crown onto the preformed neutral metallic axles. Upon mixing equimolar solutions of NDI-$[CH_2CH_2O(An)$-$PS_2NH_4]_2$ or NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$ and 15DN38C10 in acetone-d_6:D_2O (5:0.6, v/v), the slow rate of association and dissociation of the components on the NMR timescale at room temperature permits the observation of three different sets of peaks in their NMR spectra (Fig. 18), corresponding to the free axles and crown ether, and the [2]pseudorotaxane complexes. The rotaxane formation is indicated by the upfield shift of the NDI (H_a) and the crown aromatic peaks ($H_{d\text{-}f}$) due to aromatic shielding effects resulting from

the NDI-crown interaction, while the anisole peaks (H_{b-c}) shifted downfield, indicative of an "outer sphere" interaction of this group with the crown 15DN38C10.

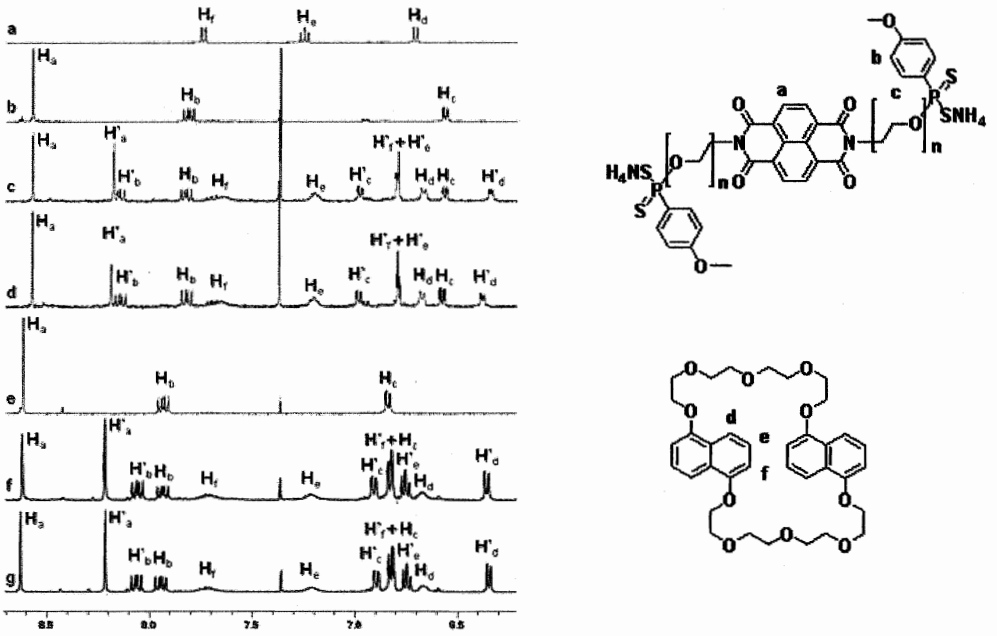


Figure 18: Partial ^{1}H-NMR spectra of a) crown 15DN38C10, b) axle NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$, c) rotaxane NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$⊂15DN38C10, d) rotaxane NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$⊂ 15DN38C10/excess NH_4^+, e) axle NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$, f) rotaxane NDI-$[CH_2CH_2O$-$CH_2CH_2O(An)PS_2NH_4]_2$⊂15DN38C10 and g) rotaxane NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$⊂ 15DN38C10/excess NH_4^+; H and H' represent uncomplexed and complexed species, respectively (for proton labeling mode see Scheme 2); the peak at 7.33 ppm is C_6H_6 carried on from the synthesis of the axles.

The observation of signals for the resonances of threaded and unthreaded species in the NMR spectra of NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ or NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$ and 15DN38C10 allows the measurement of their association constants (K_a) and free energies of complexation ($\Delta G°$) using the convenient single-point method (Table 1).[4]

The ^{1}H-NMR spectra were obtained at 25° C in acetone-d_6 / D_2O = 5 / 0.6 (v/v), using equimolar solutions ($1.66 \cdot 10^{-3}$ M) of naphthalenediimide based axles and 15DN38C10 crown-ether. The concentrations of the free axle, free crown and of their corresponding pseudorotaxanes were determined using the initial axle and crown concentrations and the integration of the NDI resonance of free and complexed species. The errors are estimated to be 10% or less. The free energies of complexation were then routinely calculated, using the formula $\Delta G° = -RT\ln K_a$.

The association constants were calculated using the formula

$$Ka = \frac{I(R)}{I(A) * (c(C) - \frac{I(R)}{I(A) + I(R)} c(A))}$$

where I(A) is the integral of the NDI hydrogen of the free axle, I(R) is the integral of the NDI hydrogen of the rotaxane, c(C) is the initial concentration of 15DN38C10, and c(A) is the initial concentration of the axle. For the association constant for NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$ and 15DN38C10, the calculation was as follows:

$$Ka = \frac{1.03}{1 * (0.00106 - \frac{1.03}{1 + 1.03} 0.00147)}$$

resulting in a K_a of 1259.1 M^{-1}.

It should be emphasized that the apparent K_a values for rotaxanes NDI-$[CH_2CH_2O$-(An)-$PS_2NH_4]_2 \subset$15DN38C10 and NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2 \subset$15DN38C10 were calculated considering a 1:1 reaction of the anionic axles with the $[15DN38C10 \cdot NH_4]^+$ inclusion complex. All our attempts to replace the NH_4^+ counter-ion with non-interacting R_4N^+ (R=Me, *n*-Pr, and *n*-Bu) cations resulted in the decomposition of the axle.

Since the dissolution of the axle produces two equivalents of NH_4^+ ions, it is reasonable to assume that the formation of the $[15DN38C10 \cdot NH_4]^+$ complex is essentially complete. When the NMR spectra of the axles NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ and NDI-$[CH_2CH_2OCH_2CH_2O$-$(An)PS_2NH_4]_2$ and crown 15DN38C10 were recorded in the presence of excess NH_4PF_6 (Fig. 18 d and g), only a small decrease of

the K_a values was observed (Table 1), as expected according to the Le Chatelier principle, while VT-NMR studies performed on NDI-[$CH_2CH_2OCH_2CH_2O$(An)PS_2NH_4]$_2$⊂15DN38C10 (1b·3 in Fig. 19) and NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2(SnMe_3)$]$_2$⊂15DN38C10 (2b-[$SnMe_3$]$_2$·3 in Fig. 19) showed that the association constants increase with decreasing the temperature.

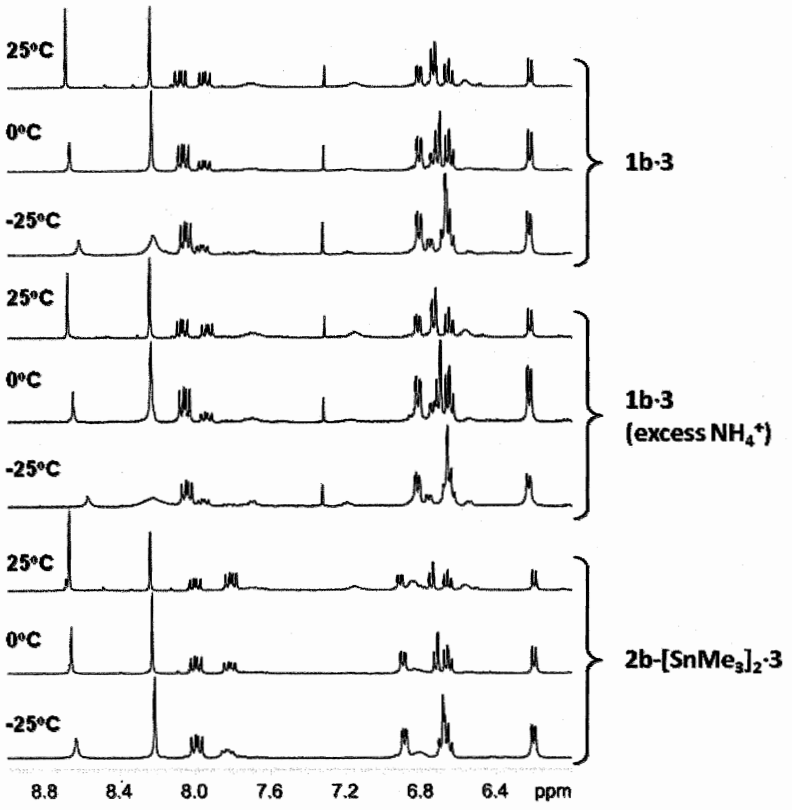


Figure 19: ^{1}H VT-NMR spectra showing the association of the axle and crown with decreasing temperature

The enthalpic ($\Delta H°$) and entropic ($-T\Delta S°$) contributions to the free energy of complexation ($\Delta G°$) can be calculated by determining the K_a values for the association of the axle and crown over a large temperature range, then building a van't Hoff plot ($R\ln K_a$ vs. T^{-1}) which should produce a straight line with a slope of $-\Delta H°$ and an intercept of $\Delta S°$. Broad peaks were observed starting around 0° C in all cases, as shown in Fig 19 for NDI-[$CH_2CH_2OCH_2CH_2O$-(An)PS_2NH_4]$_2$⊂15DN38C10, NDI-[$CH_2CH_2OCH_2CH_2O$-(An)PS_2NH_4]$_2$⊂15DN38C10 in presence of excess NH_4^+ ions and NDI-[$CH_2CH_2OCH_2CH_2O$(An)-$PS_2(SnMe_3)$]$_2$⊂15DN38C10. The broadening of these peaks increased the errors in measuring the free

axle/complexed axle ratio, thus of the K_a values at those temperatures. These errors translated into poor van't Hoff plots, hence no reliable data could be extracted from these experiments. The van't Hoff plot for NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$⊂15DN38C10 can be seen in figure 20.

Figure 20: van't Hoff plot for NDI-$[CH_2CH_2OCH_2CH_2O(An)$-$PS_2NH_4]_2$⊂15DN38C10

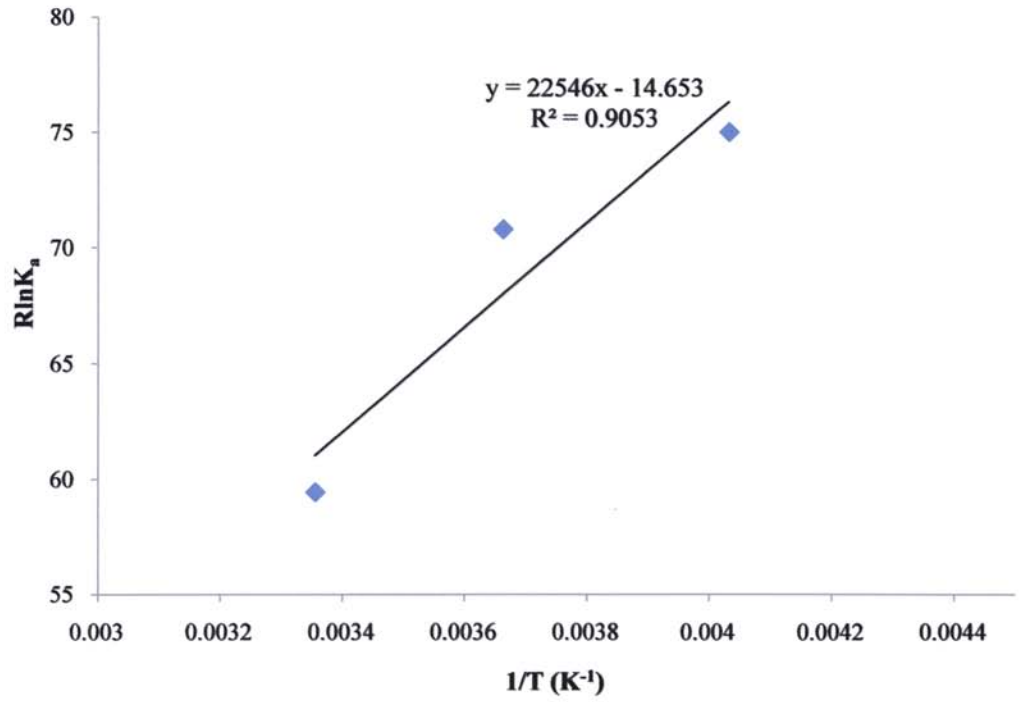


Table 1 Association constants (K_a/M^{-1})[a] and free energies of complexation ($\Delta G°$)[b] for rotaxanes NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$⊂15DN38C10 and NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(Sn$-$Me_3)]_2$⊂15DN38C10 at 25°C.

Solvent	Rotaxane	K_a (M^{-1})	$\Delta G°$ (kJmol^{-1})
Acetone-d_6:D_2O	NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$⊂15DN38C10	896.5	-16.9
5.0/0.6 (v/v)	NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$⊂15DN38C10[c]	758.7	-16.4
	NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$⊂15DN38C10	1259.1	-17.7
	NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$⊂15DN38C10[c]	1131.5	-17.4

	NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnMe_3)]_2$⊂15DN38C10	562.7	-15.7
$CDCl_3$	NDI-$[CH_2CH_2O(An)PS_2(SnMe_3)]_2$⊂15DN38C10	88.3	-11.1
	NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnMe_3)]_2$⊂15DN38C10	787.8	-16.5
	NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$⊂15DN38C10	66.1	-10.4
	NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$⊂15DN38C10	95.9	-11.3
	NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$⊂15DN38C10[d]	0.0	-
	NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$⊂15DN38C10[d]	0.0	-

[a] Determined by the single-point method using initial concentrations of axle and wheel of $1.66 \cdot 10^{-3}$ M and the integral values of the H_a resonances for threaded and unthreaded axles; errors are estimated to be 10% or less; [b] calculated using the formula $\Delta G^\circ = -RT\ln K_a$; [c] measured in the presence of excess of NH_4PF_6; [d] no rotaxane peaks were observed, the $(An)PS_2[Cu(PPh_3)_2]$ group being too large to allow threading.

Rotaxane formation starting from the neutral, bimetallic axles was studied in $CDCl_3$ (Fig. 21). As a general trend, the coordination of the $-PS_2$ donor set to the metallic centers leads to very low K_a values or no rotaxane formation at all, NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(Sn\text{-}Me_3)_2]_2$⊂15DN38C10 being the only exception to the rule, see Table 1.

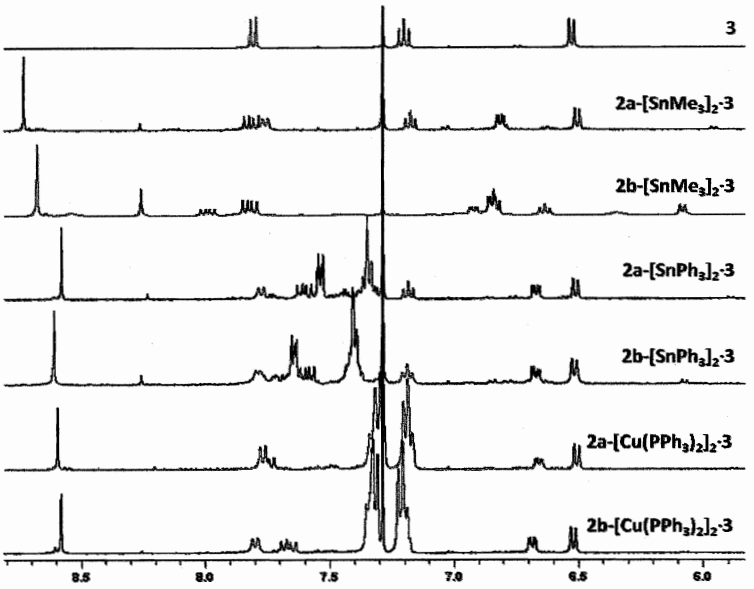


Figure 21: Rotaxane formation starting from preformed bimetallic axles and crown 15DN38C10.

These results suggest that there are two factors influencing rotaxane formation: the *size* of the stopper and the *length* of the side-arms of the axles. While for both anionic axles NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ and NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$ the size of the $(An)PS_2$ group alone is not big enough to prevent threading, in the case of NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ the shorter side-arms of the axle place its terminuses in close proximity to the NDI core, thus protecting it from the crown ether 15DN38C10, which has as a consequence a lower K_a value for NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$⊂15-DN38C10 compared to that for NDI-$[CH_2CH_2OCH_2CH_2O$-$(An)PS_2NH_4]_2$⊂15DN38C10 (896 M^{-1} vs. 1259 M^{-1}). In the case of the NDI-$[CH_2CH_2O(An)$-$PS_2(Cu(PPh_3)_2]_2$ and NDI-$[CH_2CH_2OCH_2CH_2O$-$(An)PS_2(Cu(PPh_3)_2]_2$ axles, the stoppers are big enough to prevent the slippage of crown 15DN38C10 regardless of the length of the side-arms. In the case of NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$ and NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$ axles, the size of the $(An)PS_2SnPh_3$ groups permits to some extent the threading process. However, the length of their side-arms has little influence over the K_a values (66 M^{-1} vs. 95 M^{-1}), suggesting that in this case the size of the stopper is the principal limiting factor in rotaxane formation. In the case of NDI-$[CH_2CH_2O(An)PS_2(SnMe_3)_2]_2$ and NDI-$[CH_2CH_2OCH_2CH_2O$-$(An)PS_2(SnMe_3)_2]_2$axles, the smaller size of the $(An)PS_2SnMe_3$ stopper makes threading possible, as

indicated by the K_a value of 787 M^{-1} for the NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(Sn\text{-}Me_3)_2]_2$⊂15DN38C10 rotaxane. However, NDI-$[CH_2CH_2O(An)PS_2(SnMe_3)_2]_2$⊂15DN38C10 shows a very small K_a value (88 M^{-1}), explained by the shorter side-arms of the axle which would place the $(An)PS_2SnMe_3$ stoppers in the vicinity of the NDI core, thus hampering the rotaxane formation. Comparing the association constants for the NDI-$[CH_2CH_2OCH_2CH_2O\text{-}(An)PS_2NH_4]_2$⊂15DN38C10 / NDI-$[CH_2CH_2OCH_2CH_2O(An)\text{-}PS_2(SnPh_3)_2]_2$⊂15DN38C10 pair in the acetone-water solvent system, it can be observed that the coordination of the $-PS_2$ group to the Me_3Sn(IV) center (and consequently the increase in size of the axle terminuses) significantly lowers the K_a value (1259 M^{-1} vs. 562 M^{-1}).

3.3 Solid state studies

Addition of the metallic salts to the acetone-water solutions of the anionic pseudorotaxanes resulted in the formation of mixtures of unthreaded bimetallic axles and bimetallic rotaxanes.

To further study our system, we attempted to grow crystals. Crystals for the unthreaded bimetallic compounds were grown by layering a solution of the compound in dichloromethane with hexanes. Diffusion from the layering produced orange single crystals. In the case of NDI-$[CH_2CH_2OCH_2CH_2O(An)\text{-}PS_2(SnPh_3)_2]_2$⊂15DN38C10, vapor diffusion of Et_2O into an aqueous acetone solution of the components produced deep red single crystals, which were used in X-ray diffraction experiments.

Crystallographic details for compounds NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$, NDI-$[CH_2CH_2O\text{-}(An)PS_2(Cu(PPh_3)_2]_2$, NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnMe_3)_2]_2$, and NDI-$[CH_2CH_2O(An)\text{-}PS_2(SnMe_3)_2]_2$⊂15DN38C10 are summarized in Table 2. The X-ray data were collected at 100 K on a Bruker SMART APEXII CCD diffractomer equipped with Cu Kα radiation. Intensities were collected using phi and omega scans and were corrected for Lorentz polarization and absorption effects. The *X-SEED* software platform,[5] equipped with *SHELXS* and *SHELXL* modules on a PC computer,[6] was used for all structure solution and refinement calculations and molecular graphics. The structure was solved by direct methods, and refined by anisotropic full-matrix least-squares for all non-hydrogen atoms. All hydrogen atoms were placed in calculated positions and refined using a riding model with fixed thermal parameters.

Table 2: Crystal data and details for NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$, NDI-$[CH_2CH_2O(An)$-$PS_2(Cu(PPh_3)_2]_2$, NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$, and NDI-$[CH_2CH_2OCH_2CH_2O$-$(An)PS_2(SnPh_3)_2]_2 \subset 15DN38C10$.

	NDI-$[CH_2CH_2O$-$(An)PS_2(SnPh_3)_2]_2$	NDI-$[CH_2CH_2O$-$(An)PS_2(Cu(PPh_3)_2]_2$	NDI-$[CH_2CH_2OCH_2$-$CH_2O(An)PS_2(SnPh_3)_2]_2$	NDI-$[CH_2CH_2O$-$CH_2CH_2O(An)PS_2(Sn$ $Ph_3)_2]_2 \subset 15DN38C10$
Empirical Formula	$C_{69}H_{56}Cl_4N_2O_8P_2S_4Sn_2$	$C_{106}H_{90}C_{l4}Cu_2N_2O_8P_6S_4$	$C_{72}H_{64}N_2O_{10}P_2S_4Sn_2$	$C_{216}H_{220}N_4O_{42}P_4S_8Sn_4$
FW, $g \cdot mol^{-1}$	1610.52	2102.74	1544.81	4399.24
Crystal System	Triclinic	Triclinic	Monoclinic	Triclinic
Space Group	$P\bar{1}$	$P\bar{1}$	Pc	$P\bar{1}$
T (K)	173	173	100(2)	100(2)
a, (Å)	9.1473(9)	9.2045(1)	13.7321(2)	11.6038(4)
b, (Å)	13.3655(12)	11.5410(2)	10.5102(2)	16.3167(6)
c, (Å)	14.7118(13)	23.4034(4)	23.2601(3)	27.3486(9)
α, (°)	75.801(4)	85.150(1)	90	88.799(2)
β, (°)	78.668(5)	89.605(1)	97.740(1)	78.172(2)
γ, (°)	87.853(5)	75.421(1)	90	83.306(2)
V, ($Å^3$)	1709.6(3)	2397.19(6)	3326.48(9)	5033.6(3)
Z, Z'	1	1	2	1
D_x ($mg \cdot m^{-3}$)	1.564	1.457	1.542	1.451
$F(000)$	810	1084	1568	2268
R/R_w^2 (obs data)	0.123/0.323	0.041/0.108	0.037/0.093	0.054/0.138
S	1.05	1.02	01.07	1.05
no. of reflns/params	5944/426	8375/596	8953/832	17677/1330
$\Delta\rho_{max/min}$ ($e \cdot Å^{-3}$)	2.71/-1.67	0.53/-0.61	0.70/-0.61	00.98/-0.61

I. NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$.

The molecular structure of NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$consists of two -$(An)PS_2$ moieties coordinated to two -$SnPh_3$ metallic centers in a monodentate fashion (Fig. 22a). The -$SnPh_3$ groups flank the NDI central core on both sides, with no significant non-covalent interactions between the two. The

crystal packing of NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$ is based on a combination of $\pi - \pi$ stacking and C-H$\cdots\pi$ interactions between two adjacent molecules (Fig. 22 b and c), involving a phenyl (-$SnPh_3$) ring from one molecule and the central NDI core and another phenyl ring from an adjacent molecule.

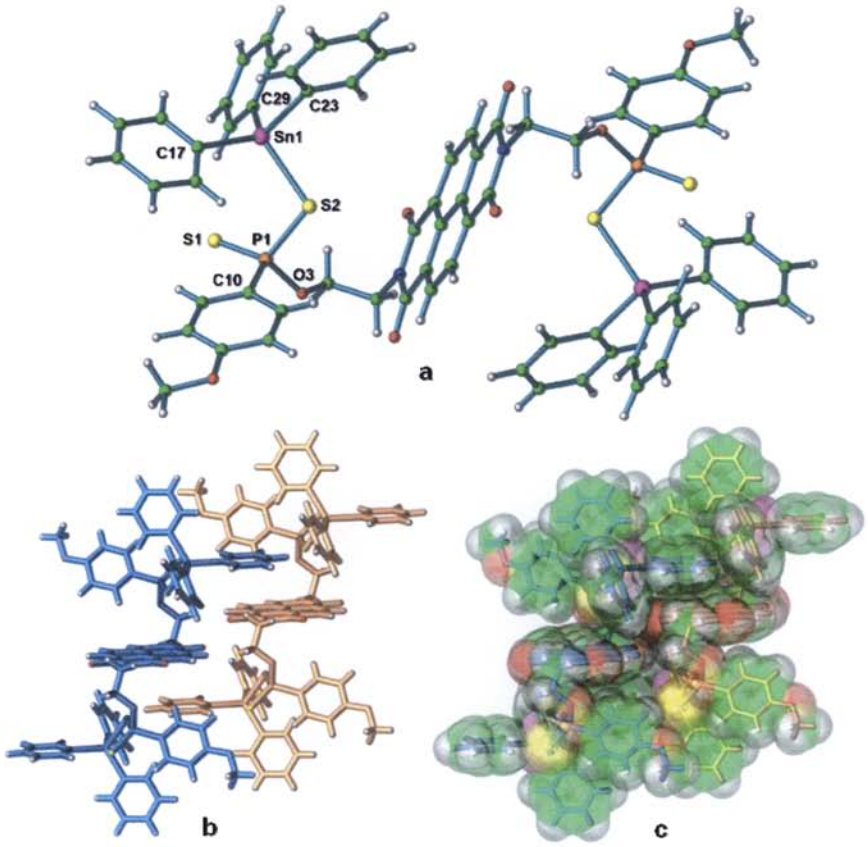


Figure 22: a) Molecular structure of NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$; selected bond lengths (Å) and angles (°): Sn1-S2=2.450(4); Sn1-C17=2.175(16); Sn1-C23=2.172(13); Sn1-C29=2.145(17); S1-P1=1.938(7); S2-P1=2.080(4); P1-O3=1.587(12); P1-C10=1.772(15); S2-Sn1-C17=109.4(4); S2-Sn1-C23=97.8(4); S2-Sn1-C29=116.0(4); Sn1-S2-P1=105.12(19); S1-P1-S2=115.2(2); color code: carbon-green; hydrogen-gray; phosphorus-orange; sulfur-yellow; metal atom (tin)-purple; b) packing of two adjacent molecules; c) space filling representation of the same two building blocks.

II. NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$.

The molecular structure of NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$consists of two -$(An)PS_2$ moieties coordinated to two -$Cu(PPh_3)_2$ metallic centers in a bidentate fashion (Fig. 23a). The anisole groups are involved in a π-π stacking interaction with the central NDI core, with several C – C distances between 3.4

and 3.6 Å. The crystal packing of NDI-$[CH_2CH_2O(An)PS_2(Cu\text{-}(PPh_3)_2]_2$is based on a combination of $\pi - \pi$ stacking and C-H$\cdots\pi$ interactions involving both -PPh_3 groups coordinated to the Cu(I) atom (Fig. 23b and c).

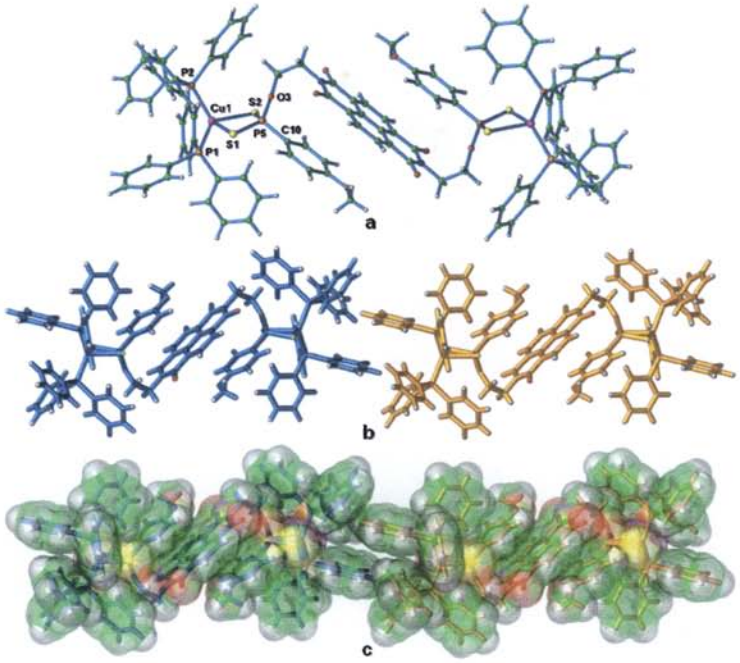


Figure 23: a) Molecular structure of NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$; selected bond lengths (Å) and angles (°): Cu1-S1=2.3870 (8); Cu1-S2=2.5484 (9); Cu1-P1=2.2676 (8); Cu1-P2=2.2714 (8); S1-P5=1.9957 (10); S2-P5=1.9850 (11); P5-O3=1.615 (2); P5-C10=1.808 (3); S1-Cu1-S2=85.30 (3); P1-Cu1-P2=124.12 (3); S1-Cu1-P1=114.62 (3); S1-Cu1-P2=112.68 (3); S2-Cu1-P1=101.19 (3); S2-Cu1-P2=110.69 (3); S1-P5-S2=114.39 (5); O3-P5-C10=103.54 (13); color code: carbon-green; hydrogen-gray; phosphorus-orange; sulfur-yellow; metal atom (copper)-purple; b) packing of two adjacent molecules; c) space filling representation of the same two building blocks.

III. NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$.

As with NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$, the molecular structure of NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$consists of two -$(An)PS_2$ moieties coordinated to two -$SnPh_3$ metallic centers in a monodentate fashion (Fig. 24a). The geometric parameters around the tin atom are virtually the same as in the case of NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$, showing that the coordination behavior of the -$(An)PS_2$ moieties are independent of the length of the side arms attached to the central NDI

core. The crystal packing of NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2(Sn\text{-}Ph_3)_2]_2$is driven by phenyl embraces of the -$SnPh_3$ groups (Fig. 24b and c).

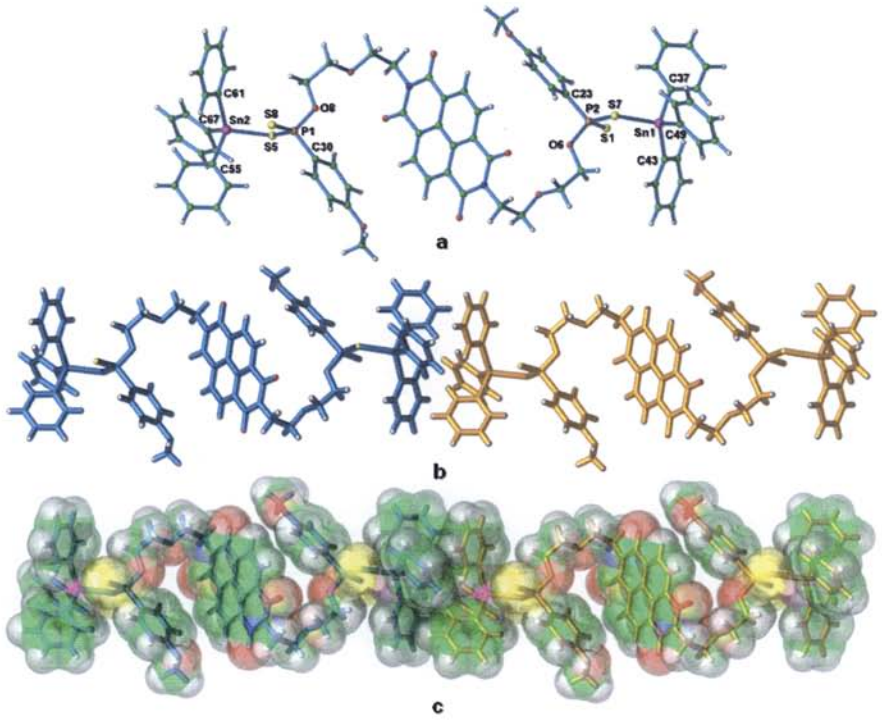


Figure 24: a) Molecular structure of NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$; selected bond lengths (Å) and angles (°): Sn1-S7=2.440(2); Sn1-C37=2.109(8); Sn1-C43=2.113(6); Sn1-C49=2.143(7); Sn2-S5=2.4326(17); Sn2-C55=2.138(7); Sn2-C61=2.123(6); Sn2-C67=2.156(7); S1-P2=1.929(3); S7-P2=2.077(2); S5-P1=2.085(2); S8-P1=1.934(2); P1-O8=1.597(5); P1-C30=1.804(7); P2-O6=1.594(5); P2-C23=1.784(7); S7-Sn1-C37=109.0(2); S7-Sn1-C43=116.24(19); S7-Sn1-C49=96.0(2); Sn1-S7-P2=103.92(9); S1-P2-S7=115.45(11); O6-P2-C23=99.9(3); S5-Sn2-C55=110.8(2); S5-Sn2-C61=115.78(19); S5-Sn2-C67=97.1(2); Sn2-S5-P1=102.22(8); S5-P1-S8=114.79(11); O8-P1-C30=100.4(3); color code: carbon-green; hydrogen-gray; phosphorus-orange; sulfur-yellow; metal atom (tin)-purple; b) packing of two adjacent molecules; c) space filling representation of the same two building blocks.

IV. NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$⊂15DN38C10.

The structure of this rotaxane (Fig. 24) shows a similar arrangement of the NDI and 15DN38C10 pair to that observed for related systems,[1,7] with the π-rich aromatic regions of 15DN38C10 stacked around

the π-deficient NDI core. There are two independent molecules in the unit cell, both having the -PS_2 groups coordinated in a monodentate fashion to the tin atom, virtually identical with the unthreaded NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$counterpart. A notable difference is that in one molecule, the Sn center is tetra-coordinate (Fig. 25a), while in the other, a water molecule expands the tin coordination number to five (Fig. 25b) and is involved in hydrogen bonding with two oxygen atoms from a neighboring crown ether macrocycle (Fig. 26). This leads to different orientation of the side-arms with respect to the central NDI/ 15DN38C10 core, with the $SnPh_3$ and anisole moieties oriented toward the outer region of the crown 15DN38C10, respectively. The naphthalene rings are π-stacked on both sides of the NDI central core. In the case of the tetracoordinate tin rotaxane, the perpendicular distance between the NDI and 15DN38C10 rings is 3.50 Å and for the pentacoordinate tin rotaxane is 3.48 Å.

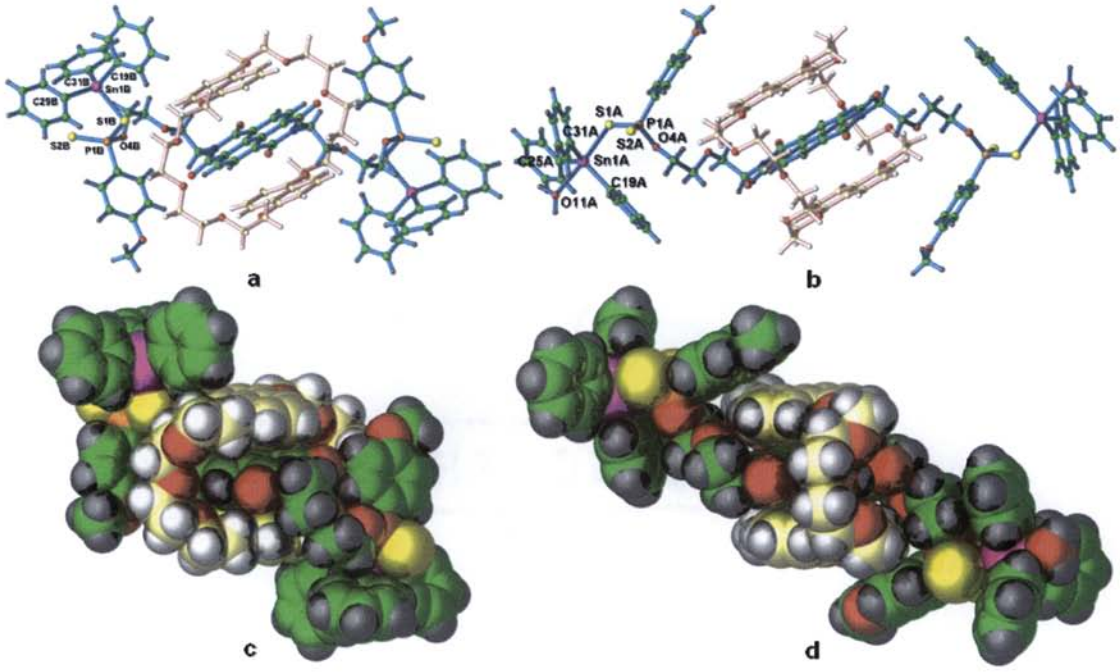


Figure 25: Molecular structures of the two independent molecules of NDI-$[CH_2CH_2OCH_2CH_2O(An)$-$PS_2(SnPh_3)_2]_2$⊂15DN38C10: a) the four-coordinate and b) the five-coordinate tin atom; selected bond lengths (Å) and angles (°): Sn1A-S1A=2.5626(14); Sn1A-O11A=2.457(4); Sn1A-C19A=2.132(5); Sn1A-C25A=2.140(5); Sn1A-C31A=2.136(5); S1A-P1A=2.0462(19); S2A-P1A=1.934(2); Sn1B-C31B=2.128(5); Sn1B-S1B=2.4427(14); Sn1B-C19B=2.135(6); Sn1B-C25B=2.116(5); S1B-

P1B=2.0758(19); S2B-P1B=1.9387(19); S1A-Sn1A-C19A=101.35(14); S1A-Sn1A-C25A=90.58(13); S1A-Sn1A-C31A=99.05(15); S1A-Sn1A-O11A=175.54(9); S1A-P1A-S2A=117.18(10); S1B-Sn1B-C31B=111.35(14); S1B-Sn1B-C19B=100.82(15); S1B-Sn1B-C25B=109.68(15); S1B-P1B-S2B=115.00(8); c) and d) space filling representation of the two independent molecules.

The hydrogen atoms from the water molecule coordinated to the tin atom is involved in two hydrogen bonds with two oxygen atoms within a crown ether wheel from a neighboring rotaxane molecule. The O···H distances are 1.91 Å and 1.73 Å, with the O-H-O angles of 173.8° and 170.1° respectively. This interaction contributes to the different orientation of the side-arms of the rotaxanes.

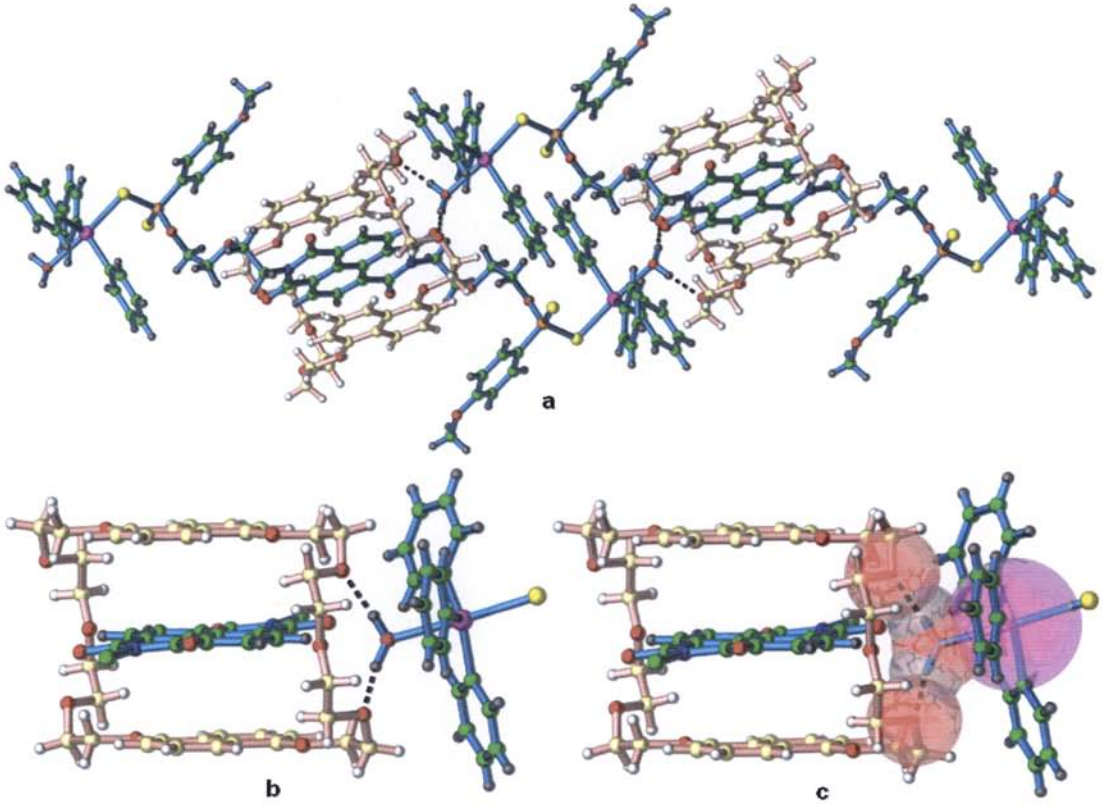


Figure 26: Hydrogen bonding involving the coordinated water molecule and the crown ether: a) two rotaxanes held together by hydrogen bonding; b) detail of the hydrogen bonds; c) space filling of the atoms involved in hydrogen bonding.

Another consequence of the hydrogen bonding is the different orientation in the solid state of the central NDI core relative to the aromatic region of the crown ether (Fig. 27). This orientation can be measured by the torsion angle defined by the $N_{NDI} - Ct_{NDI} - Ct_{15DN38C10} - C_{15DN38C10}$ angle.[8] In the case of the tetracoordinate tin rotaxane, the torsion angle is 86.8° and for the pentacoordinate tin rotaxane is 78°.

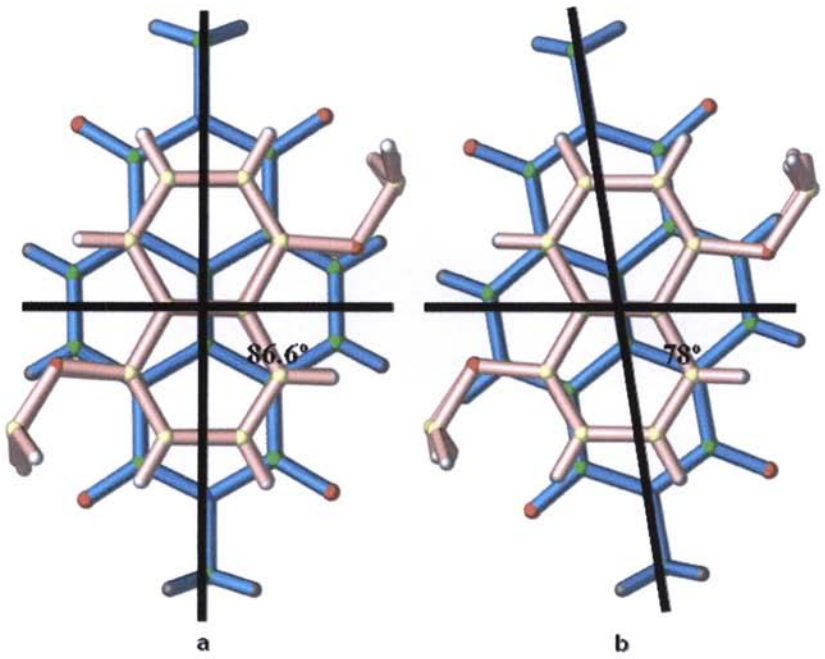


Figure 27: The different relative orientation between the NDI core relative and the aromatic region of the crown ether: a) the tetracoordinate tin rotaxane; b) the pentacoordinate tin rotaxane.

To make a step further toward our goal to prepare MORFs, we also studied the coordination of the axles to metal centers with an overall 2^+ charge, that is Ph_2SnCl_2. The solid state structures of these two compounds are presented in Figures 28 and 31.

TABLE 3 : Crystal data and details for NDI-[$CH_2CH_2O(An)PS_2]_2$-[$SnPh_2]_2$ and NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2]_2$-[$SnPh_2$]

	(NDI-[$CH_2CH_2O(An)PS_2]_2)_2$-[$SnPh_2]_2$	NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2]_2$-[$SnPh_2$]
Empirical Formula	$C_{45}H_{38}Cl_2N_2O_8P_2S_4Sn$	$C_{48}H_{44}N_2O_{10}P_2S_4Sn \cdot 2(CH_2Cl_2)$
FW, g · mol^{-1}	1114.54	1287.57
Crystal System	Triclinic	Triclinic
Space Group	*P*	*P*
T (K)	100	100
a, (Å)	10.9684 (2)	12.3562 (3)
b, (Å)	12.3642 (2)	13.0479 (2)
c, (Å)	17.6112 (3)	18.2453 (4)
α, (°)	87.540 (1)	91.405 (1)
β, (°)	88.133 (1)	105.836 (1)
γ, (°)	71.074 (1)	105.259 (1)
V, ($Å^3$)	2256.71 (7)	2715.40 (10)
Z, *Z'*	2	2
D_x ($mg \cdot m^{-3}$)	1.640	1.575
F(000)	1128	1308
R/R_w^2 (obs data)	0.027/0.074	0.045/0.119
S	1.06	1.19
no. of reflns/params	8339/579	9540/671
$\Delta\rho_{max/min}$ ($e \cdot Å^{-3}$)	0.93/−0.33	1.80/−1.27

The structure for (NDI-[$CH_2CH_2O(An)PS_2]_2)_2$-[$SnPh_2]_2$ showed that the short axle forms a dimer when reacted with Sn_2Ph_2Cl. π-π stacking is evident when multiple unit cells are aligned together (Fig. 30).

The NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2$]-[$SnPh_2$] structure formed a monomer in which both PS_2 groups on the axle are bound to the same tin atom. This was made possible due to the longer "arms" between the NDI central piece and the PS_2 ligands. Two unit cells have π-π stacking with each other when aligned with each other.

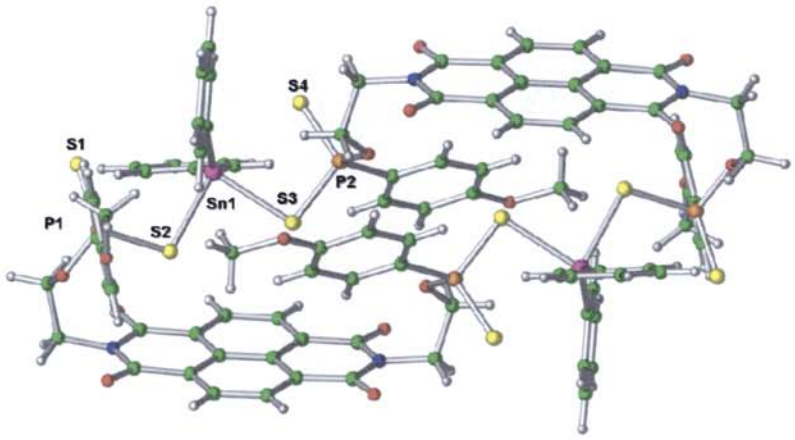


Figure 28: Molecular structure for (NDI-$[CH_2CH_2O(An)PS_2]_2)_2$-$[SnPh_2]_2$; selected bond lengths (Å) and angles (°): Sn1-S2= 2.5111(7); Sn1-S3=2.4996(6); S1-P1=1.9370(9); S2-P1=2.0627(8); S3-P2= 2.0508(8); S4-P2=1.9704(8); S1-P1-S2=114.76(4); S2-Sn1-S3=84.11(2); Sn1-S3-P2=93.87(3); S3-P2-S4=109.22(4); color code: carbon-green; hydrogen-gray; phosphorus-orange; sulfur-yellow; metal atom (tin)-purple

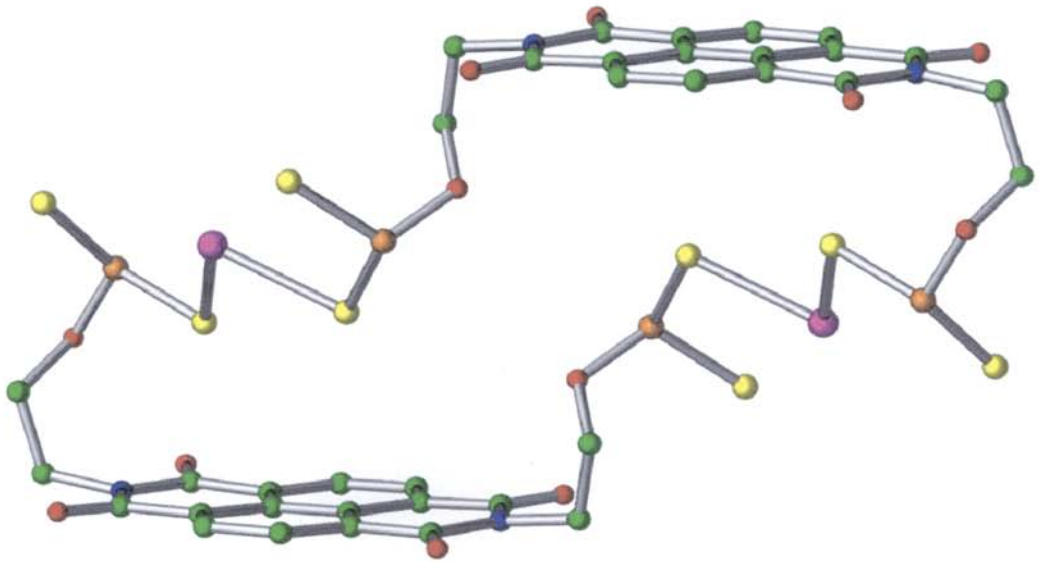


Figure 29: Molecular structure for (NDI-$[CH_2CH_2O(An)PS_2]_2)_2$-$[SnPh_2]_2$ with hydrogens, anisole groups of the axle, and phenyl ligands removed for clarity.

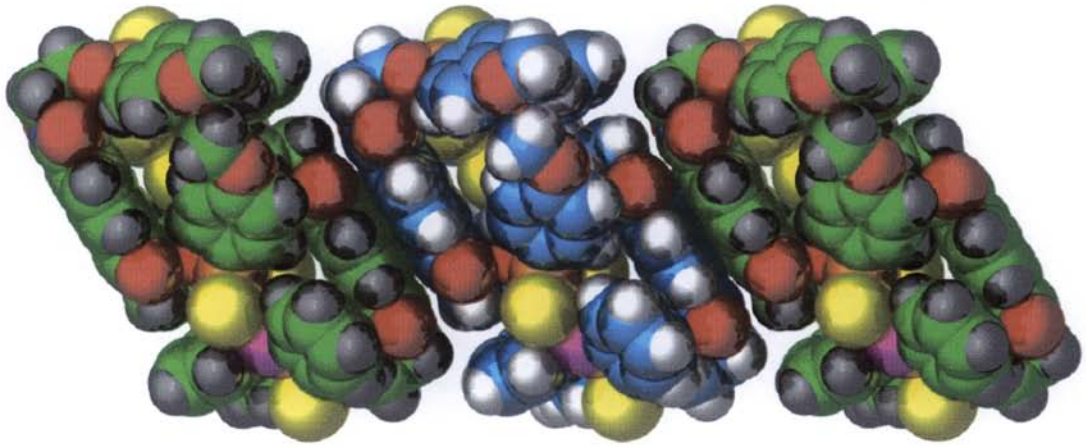


Figure 30: Multiple unit cells for (NDI-[$CH_2CH_2O(An)PS_2$]$_2$)$_2$-[$SnPh_2$]$_2$ showing π-π stacking

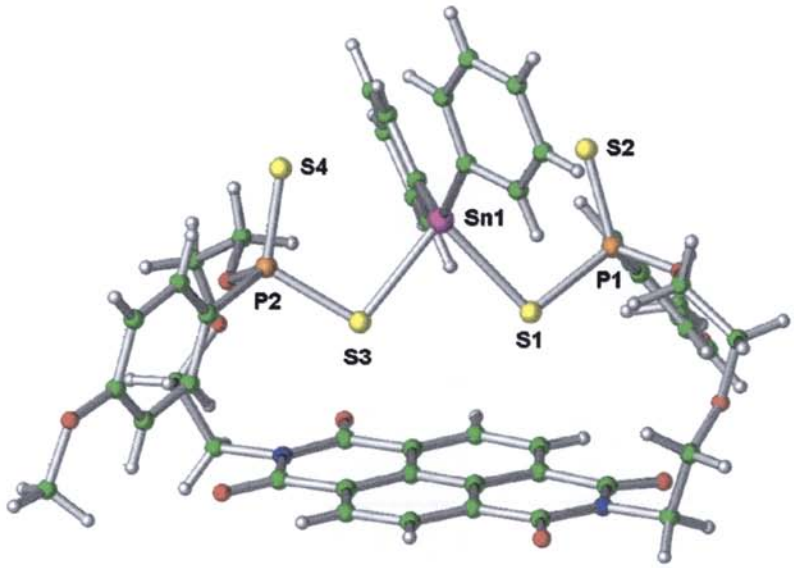


Figure 31: Molecular structure for NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2$]-[$SnPh_2$]; selected bond lengths (Å) and angles (°): S2-P1=1.942(1); S1-P1=2.075(2); S1-Sn1=2.473(1); Sn1-S3=2.490(1); P2-S3=2.061(1); S4-P2=1.952(1); S4-P2-S3=112.21(7); P2-S3-Sn1=97.60(5); S3-Sn1-S1=83.74(4) ; Sn1-S1-P1= 97.51(5) ; S1-P1-S2=111.29(7); color code: carbon-green; hydrogen-gray; phosphorus-orange; sulfur-yellow; metal atom (tin)-purple

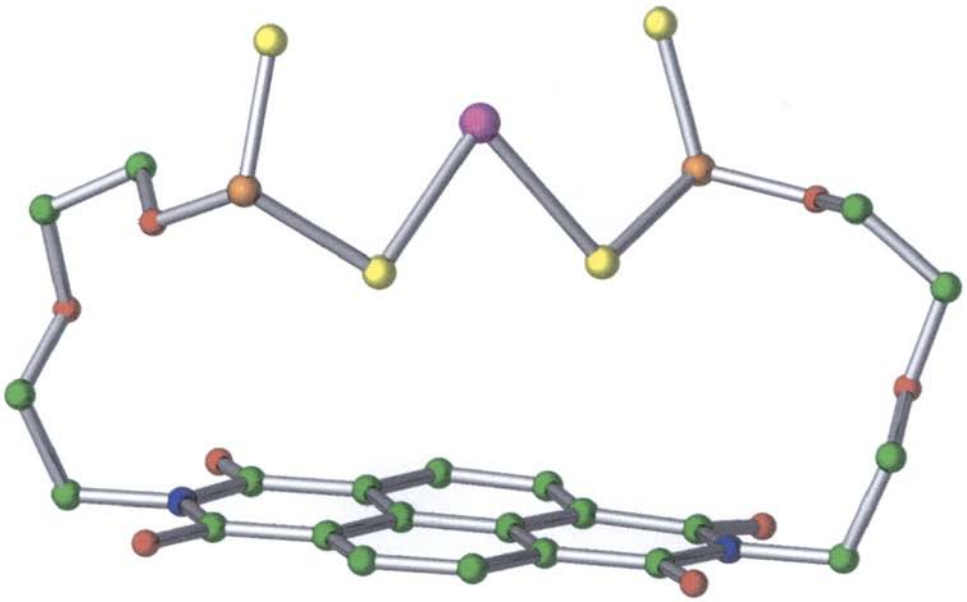


Figure 32: Molecular structure for NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2$]-[$SnPh_2$] with hydrogens, anisole groups on axle, and phenyl ligands removed for clarity

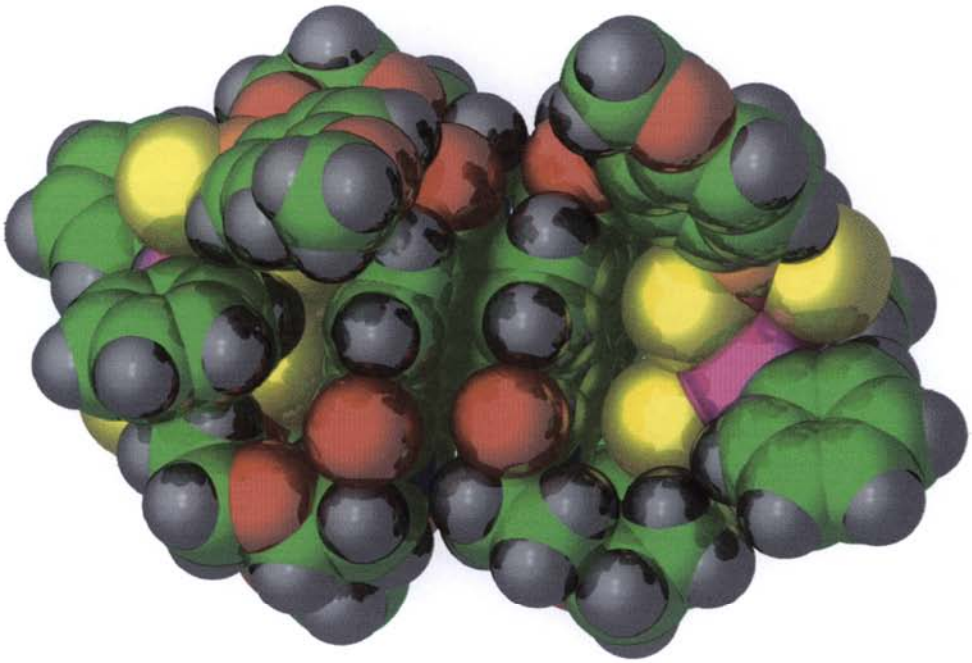


Figure 33: π-π interaction of two unit cells of NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2$]-[$SnPh_2$]

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Conclusion

NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$ and NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$ have been successfully synthesized and their structures established by ^1H NMR. Complexes of our axles bound to $SnMe_3$, $SnPh_3$, and $Cu(PPh_3)_2$ have also been successfully obtained, proving that the dithiophosphonate group on the axle is an effective ligand.

In conclusion, we have successfully designed, synthesized, and characterized ditopic anionic axles with donor properties and used them for the preparation of neutral metallo-rotaxanes. The synthesis of neutral rotaxanes from anionic axles and cationic metal building blocks is a major step towards creating neutral MORFs. While it was clear *a priori* that the metallic systems used here would generate discrete rotaxanes rather than MORFs, they were chosen to serve as "proof-of-principle" experiments and because their solubility would allow a better characterization of the system. The use of metallic systems with an overall charge of 2^+ should yield at least one-dimensional MORFs through the coordination of two $-PS_2$ groups from two different rotaxanes to the metal, since the side-arms of the axles are not long enough to allow the formation of their topological isomers, the corresponding monometallic catenanes. The NDI group can be easily functionalized with other negatively charged side-arms with donor properties, thus opening the door for the synthesis of a large variety of neutral interlocked arrays, either discrete species self-assembled *via* secondary bonds or "classic", coordinatively bounded MORFs.

FUTURE WORK

Synthesis of one-dimensional MORFs has been attempted but no crystals have been obtained yet for X-ray diffraction analysis. Without a solid state structure, it is impossible to determine if MORFs or discrete rotaxanes are formed. Two- and three- dimensional MORFs would also be excellent synthetic targets.

Addition of a second guest on the axle, possibly a pyromelliticdianhydride, will enable the rotaxanes and hence their MORFs to be used as molecular switching devices or memory for computers.

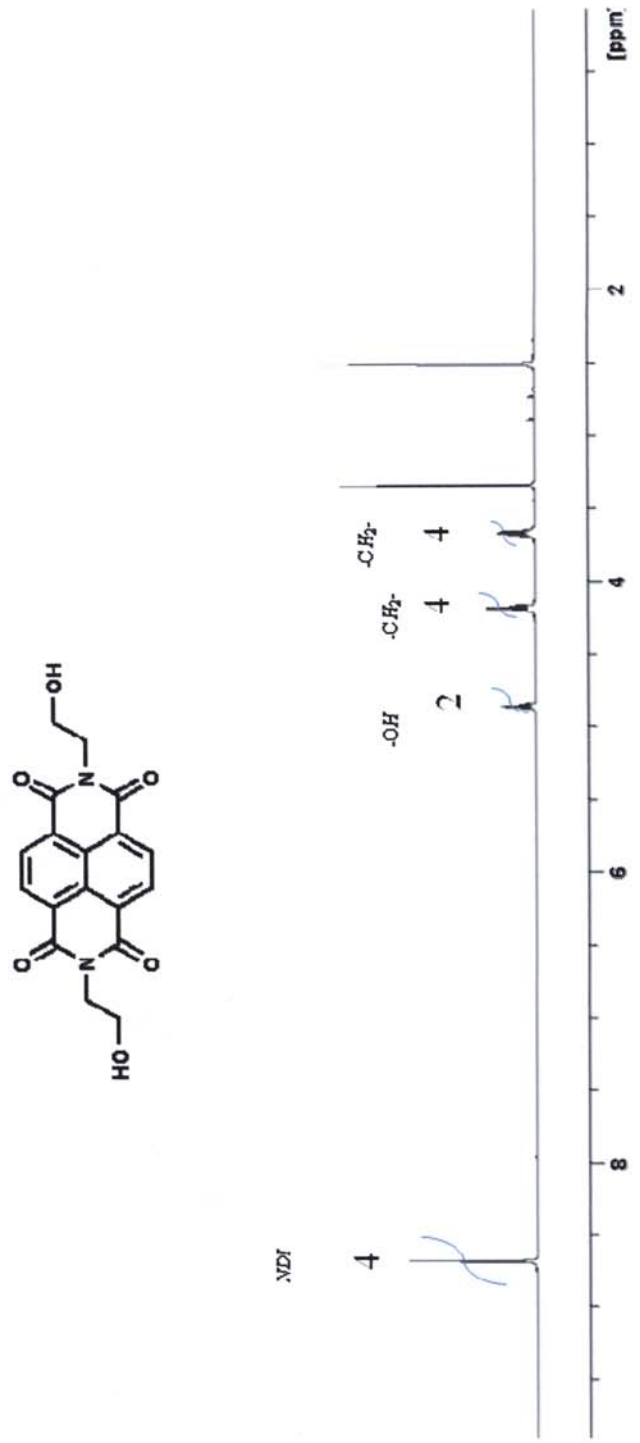

Figure A1: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2OH]_2$

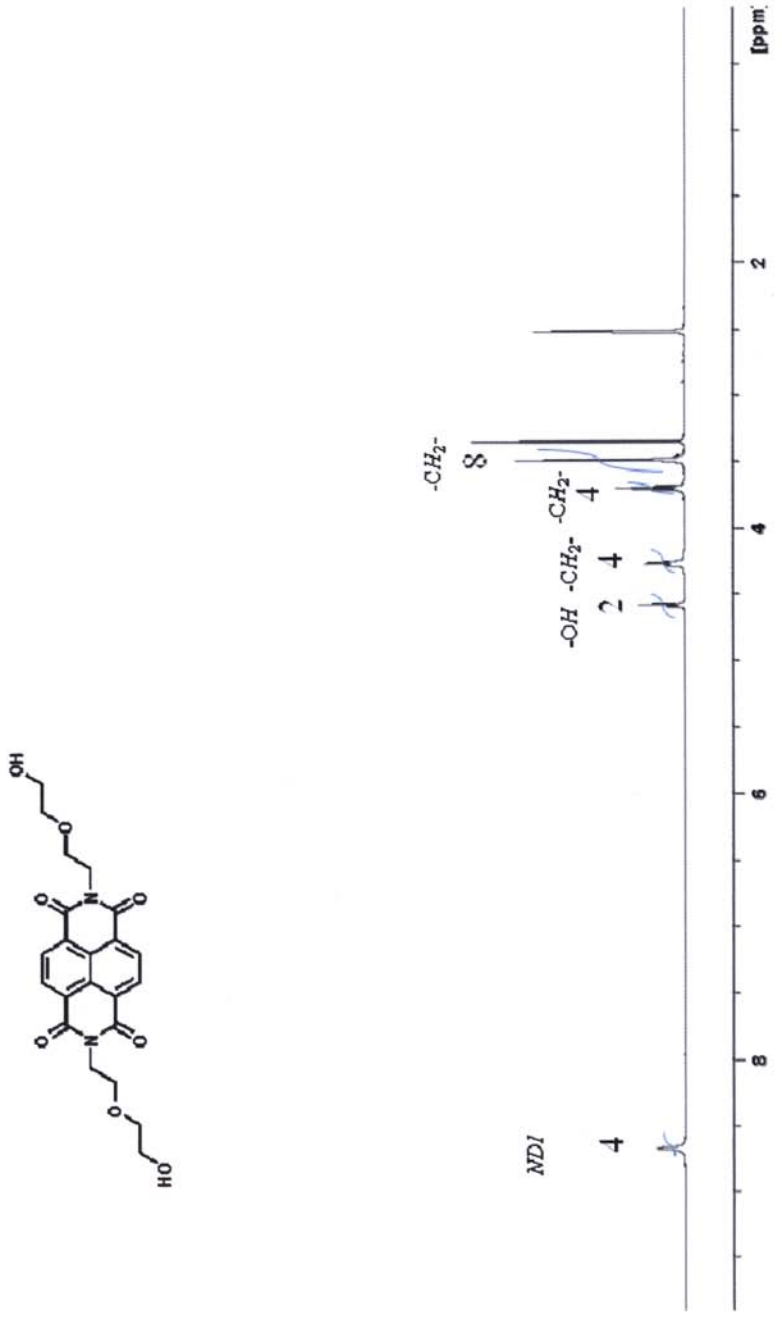

Figure A2: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2OCH_2CH_2OH]_2$

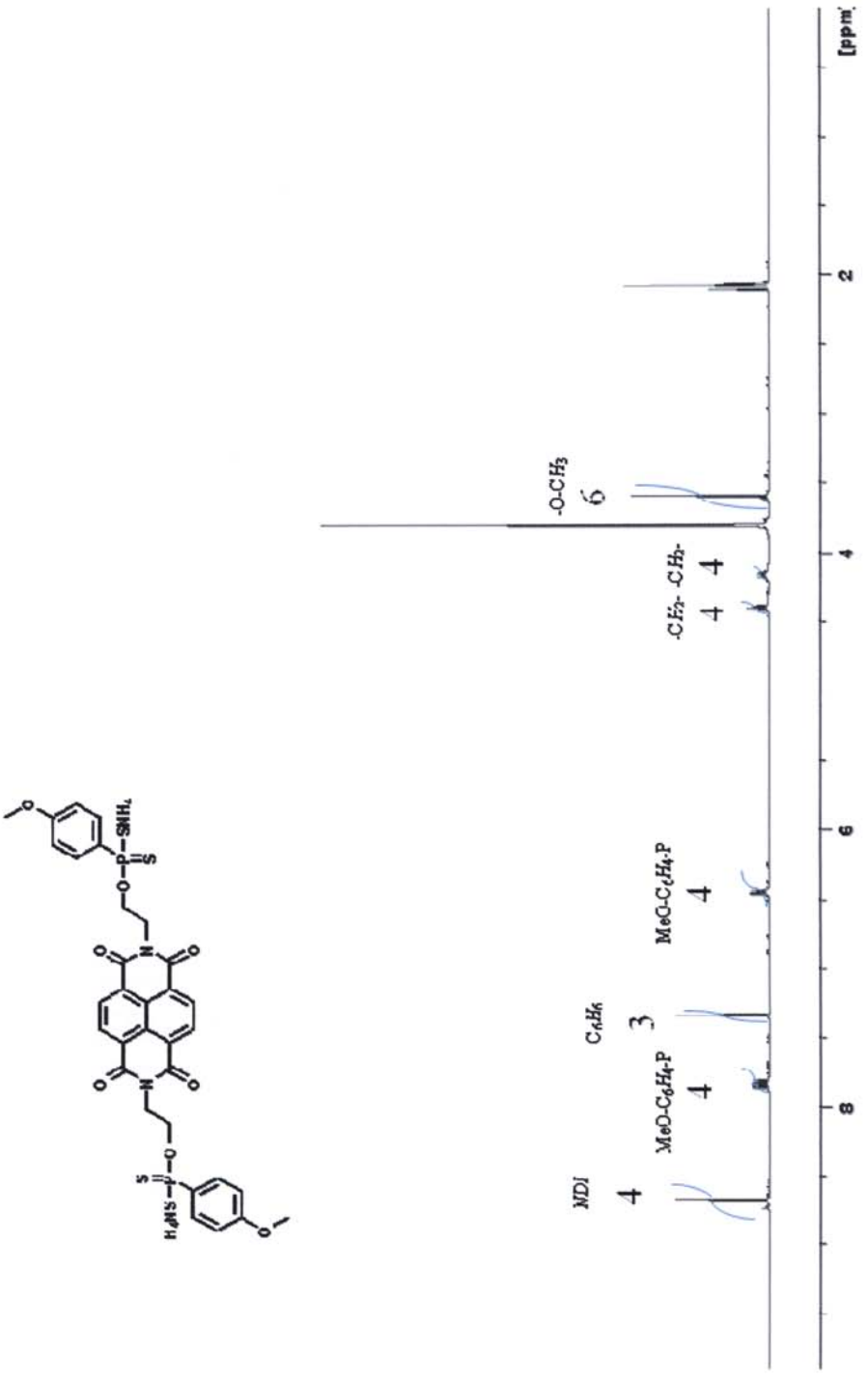

Figure A3: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2O(An)PS_2NH_4]_2$

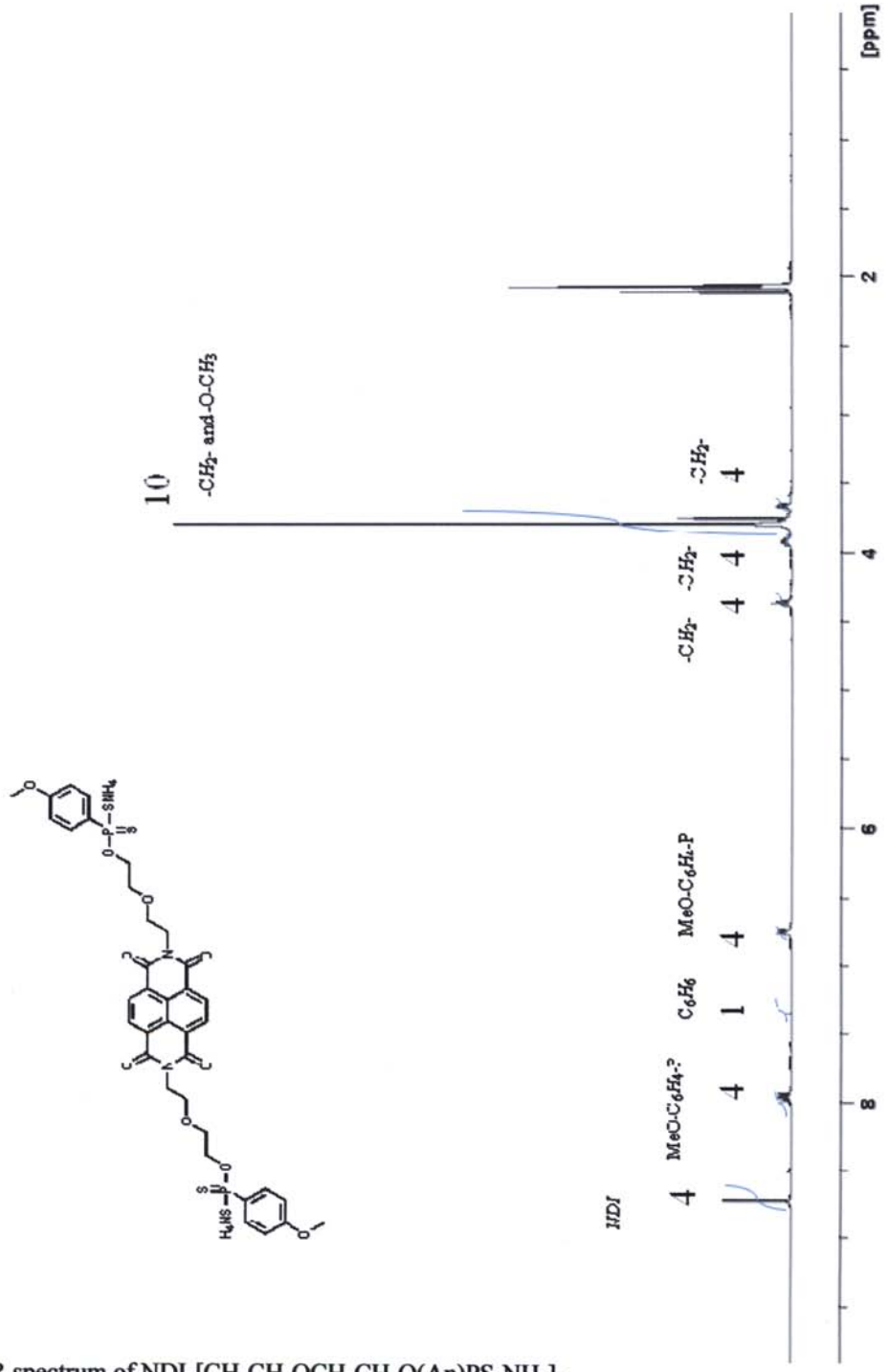

Figure A4: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2NH_4]_2$

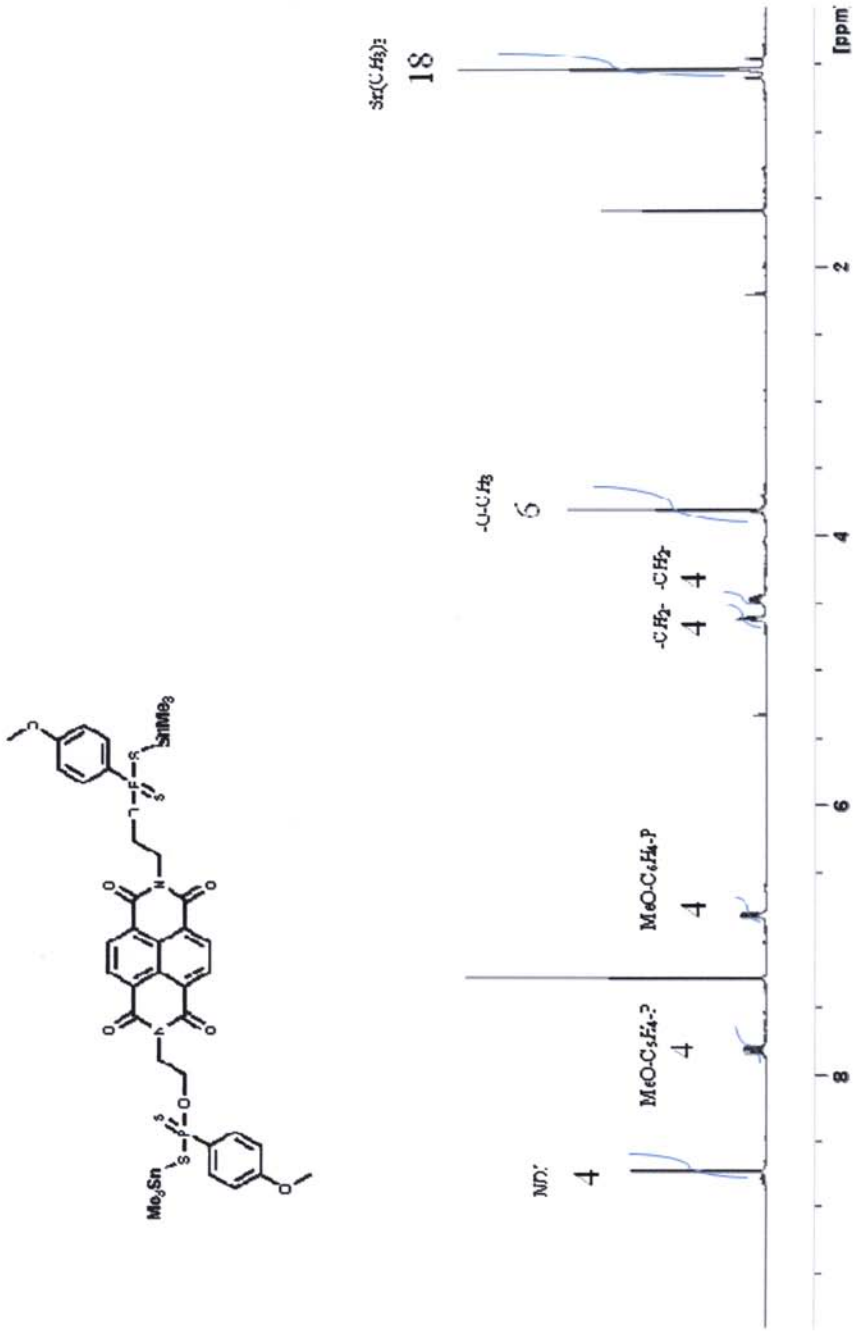

Figure A5: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2O(An)PS_2(SnMe_3)_2]_2$

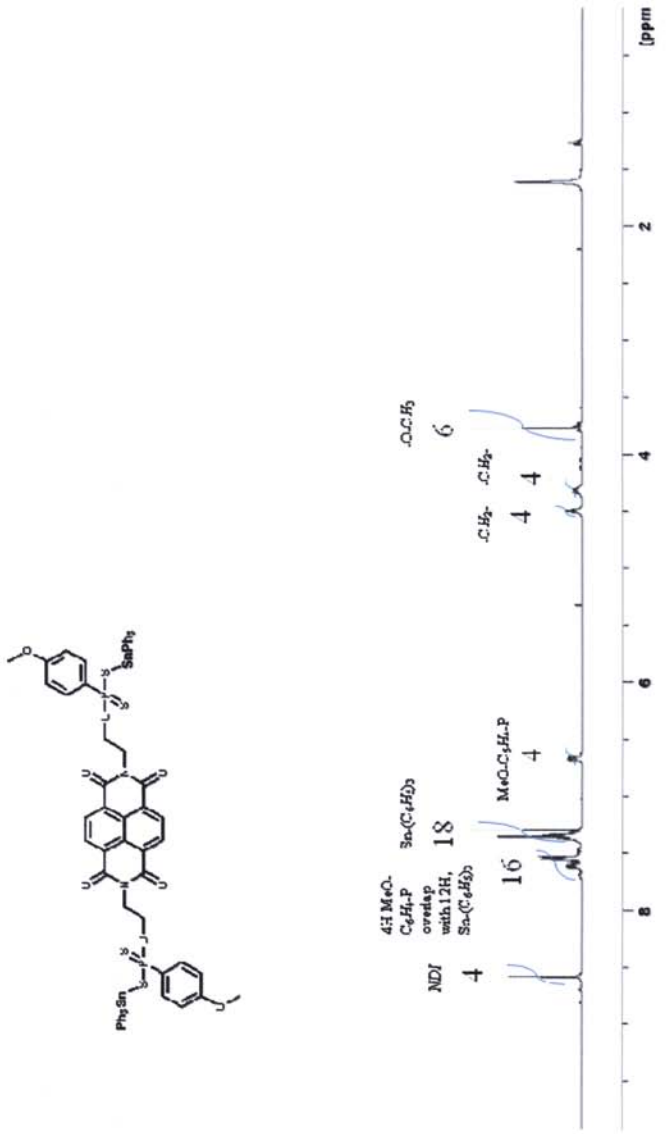

Figure A6: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$

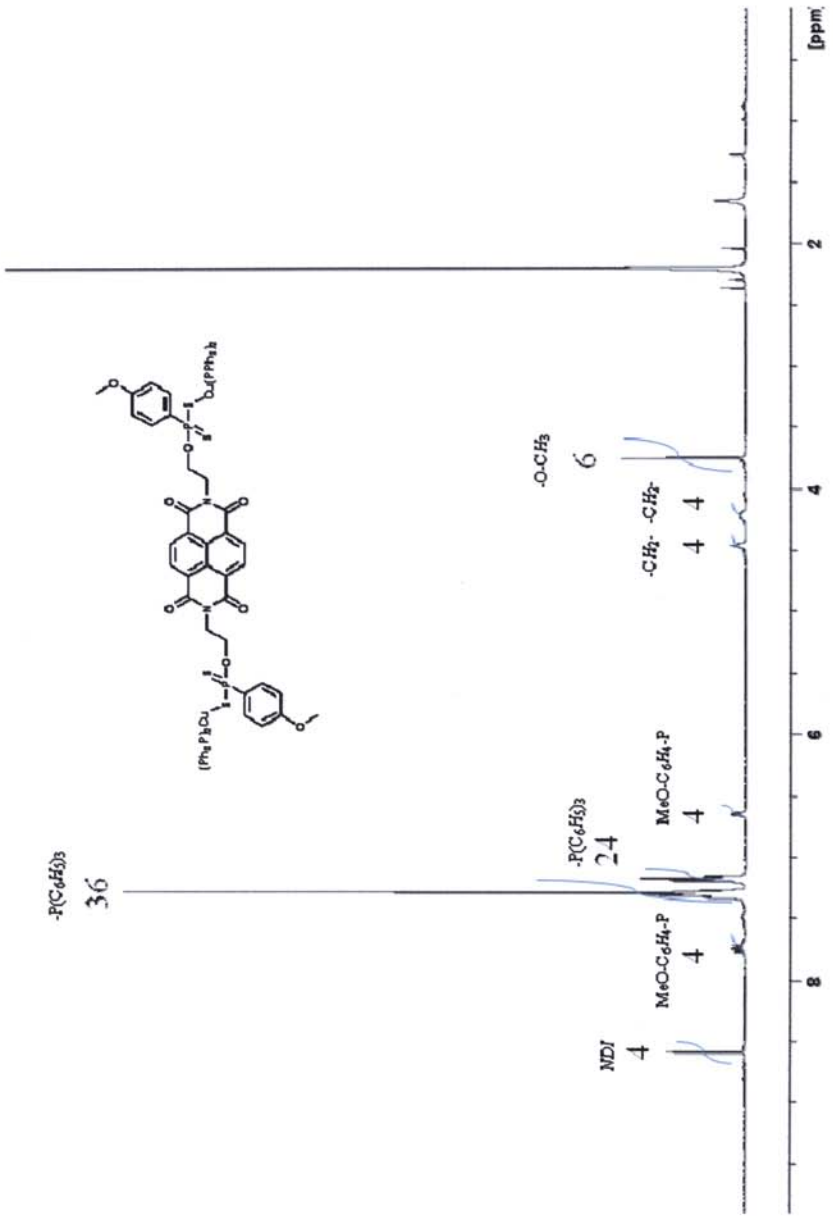

Figure A7: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$

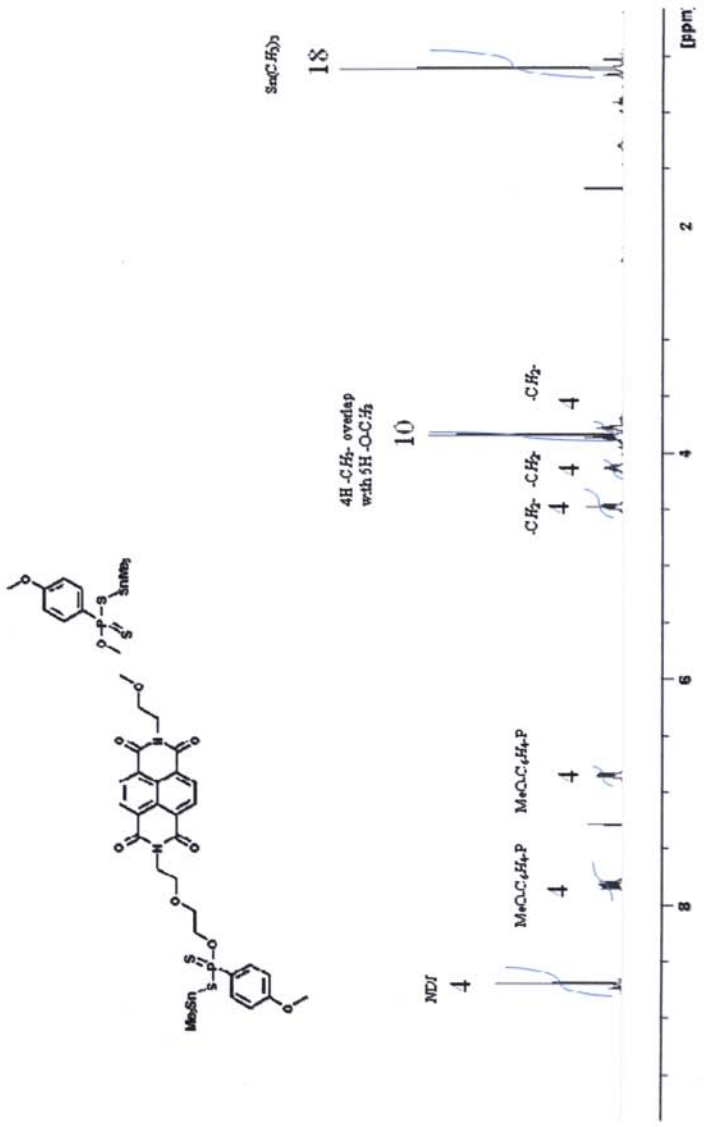

Figure A8: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnMe_3)_2]_2$

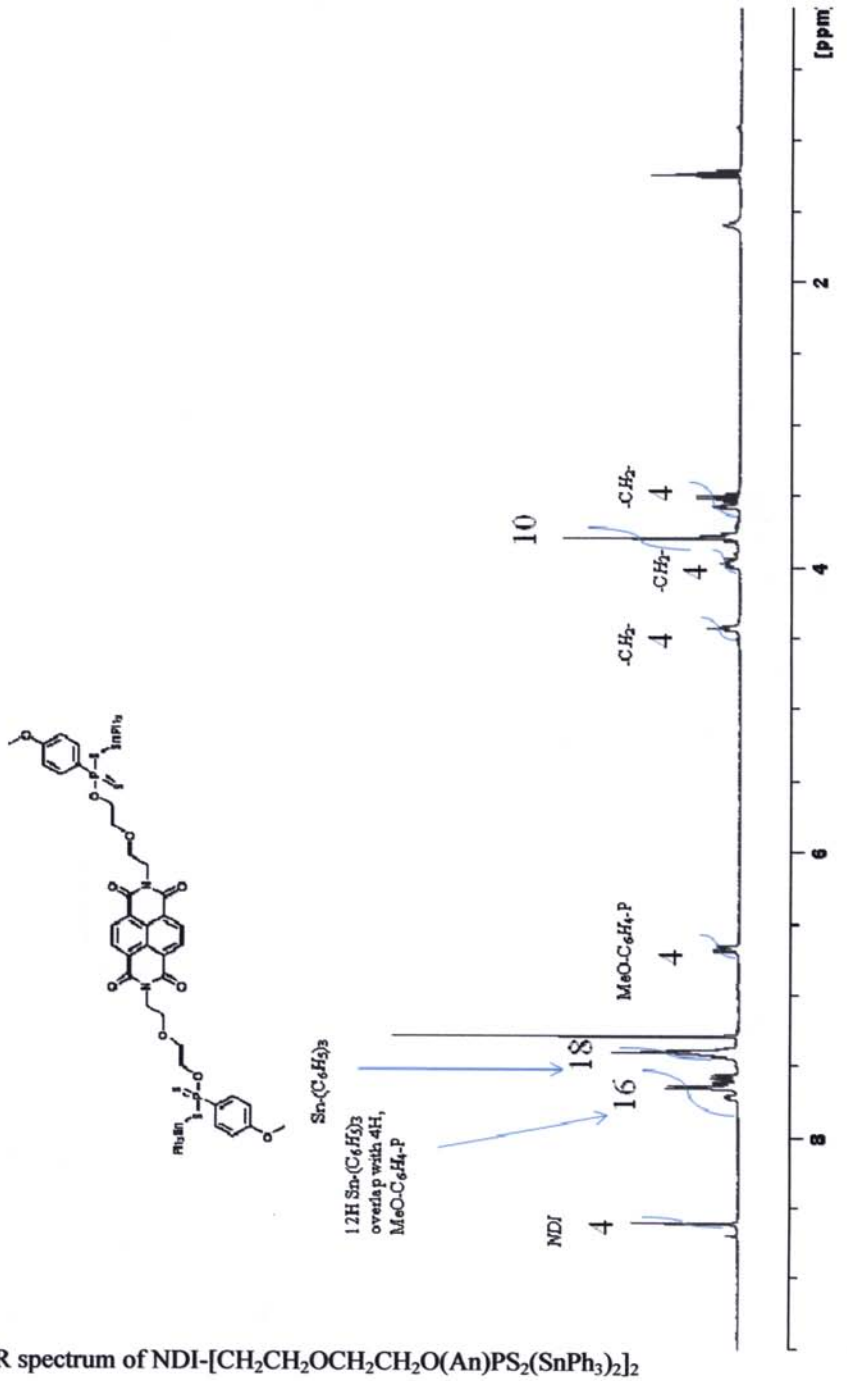

Figure A9: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$

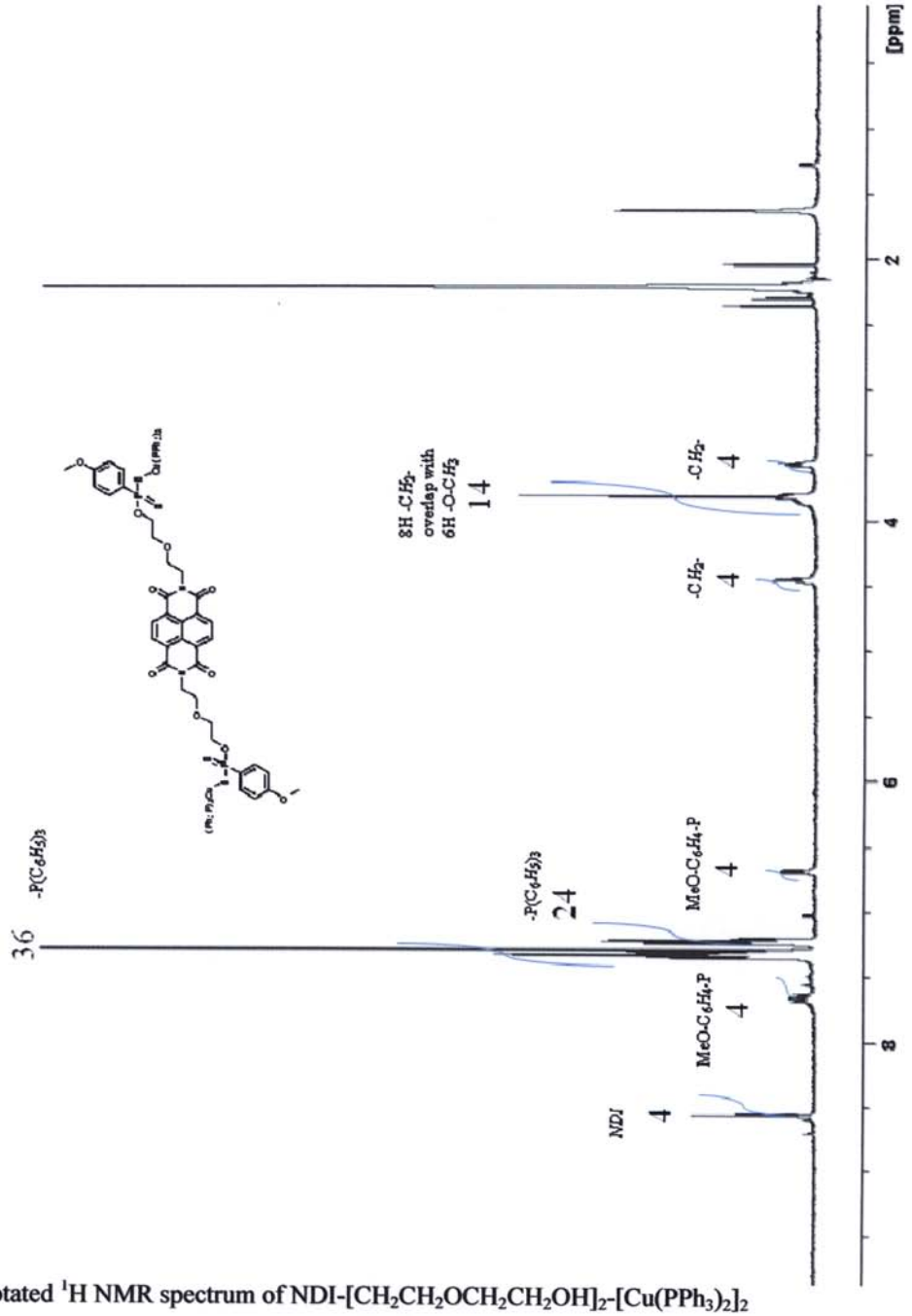

Figure A10: Annotated ^{1}H NMR spectrum of NDI-$[CH_2CH_2OCH_2CH_2OH]_2$-$[Cu(PPh_3)_2]_2$

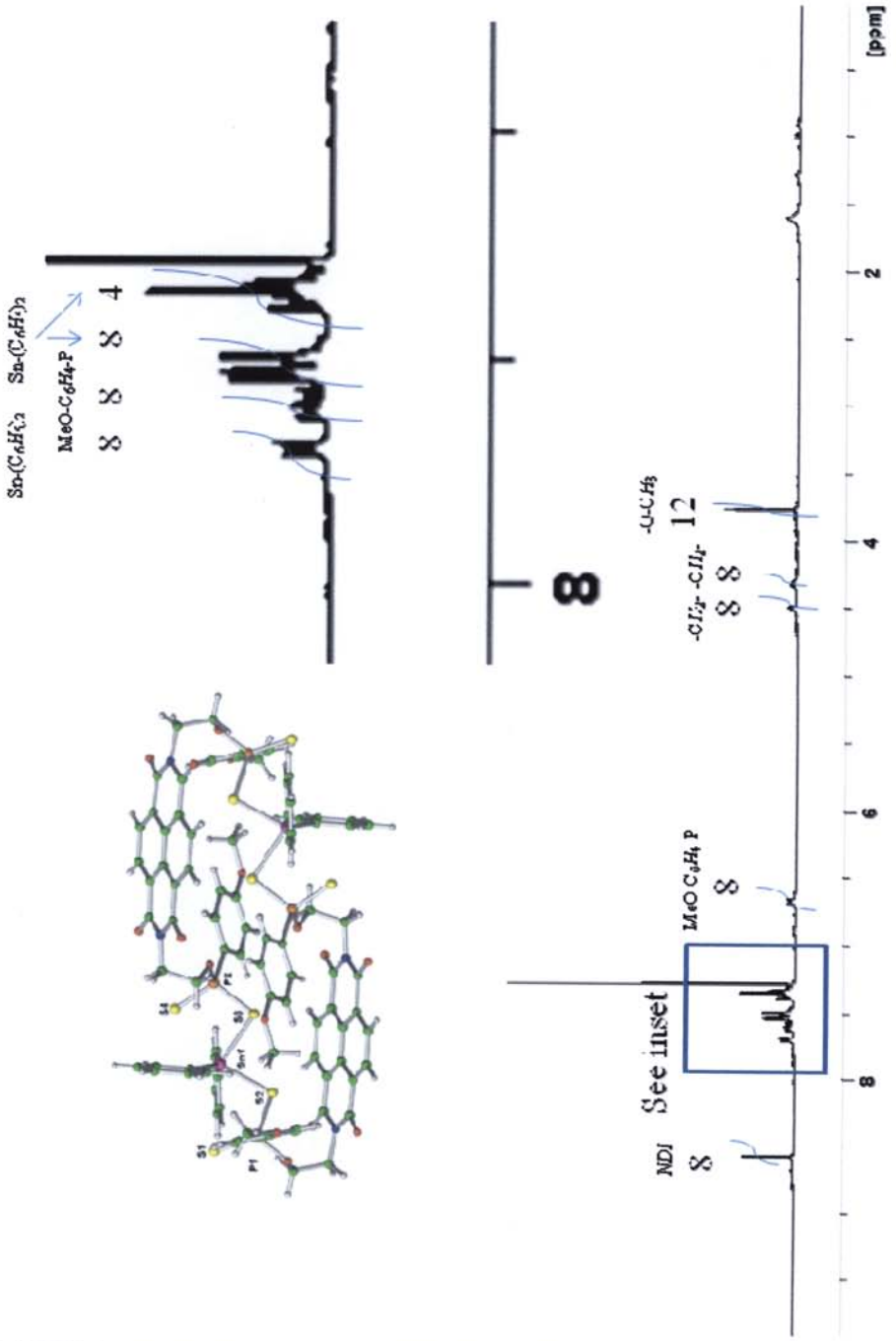

Figure A11: Annotated 'H NMR spectrum of NDI-$[CH_2CH_2O(An)PS_2]_2$-$[SnPh_2]_2$

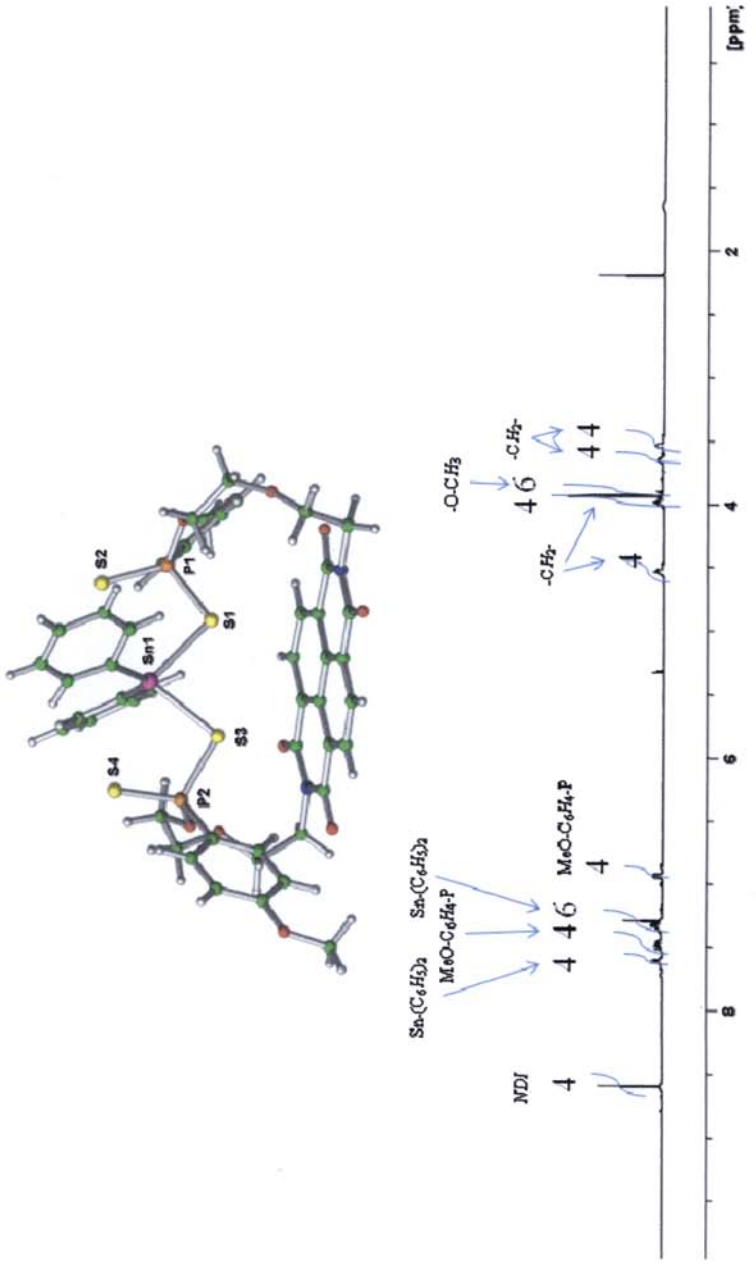

Figure A12: Annotated ^{1}H NMR spectrum of NDI- $[CH_2CH_2OCH_2CH_2OH]$-$[SnPh_2]$

Appendix 2: Crystallographic Data

Table A1: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.45548 (12)	0.34884 (8)	0.37897 (7)	0.0380 (3)	
Cl1A	0.092 (2)	0.010 (4)	0.943 (2)	0.31 (4)*	0.25
Cl1B	0.192 (2)	-0.0984 (8)	1.0103 (10)	0.049 (4)*	0.25
Cl1C	0.241 (3)	-0.1003 (9)	1.0095 (15)	0.086 (8)*	0.25
Cl1D	0.3991 (13)	-0.0125 (13)	0.9984 (11)	0.058 (4)*	0.25
Cl2A	0.3953 (17)	0.053 (4)	0.975 (3)	0.27 (3)*	0.25
Cl2B	0.2336 (19)	0.1254 (9)	0.9116 (9)	0.046 (4)*	0.25
Cl2C	0.1882 (14)	0.1166 (8)	0.9069 (6)	0.019 (3)*	0.25
Cl2D	0.140 (2)	0.081 (3)	0.9106 (12)	0.127 (11)*	0.25
S1	0.6406 (5)	0.2951 (4)	0.1490 (3)	0.0564 (12)	
S2	0.3414 (4)	0.2151 (3)	0.3268 (2)	0.0399 (9)	
P1	0.4442 (5)	0.2313 (3)	0.1846 (2)	0.0426 (10)	
O1	0.1482 (14)	-0.0341 (10)	0.2234 (8)	0.065 (4)	
O2	0.4544 (12)	-0.0706 (8)	0.4381 (8)	0.055 (3)	
O3	0.4373 (12)	0.1160 (8)	0.1749 (6)	0.046 (3)	
O4	0.0246 (12)	0.4076 (9)	-0.0699 (8)	0.057 (3)	
N1	0.2994 (19)	-0.0471 (9)	0.3307 (9)	0.059 (4)	
C1	0.159 (2)	-0.0300 (12)	0.3003 (11)	0.056 (5)	
C2	0.0401 (18)	-0.0078 (11)	0.3736 (11)	0.044 (4)	
C3	-0.099 (2)	0.0161 (12)	0.3494 (11)	0.053 (5)	
H3	-0.1125	0.0190	0.2863	0.064*	
C4	0.0590 (19)	-0.0090 (11)	0.4660 (10)	0.047 (4)	
C5	0.2036 (17)	-0.0294 (10)	0.4915 (11)	0.042 (4)	
C6	0.2180 (18)	-0.0354 (11)	0.5840 (11)	0.045 (4)	
H6	0.3115	-0.0533	0.6021	0.054*	
C7	0.328 (2)	-0.0524 (11)	0.4208 (12)	0.050 (5)	
C8	0.424 (2)	-0.0623 (13)	0.2589 (14)	0.069 (6)	
H8A	0.3876	-0.0798	0.2057	0.083*	
H8B	0.4846	-0.1207	0.2868	0.083*	
C9	0.5186 (19)	0.0326 (13)	0.2219 (12)	0.058 (5)	
H9A	0.5522	0.0515	0.2756	0.069*	
H9B	0.6080	0.0193	0.1765	0.069*	
C10	0.3173 (16)	0.2889 (12)	0.1107 (10)	0.044 (4)	
C11	0.3595 (17)	0.3751 (13)	0.0359 (10)	0.047 (4)	
H11	0.4550	0.4055	0.0271	0.056*	
C12	0.2652 (17)	0.4173 (12)	-0.0259 (9)	0.044 (4)	
H12	0.2964	0.4759	-0.0770	0.053*	

C13	0.1249 (16)	0.3740 (12)	-0.0131 (10)	0.042 (4)	
C14	0.078 (2)	0.2883 (14)	0.0622 (13)	0.063 (5)	
H14	-0.0173	0.2580	0.0714	0.076*	
C15	0.1768 (19)	0.2480 (13)	0.1239 (11)	0.054 (5)	
H15	0.1454	0.1909	0.1764	0.064*	
C16	0.0695 (19)	0.4922 (13)	-0.1487 (11)	0.053 (5)	
H16A	0.0870	0.5527	-0.1257	0.079*	
H16B	-0.0090	0.5074	-0.1867	0.079*	
H16C	0.1616	0.4751	-0.1884	0.079*	
C17	0.4338 (18)	0.4982 (12)	0.2824 (10)	0.048 (4)	
C18	0.5273 (16)	0.5755 (11)	0.2824 (9)	0.038 (4)	
H18	0.5990	0.5639	0.3225	0.046*	
C19	0.5138 (19)	0.6735 (13)	0.2207 (12)	0.054 (5)	
H19	0.5790	0.7284	0.2178	0.065*	
C20	0.4071 (18)	0.6896 (12)	0.1652 (11)	0.048 (4)	
H20	0.3971	0.7561	0.1253	0.057*	
C21	0.3148 (18)	0.6109 (13)	0.1665 (12)	0.055 (5)	
H21	0.2404	0.6229	0.1283	0.066*	
C22	0.3308 (18)	0.5117 (12)	0.2249 (10)	0.045 (4)	
H22	0.2710	0.4554	0.2243	0.054*	
C23	0.2990 (17)	0.3396 (10)	0.5126 (9)	0.039 (4)	
C24	0.2143 (17)	0.4272 (12)	0.5235 (11)	0.046 (4)	
H24	0.2283	0.4890	0.4742	0.055*	
C25	0.1104 (18)	0.4231 (11)	0.6067 (10)	0.042 (4)	
H25	0.0532	0.4819	0.6156	0.050*	
C26	0.0920 (18)	0.3333 (13)	0.6753 (10)	0.048 (4)	
H26	0.0199	0.3301	0.7321	0.057*	
C27	0.1752 (17)	0.2449 (12)	0.6655 (10)	0.046 (4)	
H27	0.1612	0.1835	0.7152	0.055*	
C28	0.2776 (16)	0.2488 (12)	0.5825 (9)	0.041 (4)	
H28	0.3331	0.1893	0.5735	0.049*	
C29	0.6712 (19)	0.3145 (11)	0.4147 (10)	0.047 (4)	
C30	0.6798 (17)	0.3077 (9)	0.5083 (10)	0.038 (4)	
H30	0.5926	0.3170	0.5524	0.045*	
C31	0.8146 (17)	0.2873 (11)	0.5392 (11)	0.045 (4)	
H31	0.8185	0.2807	0.6045	0.055*	
C32	0.9413 (17)	0.2770 (11)	0.4755 (11)	0.045 (4)	
H32	1.0344	0.2661	0.4956	0.054*	
C33	0.9328 (18)	0.2825 (11)	0.3817 (12)	0.048 (4)	
H33	1.0194	0.2722	0.3375	0.058*	
C34	0.7973 (16)	0.3030 (11)	0.3524 (11)	0.041 (4)	
H34	0.7929	0.3092	0.2873	0.049*	
C36	0.2028 (16)	0.0311 (8)	1.0241 (19)	0.073 (11)*	0.50

Table A2: Atomic displacement parameters ($Å^2$) for NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0382 (5)	0.0372 (5)	0.0368 (5)	-0.0018 (4)	-0.0069 (4)	-0.0057 (4)
S1	0.060 (3)	0.068 (3)	0.041 (2)	-0.010 (2)	-0.0024 (18)	-0.0166 (19)
S2	0.053 (2)	0.0355 (18)	0.0281 (16)	-0.0082 (17)	0.0043 (15)	-0.0096 (14)
P1	0.053 (2)	0.048 (2)	0.0277 (16)	-0.0022 (19)	-0.0006 (16)	-0.0154 (16)
O1	0.072 (8)	0.075 (8)	0.045 (6)	-0.008 (7)	-0.009 (6)	-0.008 (6)
O2	0.043 (7)	0.050 (6)	0.066 (7)	0.008 (5)	-0.011 (5)	-0.003 (5)
O3	0.053 (6)	0.054 (6)	0.037 (5)	0.013 (5)	-0.009 (4)	-0.026 (4)
O4	0.053 (7)	0.060 (7)	0.057 (6)	0.011 (6)	-0.021 (5)	-0.004 (5)
N1	0.102 (12)	0.034 (7)	0.042 (7)	0.011 (7)	-0.011 (7)	-0.014 (6)
C1	0.095 (14)	0.030 (8)	0.043 (9)	-0.016 (9)	-0.018 (9)	-0.006 (7)
C2	0.050 (9)	0.030 (7)	0.050 (8)	-0.008 (7)	-0.008 (7)	-0.008 (7)
C3	0.077 (12)	0.039 (8)	0.041 (8)	-0.005 (9)	-0.016 (8)	0.000 (7)
C4	0.068 (11)	0.026 (7)	0.038 (8)	-0.018 (7)	0.008 (7)	-0.002 (6)
C5	0.041 (9)	0.021 (6)	0.059 (9)	-0.004 (6)	-0.011 (7)	-0.001 (6)
C6	0.042 (9)	0.038 (8)	0.053 (9)	-0.009 (7)	-0.016 (7)	0.002 (7)
C7	0.059 (11)	0.023 (7)	0.056 (9)	0.008 (7)	0.005 (8)	0.001 (7)
C8	0.090 (15)	0.046 (10)	0.067 (11)	0.007 (10)	-0.014 (10)	-0.010 (9)
C9	0.050 (10)	0.070 (11)	0.053 (9)	0.030 (9)	-0.009 (8)	-0.023 (8)
C10	0.035 (8)	0.048 (8)	0.046 (8)	-0.015 (7)	0.014 (6)	-0.018 (7)
C11	0.030 (8)	0.072 (11)	0.037 (7)	-0.008 (8)	-0.009 (6)	-0.005 (7)
C12	0.044 (9)	0.059 (9)	0.027 (7)	-0.004 (8)	0.006 (6)	-0.013 (7)
C13	0.026 (8)	0.050 (9)	0.045 (8)	-0.002 (7)	-0.004 (6)	-0.005 (7)
C14	0.053 (11)	0.059 (11)	0.074 (11)	0.000 (9)	-0.025 (9)	-0.001 (9)
C15	0.060 (11)	0.049 (9)	0.045 (9)	-0.007 (9)	-0.002 (8)	-0.003 (8)
C16	0.050 (10)	0.067 (11)	0.044 (8)	0.010 (9)	-0.012 (7)	-0.016 (8)
C17	0.056 (10)	0.045 (9)	0.031 (7)	-0.010 (8)	0.000 (7)	0.009 (7)
C18	0.034 (8)	0.050 (8)	0.037 (7)	0.003 (7)	-0.016 (6)	-0.018 (6)
C19	0.050 (10)	0.046 (9)	0.059 (10)	-0.017 (8)	0.003 (8)	-0.006 (8)
C20	0.045 (9)	0.035 (8)	0.055 (9)	0.007 (7)	-0.009 (7)	0.003 (7)
C21	0.043 (9)	0.060 (10)	0.056 (9)	0.001 (9)	-0.025 (7)	0.008 (8)
C22	0.049 (10)	0.042 (8)	0.048 (8)	-0.003 (7)	-0.002 (7)	-0.022 (7)
C23	0.058 (9)	0.025 (6)	0.023 (6)	-0.008 (7)	0.018 (6)	-0.005 (5)
C24	0.045 (9)	0.048 (9)	0.045 (8)	0.003 (8)	-0.008 (7)	-0.012 (7)
C25	0.056 (10)	0.038 (7)	0.041 (7)	0.000 (7)	-0.012 (7)	-0.024 (6)
C26	0.051 (10)	0.072 (10)	0.025 (6)	-0.002 (8)	-0.002 (6)	-0.023 (7)
C27	0.044 (9)	0.051 (9)	0.038 (8)	0.001 (8)	-0.008 (7)	-0.005 (7)
C28	0.043 (8)	0.052 (8)	0.038 (7)	-0.010 (7)	-0.015 (6)	-0.024 (6)
C29	0.065 (11)	0.029 (7)	0.038 (8)	-0.012 (7)	0.001 (7)	0.003 (6)
C30	0.053 (9)	0.016 (6)	0.042 (7)	-0.013 (6)	-0.004 (7)	-0.005 (6)
C31	0.048 (9)	0.035 (8)	0.056 (9)	-0.011 (7)	-0.031 (7)	0.003 (7)

C32	0.034 (8)	0.039 (8)	0.062 (9)	-0.007 (7)	-0.017 (7)	-0.006 (7)
C33	0.039 (9)	0.033 (8)	0.066 (10)	-0.007 (7)	0.004 (7)	-0.010 (7)
C34	0.039 (8)	0.036 (8)	0.044 (8)	-0.008 (7)	-0.014 (7)	0.001 (6)

Table A3: Geometric parameters (Å, °) for NDI-$[CH_2CH_2O(An)PS_2(SnPh_3)_2]_2$

Sn1—C29	2.145 (18)	C11—C12	1.38 (2)
Sn1—C23	2.172 (12)	C11—H11	0.9500
Sn1—C17	2.175 (14)	C12—C13	1.39 (2)
Sn1—S2	2.450 (4)	C12—H12	0.9500
Cl1A—C36	1.79 (2)	C13—C14	1.40 (2)
Cl1A—Cl1A^{i}	2.11 (5)	C14—C15	1.40 (2)
Cl1B—C36	1.799 (19)	C14—H14	0.9500
Cl1C—C36	1.83 (2)	C15—H15	0.9500
Cl1D—C36	1.862 (18)	C16—H16A	0.9800
Cl1D—Cl1D^{ii}	1.90 (3)	C16—H16B	0.9800
Cl2A—C36	1.77 (2)	C16—H16C	0.9800
Cl2B—C36	1.80 (2)	C17—C22	1.36 (2)
Cl2C—C36	1.85 (2)	C17—C18	1.37 (2)
Cl2D—C36	1.83 (2)	C18—C19	1.42 (2)
S1—P1	1.938 (6)	C18—H18	0.9500
S2—P1	2.080 (5)	C19—C20	1.37 (2)
P1—O3	1.587 (11)	C19—H19	0.9500
P1—C10	1.773 (17)	C20—C21	1.37 (2)
O1—C1	1.171 (19)	C20—H20	0.9500
O2—C7	1.24 (2)	C21—C22	1.41 (2)
O3—C9	1.426 (18)	C21—H21	0.9500
O4—C13	1.352 (18)	C22—H22	0.9500
O4—C16	1.413 (18)	C23—C28	1.376 (18)
N1—C7	1.38 (2)	C23—C24	1.40 (2)
N1—C1	1.43 (2)	C24—C25	1.39 (2)
N1—C8	1.44 (2)	C24—H24	0.9500
C1—C2	1.45 (2)	C25—C26	1.36 (2)
C3—H3	0.9500	C25—H25	0.9500
C2—C3	1.40 (2)	C26—C27	1.40 (2)
C2—C4	1.40 (2)	C26—H26	0.9500
C3—C6^{iii}	1.37 (2)	C27—C28	1.38 (2)
C4—C4^{iii}	1.38 (3)	C27—H27	0.9500
C4—C5	1.44 (2)	C28—H28	0.9500
C5—C6	1.37 (2)	C29—C34	1.35 (2)
C5—C7	1.46 (2)	C29—C30	1.38 (2)
C6—H6	0.9500	C30—C31	1.39 (2)
C6—C3^{iii}	1.37 (2)	C30—H30	0.9500

C8—C9	1.49 (2)	C31—C32	1.37 (2)
C8—H8A	0.9900	C32—H32	0.9500
C8—H8B	0.9900	C31—H31	0.9500
C9—H9A	0.9900	C32—C33	1.38 (2)
C9—H9B	0.9900	C33—C34	1.39 (2)
C10—C15	1.37 (2)	C33—H33	0.9500
C10—C11	1.39 (2)	C34—H34	0.9500
C29—Sn1—C23	106.7 (6)	Cl2A—C36—Cl2B	68.0 (18)
C29—Sn1—C17	116.2 (6)	Cl1A—C36—Cl2B	66.2 (18)
C23—Sn1—C17	108.9 (5)	Cl2A—C36—Cl1B	98 (2)
C29—Sn1—S2	116.0 (4)	Cl1A—C36—Cl1B	62.5 (19)
C23—Sn1—S2	97.8 (4)	Cl2B—C36—Cl1B	112.5 (16)
C17—Sn1—S2	109.4 (5)	Cl2A—C36—Cl2D	95.5 (19)
C36—Cl1A—Cl1A^{i}	87.1 (17)	Cl1B—C36—Cl2D	89.9 (17)
C36—Cl1D—Cl1D^{ii}	145.7 (17)	Cl2A—C36—Cl1C	85 (2)
P1—S2—Sn1	105.14 (18)	Cl1A—C36—Cl1C	73 (2)
O3—P1—C10	99.5 (7)	Cl2B—C36—Cl1C	112.2 (17)
O3—P1—S1	115.8 (5)	Cl2D—C36—Cl1C	96.4 (18)
C10—P1—S1	114.7 (5)	Cl2A—C36—Cl2C	81.0 (18)
O3—P1—S2	101.1 (4)	Cl1A—C36—Cl2C	52.9 (17)
C10—P1—S2	108.9 (5)	Cl1C—C36—Cl2C	108.8 (16)
S1—P1—S2	115.2 (3)	Cl1B—C36—Cl1D	74.0 (11)
C9—O3—P1	124.4 (11)	Cl2D—C36—Cl1D	108.8 (16)
C13—O4—C16	116.4 (12)	Cl1C—C36—Cl1D	60.3 (11)
C7—N1—C1	127.6 (15)	Cl2C—C36—Cl1D	100.6 (13)
C7—N1—C8	116.9 (16)	C6^{iii}—C3—H3	120.0
C1—N1—C8	115.6 (15)	C2—C3—H3	120.0
O1—C1—N1	121.0 (17)	C5—C6—H6	119.0
O1—C1—C2	126.0 (18)	C3^{iii}—C6—H6	120.0
N1—C1—C2	113.0 (14)	N1—C8—H8A	110.0
C3—C2—C4	119.2 (15)	C9—C8—H8A	109.0
C3—C2—C1	117.6 (15)	N1—C8—H8B	110.0
C4—C2—C1	123.2 (15)	C9—C8—H8B	109.0
C6^{iii}—C3—C2	120.5 (15)	H8A—C8—H8B	108.0
C4^{iii}—C4—C2	121 (2)	O3—C9—H9A	109.0
C4^{iii}—C4—C5	118.8 (19)	C8—C9—H9A	109.0
C2—C4—C5	120.2 (14)	O3—C9—H9B	110.0
C6—C5—C4	119.2 (14)	C8—C9—H9B	110.0
C6—C5—C7	121.7 (15)	H9A—C9—H9B	108.0
C4—C5—C7	118.9 (15)	C12—C11—H11	119.0
C3^{iii}—C6—C5	121.1 (15)	C10—C11—H11	119.0
O2—C7—N1	120.9 (15)	C11—C12—H12	120.0
O2—C7—C5	122.2 (16)	C13—C12—H12	120.0

N1—C7—C5	116.8 (16)	C13—C14—H14	121.0
N1—C8—C9	110.4 (15)	C15—C14—H14	121.0
O3—C9—C8	110.6 (15)	C10—C15—H15	120.0
C15—C10—C11	118.4 (15)	C14—C15—H15	120.0
C15—C10—P1	121.1 (12)	O4—C16—H16A	109.0
C11—C10—P1	120.5 (12)	O4—C16—H16B	109.9
C12—C11—C10	121.3 (14)	H16A—C16—H16B	109.0
C11—C12—C13	119.8 (14)	O4—C16—H16C	109.0
O4—C13—C12	125.0 (13)	H16A—C16—H16C	110.0
O4—C13—C14	114.7 (14)	H16B—C16—H16C	109.0
C12—C13—C14	120.3 (15)	C17—C18—H18	121.0
C13—C14—C15	118.2 (16)	C19—C18—H18	121.0
C10—C15—C14	121.9 (15)	C20—C19—H19	120.0
C22—C17—C18	122.7 (14)	C18—C19—H19	120.0
C22—C17—Sn1	120.3 (12)	C21—C20—H20	120.0
C18—C17—Sn1	117.1 (11)	C19—C20—H20	120.0
C17—C18—C19	117.9 (14)	C20—C21—H21	120.0
C20—C19—C18	120.2 (15)	C22—C21—H21	120.0
C21—C20—C19	120.8 (14)	C17—C22—H22	120.0
C20—C21—C22	119.6 (15)	C21—C22—H22	120.0
C17—C22—C21	118.8 (15)	C24—C25—H25	121.0
C28—C23—C24	120.9 (12)	C25—C26—H26	119.0
C28—C23—Sn1	120.9 (10)	C27—C26—H26	119.0
C24—C23—Sn1	118.1 (9)	C28—C27—H27	121.0
C25—C24—C23	119.6 (13)	C26—C27—H27	121
C26—C25—C24	118.7 (14)	C27—C28—H28	119.0
C25—C26—C27	122.5 (13)	C23—C28—H28	120.0
C28—C27—C26	118.8 (14)	C29—C30—H30	119.0
C23—C28—C27	119.5 (14)	C31—C30—H30	120.0
C34—C29—C30	118.7 (16)	C32—C31—H31	120.0
C34—C29—Sn1	125.4 (12)	C30—C31—H31	120.0
C30—C29—Sn1	115.9 (11)	C31—C32—H32	120.0
C29—C30—C31	120.8 (15)	C33—C32—H32	120.0
C32—C31—C30	119.9 (15)	C32—C33—H33	120.0
C31—C32—C33	119.4 (15)	C34—C33—H33	120.0
C32—C33—C34	119.6 (14)	C29—C34—H34	119.0
C29—C34—C33	121.4 (15)	C33—C34—H34	119.0
Cl2A—C36—Cl1A	115 (2)		
C23—Sn1—S1—P1	15.4 (12)	S1—Sn1—C17—C18	-104.2 (12)
C17—Sn1—S1—P1	-104.0 (5)	C22—C17—C18—C19	1 (2)
C29—Sn1—S1—P1	137.8 (4)	C17—C18—C19—C20	4 (2)
Sn1—S1—P1—O3	-133.7 (4)	C18—C19—C20—C21	-1 (3)
Sn1—S1—P1—C10	111.3 (6)	C19—C20—C21—C22	-3 (3)

Sn1—S1—P1—S2	-16.3 (2)	C18—C17—C22—C21	-3 (2)
C10—P1—O3—C9	-180.0 (12)	C20—C21—C22—C17	3 (2)
S2—P1—O3—C9	-67.7 (11)	C17—Sn1—C23—C24	-3.9 (14)
S1—P1—O3—C9	57.4 (12)	C29—Sn1—C23—C24	122.3 (12)
$C5^{iv}$—C1—C2—C3	0.7 (17)	S1—Sn1—C23—C24	-118.8 (13)
C1—C2—C3—$C3^{iv}$	-1.1 (15)	C29—Sn1—C23—C28	-61.2 (13)
$C3^{iv}$—C3—C4—C5	3 (3)	S1—Sn1—C23—C28	58 (2)
C2—C3—C4—C5	4 (2)	C28—C23—C24—C25	2 (2)
C3—C4—C5—$C1^{iv}$	-2 (2)	Sn1—C23—C24—C25	178.2 (12)
C5—C4—C6—O2	-3 (3)	C23—C24—C25—C26	0 (2)
C1—C2—C7—O1	-0.8 (8)	C24—C25—C26—C27	3 (2)
P1—O3—C9—C8	139.3 (13)	C25—C26—C27—C28	-3 (2)
O3—P1—C10—C11	-126.1 (13)	C24—C23—C28—C27	-2 (2)
S2—P1—C10—C11	128.7 (12)	Sn1—C23—C28—C27	-179.5 (11)
S1—P1—C10—C11	-2.0 (15)	C26—C27—C28—C23	1 (2)
O3—P1—C10—C15	51.9 (14)	C23—Sn1—C29—C30	-8.8 (12)
S2—P1—C10—C15	-53.3 (15)	C17—Sn1—C29—C30	112.9 (11)
C15—C10—C11—C12	-2 (2)	S1—Sn1—C29—C30	-172.1 (11)
C10—C11—C12—C13	1 (2)	C23—Sn1—C29—C34	173.7 (13)
C16—O4—C13—C12	-1 (2)	C17—Sn1—C29—C34	-64.6 (15)
C11—C12—C13—C14	1 (3)	S1—Sn1—C29—C34	10.4 (13)
C12—C13—C14—C15	-1 (3)	C34—C29—C30—C31	1 (3)
C13—C14—C15—C10	-2 (3)	Sn1—C29—C30—C31	-179.0 (11)
C11—C10—C15—C14	2 (3)	C29—C30—C31—C32	0 (3)
C23—Sn1—C17—C22	-86.9 (13)	C30—C31—C32—C33	-1 (3)
C29—Sn1—C17—C22	152.6 (12)	C31—C32—C33—C34	1 (3)
S1—Sn1—C17—C22	75.6 (12)	C32—C33—C34—C29	0 (2)
C23—Sn1—C17—C18	93.3 (12)	C30—C29—C34—C33	-1 (2)
C29—Sn1—C17—C18	-27.2 (14)	Sn1—C29—C34—C33	178.9 (11)
Symmetry codes: (i) *-x, -y, -z+2*; (ii) *-x+1, -y, -z+2*; (iii) *-x, -y, -z+1*; (iv) *-x, -y, -z*.			

Table A4: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for NDI-[CH_2CH_2O(An)PS_2(Cu(PPh_3)$_2$]$_2$

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.01745 (5)	0.81093 (4)	0.294382 (18)	0.01873 (12)
Cl1	0.32008 (11)	0.19499 (9)	0.17802 (4)	0.0442 (2)
Cl2	0.15977 (12)	0.15583 (8)	0.07839 (4)	0.0435 (2)
S1	0.25447 (8)	0.83414 (7)	0.26042 (3)	0.02095 (17)
S2	0.02714 (9)	0.67745 (7)	0.21236 (3)	0.02293 (17)
P1	0.03117 (8)	0.67577 (6)	0.37160 (3)	0.01646 (16)
P2	-0.16884 (8)	0.98220 (7)	0.27892 (3)	0.01635 (16)
P5	0.20183 (9)	0.74649 (7)	0.19684 (3)	0.01961 (17)

O1	0.0425 (2)	0.6571 (2)	0.02193 (10)	0.0283 (5)
O2	0.4030 (2)	0.85799 (18)	0.04049 (9)	0.0233 (5)
O3	0.1720 (3)	0.8410 (2)	0.14062 (9)	0.0264 (5)
O4	0.7567 (3)	0.3922 (2)	0.13217 (11)	0.0345 (6)
N1	0.2229 (3)	0.7577 (2)	0.02971 (10)	0.0193 (5)
C1	0.1754 (3)	0.6544 (3)	0.02053 (13)	0.0220 (7)
C2	0.2926 (3)	0.5463 (3)	0.00924 (12)	0.0196 (6)
C3	0.4444 (3)	0.5510 (3)	0.00625 (12)	0.0179 (6)
C4	0.4865 (3)	0.6582 (3)	0.01570 (12)	0.0187 (6)
C5	0.3721 (3)	0.7654 (3)	0.03008 (12)	0.0197 (6)
C6	0.6349 (3)	0.6614 (3)	0.01156 (13)	0.0220 (7)
H6	0.6626	0.7335	0.0174	0.026*
C7	0.2548 (3)	0.4404 (3)	0.00116 (13)	0.0232 (7)
H7	0.1531	0.4367	0.0043	0.028*
C8	0.1051 (3)	0.8655 (3)	0.04121 (13)	0.0226 (7)
H8A	0.0208	0.8757	0.0137	0.027*
H8B	0.1461	0.9370	0.0351	0.027*
C9	0.0473 (3)	0.8582 (3)	0.10132 (13)	0.0239 (7)
H9A	-0.0289	0.9331	0.1079	0.029*
H9B	-0.0002	0.7901	0.1073	0.029*
C10	0.3690 (4)	0.6352 (3)	0.17940 (13)	0.0234 (7)
C11	0.5071 (4)	0.6613 (3)	0.18411 (15)	0.0291 (7)
H11	0.5110	0.7356	0.1979	0.035*
C12	0.6400 (4)	0.5828 (3)	0.16932 (15)	0.0292 (7)
H12	0.7333	0.6028	0.1730	0.035*
C13	0.6339 (4)	0.4748 (3)	0.14910 (13)	0.0260 (7)
C14	0.4974 (4)	0.4445 (3)	0.14549 (14)	0.0266 (7)
H14	0.4946	0.3689	0.1330	0.032*
C15	0.3655 (4)	0.5242 (3)	0.16011 (13)	0.0246 (7)
H15	0.2725	0.5035	0.1570	0.030*
C16	0.8991 (4)	0.4221 (4)	0.13472 (17)	0.0402 (9)
H16A	0.8948	0.4963	0.1103	0.060*
H16B	0.9781	0.3566	0.1212	0.060*
H16C	0.9215	0.4339	0.1744	0.060*
C17	0.2487 (3)	0.4910 (3)	0.32702 (14)	0.0242 (7)
H17	0.2174	0.5335	0.2908	0.029*
C18	0.3596 (3)	0.3841 (3)	0.32957 (15)	0.0275 (7)
H18	0.4023	0.3534	0.2951	0.033*
C19	0.4089 (4)	0.3216 (3)	0.38199 (16)	0.0312 (8)
H19	0.4850	0.2485	0.3835	0.037*
C20	0.3466 (4)	0.3663 (3)	0.43176 (16)	0.0313 (8)
H20	0.3806	0.3242	0.4678	0.038*
C21	0.2334 (3)	0.4734 (3)	0.42951 (14)	0.0249 (7)

H21	0.1909	0.5034	0.4641	0.030*
C22	0.1823 (3)	0.5368 (3)	0.37690 (13)	0.0181 (6)
C23	0.0490 (3)	0.7350 (3)	0.44087 (12)	0.0204 (6)
C24	0.1755 (4)	0.7758 (3)	0.45059 (15)	0.0302 (8)
H24	0.2495	0.7724	0.4218	0.036*
C25	0.1941 (4)	0.8216 (3)	0.50231 (15)	0.0381 (9)
H25	0.2816	0.8483	0.5089	0.046*
C26	0.0866 (5)	0.8287 (3)	0.54435 (15)	0.0378 (9)
H26	0.1009	0.8594	0.5797	0.045*
C27	-0.0424 (4)	0.7909 (3)	0.53472 (14)	0.0303 (8)
H27	-0.1179	0.7976	0.5630	0.036*
C28	-0.0600 (4)	0.7432 (3)	0.48308 (13)	0.0221 (7)
H28	-0.1472	0.7159	0.4766	0.027*
C29	-0.1394 (3)	0.6223 (3)	0.37796 (13)	0.0180 (6)
C30	-0.1541 (4)	0.5267 (3)	0.41640 (13)	0.0243 (7)
H30	-0.0698	0.4812	0.4386	0.029*
C31	-0.2908 (4)	0.4981 (3)	0.42230 (14)	0.0283 (7)
H31	-0.3002	0.4331	0.4486	0.034*
C32	-0.4147 (4)	0.5641 (3)	0.38986 (15)	0.0287 (7)
H32	-0.5094	0.5461	0.3950	0.034*
C33	-0.4000 (4)	0.6549 (3)	0.35044 (15)	0.0278 (7)
H33	-0.4838	0.6986	0.3274	0.033*
C34	-0.2635 (3)	0.6830 (3)	0.34417 (13)	0.0223 (7)
H34	-0.2539	0.7452	0.3162	0.027*
C35	-0.3269 (3)	0.9886 (2)	0.32740 (12)	0.0176 (6)
C36	-0.2917 (4)	0.9665 (3)	0.38582 (13)	0.0219 (6)
H36	-0.1902	0.9517	0.3983	0.026*
C37	-0.4033 (4)	0.9659 (3)	0.42586 (13)	0.0246 (7)
H37	-0.3786	0.9526	0.4656	0.030*
C38	-0.5512 (4)	0.9848 (3)	0.40773 (14)	0.0266 (7)
H38	-0.6277	0.9833	0.4350	0.032*
C39	-0.5865 (4)	1.0055 (3)	0.35060 (15)	0.0284 (7)
H39	-0.6881	1.0188	0.3384	0.034*
C40	-0.4755 (3)	1.0075 (3)	0.30976 (14)	0.0234 (7)
H40	-0.5015	1.0217	0.2701	0.028*
C41	-0.2498 (3)	1.0028 (3)	0.20649 (12)	0.0182 (6)
C42	-0.3037 (3)	0.9098 (3)	0.18707 (13)	0.0222 (7)
H42	-0.3023	0.8403	0.2122	0.027*
C43	-0.3590 (4)	0.9180 (3)	0.13155 (14)	0.0267 (7)
H43	-0.3972	0.8550	0.1191	0.032*
C44	-0.3589 (4)	1.0172 (3)	0.09424 (13)	0.0270 (7)
H44	-0.3961	1.0223	0.0561	0.032*
C45	-0.3041 (4)	1.1097 (3)	0.11274 (13)	0.0258 (7)

H45	-0.3038	1.1781	0.0872	0.031*
C46	-0.2497 (3)	1.1022 (3)	0.16845 (13)	0.0216 (6)
H46	-0.2121	1.1656	0.1807	0.026*
C47	-0.1283 (3)	1.1273 (3)	0.28721 (12)	0.0202 (6)
C48	-0.2439 (4)	1.2308 (3)	0.29076 (14)	0.0239 (7)
H48	-0.3454	1.2260	0.2902	0.029*
C49	-0.2118 (4)	1.3404 (3)	0.29511 (14)	0.0296 (8)
H49	-0.2910	1.4109	0.2968	0.035*
C50	-0.0641 (4)	1.3471 (3)	0.29702 (15)	0.0335 (8)
H50	-0.0420	1.4221	0.3008	0.040*
C51	0.0501 (4)	1.2462 (3)	0.29353 (17)	0.0360 (9)
H51	0.1514	1.2514	0.2946	0.043*
C52	0.0183 (4)	1.1360 (3)	0.28839 (15)	0.0289 (7)
H52	0.0981	1.0662	0.2857	0.035*
C53	0.2475 (5)	0.0902 (3)	0.14386 (18)	0.0413 (9)
H53A	0.3301	0.0194	0.1369	0.050*
H53B	0.1740	0.0626	0.1691	0.050*

Table A5: Atomic displacement parameters ($Å^2$) for NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0168 (2)	0.0198 (2)	0.0177 (2)	-0.00231 (18)	0.00297 (17)	0.00260 (17)
Cl1	0.0427 (5)	0.0487 (6)	0.0448 (5)	-0.0196 (5)	-0.0099 (4)	0.0014 (4)
Cl2	0.0595 (6)	0.0318 (5)	0.0387 (5)	-0.0103 (4)	-0.0084 (4)	-0.0028 (4)
S1	0.0177 (4)	0.0246 (4)	0.0212 (4)	-0.0057 (3)	0.0025 (3)	-0.0045 (3)
S2	0.0213 (4)	0.0255 (4)	0.0234 (4)	-0.0085 (3)	0.0017 (3)	-0.0018 (3)
P1	0.0149 (4)	0.0174 (4)	0.0161 (4)	-0.0033 (3)	0.0015 (3)	0.0016 (3)
P2	0.0153 (4)	0.0171 (4)	0.0156 (4)	-0.0029 (3)	0.0009 (3)	0.0007 (3)
P5	0.0200 (4)	0.0203 (4)	0.0189 (4)	-0.0059 (3)	0.0023 (3)	-0.0011 (3)
O1	0.0194 (12)	0.0270 (13)	0.0399 (14)	-0.0066 (10)	0.0003 (10)	-0.0084 (10)
O2	0.0257 (12)	0.0197 (11)	0.0256 (12)	-0.0074 (10)	0.0020 (9)	-0.0029 (9)
O3	0.0311 (12)	0.0304 (13)	0.0197 (11)	-0.0132 (10)	-0.0032 (9)	0.0020 (9)
O4	0.0315 (13)	0.0301 (14)	0.0365 (14)	0.0016 (11)	0.0088 (11)	-0.0022 (10)
N1	0.0200 (13)	0.0196 (13)	0.0180 (13)	-0.0047 (11)	0.0026 (10)	-0.0012 (10)
C1	0.0207 (16)	0.0291 (17)	0.0171 (15)	-0.0089 (14)	-0.0001 (12)	0.0001 (12)
C2	0.0201 (15)	0.0233 (16)	0.0159 (15)	-0.0063 (13)	0.0023 (12)	-0.0019 (12)
C3	0.0205 (15)	0.0198 (15)	0.0138 (14)	-0.0061 (12)	0.0000 (11)	0.0002 (11)
C4	0.0214 (15)	0.0210 (16)	0.0139 (14)	-0.0063 (13)	0.0015 (12)	0.0003 (11)
C5	0.0251 (16)	0.0222 (16)	0.0128 (14)	-0.0085 (14)	0.0002 (12)	0.0009 (11)
C6	0.0240 (16)	0.0220 (16)	0.0229 (16)	-0.0109 (14)	0.0013 (13)	-0.0025 (12)
C7	0.0174 (15)	0.0303 (18)	0.0251 (17)	-0.0120 (14)	0.0022 (13)	-0.0021 (13)
C8	0.0213 (16)	0.0199 (16)	0.0238 (16)	-0.0007 (13)	-0.0038 (13)	-0.0001 (12)
C9	0.0190 (16)	0.0256 (17)	0.0240 (17)	-0.0002 (13)	-0.0006 (13)	-0.0009 (13)

C10	0.0245 (16)	0.0234 (17)	0.0219 (16)	-0.0060 (14)	0.0043 (13)	0.0000 (12)
C11	0.0237 (17)	0.0250 (18)	0.040 (2)	-0.0071 (14)	0.0096 (15)	-0.0084 (14)
C12	0.0220 (17)	0.0300 (19)	0.0347 (19)	-0.0043 (15)	0.0060 (14)	-0.0041 (14)
C13	0.0261 (17)	0.0259 (18)	0.0202 (16)	0.0022 (14)	0.0036 (13)	0.0038 (13)
C14	0.0338 (19)	0.0169 (16)	0.0281 (18)	-0.0049 (14)	0.0056 (14)	-0.0017 (13)
C15	0.0266 (17)	0.0239 (17)	0.0241 (16)	-0.0080 (14)	0.0036 (13)	-0.0018 (13)
C16	0.0253 (19)	0.045 (2)	0.043 (2)	0.0051 (17)	0.0051 (16)	-0.0052 (17)
C17	0.0191 (16)	0.0244 (17)	0.0268 (17)	-0.0012 (14)	-0.0024 (13)	-0.0018 (13)
C18	0.0192 (16)	0.0264 (18)	0.0360 (19)	-0.0026 (14)	0.0024 (14)	-0.0085 (14)
C19	0.0197 (16)	0.0191 (17)	0.052 (2)	-0.0016 (14)	0.0012 (15)	0.0038 (15)
C20	0.0210 (17)	0.0305 (19)	0.037 (2)	-0.0023 (15)	0.0008 (15)	0.0142 (15)
C21	0.0163 (15)	0.0285 (18)	0.0274 (17)	-0.0041 (14)	0.0053 (13)	0.0062 (13)
C22	0.0127 (14)	0.0156 (15)	0.0253 (16)	-0.0041 (12)	0.0030 (12)	0.0029 (12)
C23	0.0273 (17)	0.0175 (15)	0.0151 (15)	-0.0042 (13)	-0.0009 (12)	0.0016 (11)
C24	0.0337 (19)	0.0342 (19)	0.0255 (18)	-0.0158 (16)	0.0029 (14)	0.0029 (14)
C25	0.048 (2)	0.048 (2)	0.0294 (19)	-0.0317 (19)	-0.0046 (17)	0.0002 (16)
C26	0.063 (3)	0.035 (2)	0.0213 (18)	-0.0227 (19)	-0.0038 (17)	-0.0005 (14)
C27	0.041 (2)	0.0266 (18)	0.0210 (17)	-0.0045 (16)	0.0051 (15)	-0.0010 (13)
C28	0.0224 (16)	0.0206 (16)	0.0216 (16)	-0.0031 (13)	0.0013 (13)	0.0016 (12)
C29	0.0172 (15)	0.0178 (15)	0.0185 (15)	-0.0023 (12)	0.0035 (12)	-0.0045 (11)
C30	0.0210 (16)	0.0297 (18)	0.0218 (16)	-0.0073 (14)	-0.0039 (13)	0.0030 (13)
C31	0.0287 (18)	0.0318 (19)	0.0265 (17)	-0.0142 (15)	0.0009 (14)	0.0046 (14)
C32	0.0193 (16)	0.0335 (19)	0.0361 (19)	-0.0106 (15)	0.0023 (14)	-0.0068 (15)
C33	0.0199 (16)	0.0206 (17)	0.040 (2)	0.0007 (14)	-0.0074 (14)	-0.0028 (14)
C34	0.0217 (16)	0.0183 (16)	0.0256 (17)	-0.0039 (13)	-0.0013 (13)	0.0011 (12)
C35	0.0198 (15)	0.0120 (14)	0.0190 (15)	-0.0006 (12)	0.0039 (12)	-0.0001 (11)
C36	0.0223 (16)	0.0216 (16)	0.0216 (16)	-0.0050 (13)	-0.0002 (13)	-0.0018 (12)
C37	0.0314 (18)	0.0278 (17)	0.0150 (15)	-0.0088 (15)	0.0053 (13)	-0.0003 (12)
C38	0.0299 (18)	0.0239 (17)	0.0270 (17)	-0.0082 (14)	0.0141 (14)	-0.0057 (13)
C39	0.0183 (16)	0.0332 (19)	0.0343 (19)	-0.0073 (14)	0.0042 (14)	-0.0049 (14)
C40	0.0211 (16)	0.0273 (17)	0.0202 (16)	-0.0038 (14)	0.0005 (13)	-0.0003 (12)
C41	0.0133 (14)	0.0215 (16)	0.0176 (15)	-0.0010 (12)	0.0030 (11)	-0.0001 (12)
C42	0.0216 (16)	0.0220 (16)	0.0226 (16)	-0.0058 (13)	0.0013 (13)	0.0020 (12)
C43	0.0253 (17)	0.0286 (18)	0.0268 (17)	-0.0076 (15)	-0.0016 (14)	-0.0034 (13)
C44	0.0298 (18)	0.0324 (19)	0.0160 (16)	-0.0033 (15)	-0.0037 (13)	-0.0006 (13)
C45	0.0317 (18)	0.0240 (17)	0.0180 (16)	-0.0014 (14)	0.0026 (13)	0.0021 (12)
C46	0.0215 (16)	0.0221 (16)	0.0202 (16)	-0.0038 (13)	0.0038 (12)	-0.0010 (12)
C47	0.0248 (16)	0.0220 (16)	0.0139 (14)	-0.0063 (13)	-0.0004 (12)	0.0000 (11)
C48	0.0213 (16)	0.0219 (17)	0.0267 (17)	-0.0020 (14)	0.0071 (13)	-0.0032 (13)
C49	0.0361 (19)	0.0215 (17)	0.0295 (18)	-0.0035 (15)	0.0072 (15)	-0.0053 (13)
C50	0.048 (2)	0.0249 (19)	0.0329 (19)	-0.0162 (17)	0.0069 (16)	-0.0098 (14)
C51	0.0269 (19)	0.035 (2)	0.051 (2)	-0.0156 (17)	0.0033 (17)	-0.0116 (17)
C52	0.0228 (17)	0.0268 (18)	0.037 (2)	-0.0034 (15)	0.0008 (14)	-0.0080 (14)

C53	0.042 (2)	0.033 (2)	0.048 (2)	-0.0106 (18)	-0.0082 (18)	0.0073 (17)

Table A6: Geometric parameters (Å, °) for NDI-$[CH_2CH_2O(An)PS_2(Cu(PPh_3)_2]_2$

Cu1—P1	2.2676 (8)	C20—C21	1.399 (5)
Cu1—P2	2.2714 (8)	C20—H20	0.9500
Cu1—S1	2.3870 (8)	C21—C22	1.398 (4)
Cu1—S2	2.5484 (9)	C21—H21	0.9500
Cu1—P5	2.8710 (9)	C23—C24	1.388 (4)
Cl1—C53	1.768 (4)	C23—C28	1.395 (4)
Cl2—C53	1.757 (4)	C24—C25	1.389 (5)
S1—P5	1.9957 (10)	C24—H24	0.9500
S2—P5	1.9850 (11)	C25—C26	1.383 (5)
P1—C29	1.827 (3)	C25—H25	0.9500
P1—C22	1.835 (3)	C26—C27	1.390 (5)
P1—C23	1.836 (3)	C26—H26	0.9500
P2—C41	1.829 (3)	C27—C28	1.397 (4)
P2—C35	1.829 (3)	C27—H27	0.9500
P2—C47	1.830 (3)	C28—H28	0.9500
P5—O3	1.615 (2)	C29—C34	1.391 (4)
P5—C10	1.808 (3)	C29—C30	1.396 (4)
O1—C1	1.216 (4)	C30—C31	1.383 (4)
O2—C5	1.217 (4)	C30—H30	0.9500
O3—C9	1.439 (4)	C31—C32	1.390 (5)
O4—C13	1.363 (4)	C31—H31	0.9500
O4—C16	1.440 (4)	C32—C33	1.369 (5)
N1—C5	1.398 (4)	C32—H32	0.9500
N1—C1	1.402 (4)	C33—C34	1.379 (4)
N1—C8	1.473 (4)	C33—H33	0.9500
C1—C2	1.471 (4)	C34—H34	0.9500
C2—C7	1.379 (4)	C35—C40	1.390 (4)
C2—C3	1.413 (4)	C35—C36	1.395 (4)
C3—C3^{i}	1.403 (6)	C36—C37	1.387 (4)
C3—C4	1.420 (4)	C36—H36	0.9500
C4—C6	1.378 (4)	C37—C38	1.386 (5)
C4—C5	1.471 (4)	C37—H37	0.9500
C6—C7^{i}	1.398 (5)	C38—C39	1.365 (5)
C6—H6	0.9500	C38—H38	0.9500
C7—C6^{i}	1.398 (5)	C39—C40	1.397 (5)
C7—H7	0.9500	C39—H39	0.9500
C8—C9	1.504 (4)	C40—H40	0.9500
C8—H8A	0.9900	C41—C46	1.391 (4)
C8—H8B	0.9900	C41—C42	1.400 (4)

C9—H9A	0.9900	C42—C43	1.386 (4)
C9—H9B	0.9900	C42—H42	0.9500
C10—C11	1.386 (4)	C43—C44	1.381 (5)
C10—C15	1.402 (4)	C43—H43	0.9500
C11—C12	1.388 (5)	C44—C45	1.390 (5)
C11—H11	0.9500	C44—H44	0.9500
C12—C13	1.384 (5)	C45—C46	1.388 (4)
C12—H12	0.9500	C45—H45	0.9500
C13—C14	1.391 (5)	C46—H46	0.9500
C14—C15	1.386 (5)	C47—C52	1.379 (4)
C14—H14	0.9500	C47—C48	1.394 (4)
C15—H15	0.9500	C48—C49	1.381 (4)
C16—H16A	0.9800	C48—H48	0.9500
C16—H16B	0.9800	C49—C50	1.382 (5)
C16—H16C	0.9800	C49—H49	0.9500
C17—C18	1.387 (4)	C50—C51	1.366 (5)
C17—C22	1.396 (4)	C50—H50	0.9500
C17—H17	0.9500	C51—C52	1.390 (5)
C18—C19	1.387 (5)	C51—H51	0.9500
C18—H18	0.9500	C52—H52	0.9500
C19—C20	1.377 (5)	C53—H53A	0.9900
C19—H19	0.9500	C53—H53B	0.9900
P1—Cu1—P2	124.12 (3)	C19—C20—C21	120.3 (3)
P1—Cu1—S1	114.62 (3)	C19—C20—H20	119.9
P2—Cu1—S1	112.68 (3)	C21—C20—H20	119.9
P1—Cu1—S2	101.19 (3)	C22—C21—C20	120.7 (3)
P2—Cu1—S2	110.69 (3)	C22—C21—H21	119.7
S1—Cu1—S2	85.30 (3)	C20—C21—H21	119.7
P1—Cu1—P5	119.79 (3)	C17—C22—C21	118.1 (3)
P2—Cu1—P5	114.70 (3)	C17—C22—P1	119.6 (2)
S1—Cu1—P5	43.41 (2)	C21—C22—P1	122.3 (2)
S2—Cu1—P5	42.45 (2)	C24—C23—C28	119.2 (3)
P5—S1—Cu1	81.32 (3)	C24—C23—P1	117.9 (2)
P5—S2—Cu1	77.49 (3)	C28—C23—P1	122.9 (2)
C29—P1—C22	103.53 (13)	C23—C24—C25	120.1 (3)
C29—P1—C23	104.29 (14)	C23—C24—H24	120.0
C22—P1—C23	101.83 (14)	C25—C24—H24	120.0
C29—P1—Cu1	111.18 (10)	C26—C25—C24	120.7 (3)
C22—P1—Cu1	119.69 (10)	C26—C25—H25	119.6
C23—P1—Cu1	114.63 (10)	C24—C25—H25	119.6
C41—P2—C35	105.59 (13)	C25—C26—C27	119.9 (3)
C41—P2—C47	102.78 (13)	C25—C26—H26	120.1
C35—P2—C47	101.05 (13)	C27—C26—H26	120.1

C41—P2—Cu1	112.94 (10)	C26—C27—C28	119.4 (3)
C35—P2—Cu1	113.44 (9)	C26—C27—H27	120.3
C47—P2—Cu1	119.40 (10)	C28—C27—H27	120.3
O3—P5—C10	103.54 (13)	C23—C28—C27	120.7 (3)
O3—P5—S2	111.11 (9)	C23—C28—H28	119.6
C10—P5—S2	112.80 (11)	C27—C28—H28	119.6
O3—P5—S1	106.35 (9)	C34—C29—C30	118.1 (3)
C10—P5—S1	107.89 (11)	C34—C29—P1	118.2 (2)
S2—P5—S1	114.39 (5)	C30—C29—P1	123.6 (2)
O3—P5—Cu1	117.00 (9)	C31—C30—C29	120.3 (3)
C10—P5—Cu1	138.81 (10)	C31—C30—H30	119.8
S2—P5—Cu1	60.06 (3)	C29—C30—H30	119.8
S1—P5—Cu1	55.28 (3)	C30—C31—C32	120.2 (3)
C9—O3—P5	124.56 (19)	C30—C31—H31	119.9
C13—O4—C16	117.1 (3)	C32—C31—H31	119.9
C5—N1—C1	125.4 (3)	C33—C32—C31	119.9 (3)
C5—N1—C8	117.9 (2)	C33—C32—H32	120.0
C1—N1—C8	116.7 (2)	C31—C32—H32	120.0
O1—C1—N1	120.0 (3)	C32—C33—C34	119.9 (3)
O1—C1—C2	123.1 (3)	C32—C33—H33	120.0
N1—C1—C2	116.9 (3)	C34—C33—H33	120.0
C7—C2—C3	119.8 (3)	C33—C34—C29	121.4 (3)
C7—C2—C1	120.3 (3)	C33—C34—H34	119.3
C3—C2—C1	119.9 (3)	C29—C34—H34	119.3
$C3^{i}$—C3—C2	119.8 (3)	C40—C35—C36	118.9 (3)
$C3^{i}$—C3—C4	119.3 (3)	C40—C35—P2	124.6 (2)
C2—C3—C4	120.9 (3)	C36—C35—P2	116.4 (2)
C6—C4—C3	119.9 (3)	C37—C36—C35	120.7 (3)
C6—C4—C5	120.0 (3)	C37—C36—H36	119.7
C3—C4—C5	120.1 (3)	C35—C36—H36	119.7
O2—C5—N1	120.7 (3)	C38—C37—C36	119.9 (3)
O2—C5—C4	122.6 (3)	C38—C37—H37	120.1
N1—C5—C4	116.6 (2)	C36—C37—H37	120.1
C4—C6—$C7^{i}$	120.7 (3)	C39—C38—C37	119.9 (3)
C4—C6—H6	119.7	C39—C38—H38	120.1
$C7^{i}$—C6—H6	119.7	C37—C38—H38	120.1
C2—C7—$C6^{i}$	120.5 (3)	C38—C39—C40	121.0 (3)
C2—C7—H7	119.7	C38—C39—H39	119.5
$C6^{i}$—C7—H7	119.7	C40—C39—H39	119.5
N1—C8—C9	112.3 (2)	C35—C40—C39	119.7 (3)
N1—C8—H8A	109.1	C35—C40—H40	120.2
C9—C8—H8A	109.1	C39—C40—H40	120.2
N1—C8—H8B	109.1	C46—C41—C42	118.6 (3)

C9—C8—H8B	109.1	C46—C41—P2	123.1 (2)
H8A—C8—H8B	107.9	C42—C41—P2	118.2 (2)
O3—C9—C8	108.3 (2)	C43—C42—C41	120.6 (3)
O3—C9—H9A	110.0	C43—C42—H42	119.7
C8—C9—H9A	110.0	C41—C42—H42	119.7
O3—C9—H9B	110.0	C44—C43—C42	120.3 (3)
C8—C9—H9B	110.0	C44—C43—H43	119.8
H9A—C9—H9B	108.4	C42—C43—H43	119.8
C11—C10—C15	118.2 (3)	C43—C44—C45	119.7 (3)
C11—C10—P5	118.7 (2)	C43—C44—H44	120.2
C15—C10—P5	123.1 (2)	C45—C44—H44	120.2
C10—C11—C12	122.3 (3)	C46—C45—C44	120.1 (3)
C10—C11—H11	118.9	C46—C45—H45	119.9
C12—C11—H11	118.9	C44—C45—H45	119.9
C13—C12—C11	118.7 (3)	C45—C46—C41	120.7 (3)
C13—C12—H12	120.6	C45—C46—H46	119.7
C11—C12—H12	120.6	C41—C46—H46	119.7
O4—C13—C12	123.7 (3)	C52—C47—C48	118.9 (3)
O4—C13—C14	115.9 (3)	C52—C47—P2	120.0 (2)
C12—C13—C14	120.3 (3)	C48—C47—P2	121.0 (2)
C15—C14—C13	120.3 (3)	C49—C48—C47	120.4 (3)
C15—C14—H14	119.9	C49—C48—H48	119.8
C13—C14—H14	119.9	C47—C48—H48	119.8
C14—C15—C10	120.2 (3)	C48—C49—C50	119.8 (3)
C14—C15—H15	119.9	C48—C49—H49	120.1
C10—C15—H15	119.9	C50—C49—H49	120.1
O4—C16—H16A	109.5	C51—C50—C49	120.3 (3)
O4—C16—H16B	109.5	C51—C50—H50	119.8
H16A—C16—H16B	109.5	C49—C50—H50	119.8
O4—C16—H16C	109.5	C50—C51—C52	120.1 (3)
H16A—C16—H16C	109.5	C50—C51—H51	120.0
H16B—C16—H16C	109.5	C52—C51—H51	120.0
C18—C17—C22	120.8 (3)	C47—C52—C51	120.5 (3)
C18—C17—H17	119.6	C47—C52—H52	119.8
C22—C17—H17	119.6	C51—C52—H52	119.8
C19—C18—C17	120.5 (3)	Cl2—C53—Cl1	110.4 (2)
C19—C18—H18	119.7	Cl2—C53—H53A	109.6
C17—C18—H18	119.7	Cl1—C53—H53A	109.6
C20—C19—C18	119.6 (3)	Cl2—C53—H53B	109.6
C20—C19—H19	120.2	Cl1—C53—H53B	109.6
C18—C19—H19	120.2	H53A—C53—H53B	108.1
P1—Cu1—S1—P5	108.11 (4)	P5—C10—C11—C12	-177.3 (3)
P2—Cu1—S1—P5	-102.54 (4)	C10—C11—C12—C13	0.1 (5)

S2—Cu1—S1—P5	7.94 (3)	C16—O4—C13—C12	-1.3 (5)
P1—Cu1—S2—P5	-122.28 (4)	C16—O4—C13—C14	179.1 (3)
P2—Cu1—S2—P5	104.41 (4)	C11—C12—C13—O4	178.5 (3)
S1—Cu1—S2—P5	-8.08 (3)	C11—C12—C13—C14	-2.0 (5)
P2—Cu1—P1—C29	56.00 (11)	O4—C13—C14—C15	-178.1 (3)
S1—Cu1—P1—C29	-158.62 (10)	C12—C13—C14—C15	2.4 (5)
S2—Cu1—P1—C29	-68.69 (10)	C13—C14—C15—C10	-0.9 (5)
P5—Cu1—P1—C29	-109.81 (10)	C11—C10—C15—C14	-1.0 (5)
P2—Cu1—P1—C22	176.64 (11)	P5—C10—C15—C14	177.7 (2)
S1—Cu1—P1—C22	-37.98 (11)	C22—C17—C18—C19	-1.2 (5)
S2—Cu1—P1—C22	51.95 (11)	C17—C18—C19—C20	0.1 (5)
P5—Cu1—P1—C22	10.84 (12)	C18—C19—C20—C21	0.6 (5)
P2—Cu1—P1—C23	-61.96 (12)	C19—C20—C21—C22	-0.2 (5)
S1—Cu1—P1—C23	83.42 (12)	C18—C17—C22—C21	1.5 (4)
S2—Cu1—P1—C23	173.35 (11)	C18—C17—C22—P1	-177.9 (2)
P5—Cu1—P1—C23	132.23 (11)	C20—C21—C22—C17	-0.8 (4)
P1—Cu1—P2—C41	-130.97 (11)	C20—C21—C22—P1	178.6 (2)
S1—Cu1—P2—C41	83.07 (11)	C29—P1—C22—C17	98.8 (2)
S2—Cu1—P2—C41	-10.53 (11)	C23—P1—C22—C17	-153.1 (2)
P5—Cu1—P2—C41	35.49 (11)	Cu1—P1—C22—C17	-25.6 (3)
P1—Cu1—P2—C35	-10.86 (11)	C29—P1—C22—C21	-80.5 (3)
S1—Cu1—P2—C35	-156.82 (11)	C23—P1—C22—C21	27.5 (3)
S2—Cu1—P2—C35	109.57 (11)	Cu1—P1—C22—C21	155.1 (2)
P5—Cu1—P2—C35	155.59 (10)	C29—P1—C23—C24	175.9 (2)
P1—Cu1—P2—C47	108.09 (11)	C22—P1—C23—C24	68.5 (3)
S1—Cu1—P2—C47	-37.87 (12)	Cu1—P1—C23—C24	-62.3 (3)
S2—Cu1—P2—C47	-131.48 (11)	C29—P1—C23—C28	-5.6 (3)
P5—Cu1—P2—C47	-85.46 (11)	C22—P1—C23—C28	-113.1 (3)
Cu1—S2—P5—O3	-109.83 (10)	Cu1—P1—C23—C28	116.2 (2)
Cu1—S2—P5—C10	134.42 (11)	C28—C23—C24—C25	1.4 (5)
Cu1—S2—P5—S1	10.61 (4)	P1—C23—C24—C25	179.9 (3)
Cu1—S1—P5—O3	111.85 (9)	C23—C24—C25—C26	-0.9 (6)
Cu1—S1—P5—C10	-137.60 (11)	C24—C25—C26—C27	-0.7 (6)
Cu1—S1—P5—S2	-11.19 (5)	C25—C26—C27—C28	1.7 (5)
P1—Cu1—P5—O3	172.85 (9)	C24—C23—C28—C27	-0.4 (5)
P2—Cu1—P5—O3	5.76 (10)	P1—C23—C28—C27	-178.9 (2)
S1—Cu1—P5—O3	-91.80 (10)	C26—C27—C28—C23	-1.1 (5)
S2—Cu1—P5—O3	99.97 (10)	C22—P1—C29—C34	-141.6 (2)
P1—Cu1—P5—C10	-18.33 (16)	C23—P1—C29—C34	112.2 (3)
P2—Cu1—P5—C10	174.58 (16)	Cu1—P1—C29—C34	-11.9 (3)
S1—Cu1—P5—C10	77.03 (16)	C22—P1—C29—C30	40.9 (3)
S2—Cu1—P5—C10	-91.21 (16)	C23—P1—C29—C30	-65.3 (3)
P1—Cu1—P5—S2	72.88 (4)	Cu1—P1—C29—C30	170.6 (2)

P2—Cu1—P5—S2	-94.21 (4)	C34—C29—C30—C31	-3.1 (5)
S1—Cu1—P5—S2	168.23 (5)	P1—C29—C30—C31	174.4 (2)
P1—Cu1—P5—S1	-95.35 (4)	C29—C30—C31—C32	0.2 (5)
P2—Cu1—P5—S1	97.56 (4)	C30—C31—C32—C33	2.4 (5)
S2—Cu1—P5—S1	-168.23 (5)	C31—C32—C33—C34	-1.9 (5)
C10—P5—O3—C9	111.5 (2)	C32—C33—C34—C29	-1.2 (5)
S2—P5—O3—C9	-9.8 (3)	C30—C29—C34—C33	3.7 (5)
S1—P5—O3—C9	-134.9 (2)	P1—C29—C34—C33	-173.9 (2)
Cu1—P5—O3—C9	-76.0 (2)	C41—P2—C35—C40	-0.9 (3)
C5—N1—C1—O1	178.9 (3)	C47—P2—C35—C40	105.9 (3)
C8—N1—C1—O1	0.5 (4)	Cu1—P2—C35—C40	-125.1 (2)
C5—N1—C1—C2	-1.3 (4)	C41—P2—C35—C36	175.6 (2)
C8—N1—C1—C2	-179.8 (2)	C47—P2—C35—C36	-77.6 (2)
O1—C1—C2—C7	-1.8 (5)	Cu1—P2—C35—C36	51.4 (2)
N1—C1—C2—C7	178.5 (3)	C40—C35—C36—C37	-1.4 (4)
O1—C1—C2—C3	177.7 (3)	P2—C35—C36—C37	-178.1 (2)
N1—C1—C2—C3	-2.0 (4)	C35—C36—C37—C38	1.4 (5)
C7—C2—C3—C3^{i}	1.5 (5)	C36—C37—C38—C39	-0.9 (5)
C1—C2—C3—C3^{i}	-178.1 (3)	C37—C38—C39—C40	0.3 (5)
C7—C2—C3—C4	-178.6 (3)	C36—C35—C40—C39	0.8 (5)
C1—C2—C3—C4	1.9 (4)	P2—C35—C40—C39	177.2 (2)
C3^{i}—C3—C4—C6	1.1 (5)	C38—C39—C40—C35	-0.3 (5)
C2—C3—C4—C6	-178.9 (3)	C35—P2—C41—C46	114.7 (3)
C3^{i}—C3—C4—C5	-178.7 (3)	C47—P2—C41—C46	9.2 (3)
C2—C3—C4—C5	1.4 (4)	Cu1—P2—C41—C46	-120.8 (2)
C1—N1—C5—O2	-177.3 (3)	C35—P2—C41—C42	-70.4 (3)
C8—N1—C5—O2	1.1 (4)	C47—P2—C41—C42	-175.9 (2)
C1—N1—C5—C4	4.4 (4)	Cu1—P2—C41—C42	54.1 (3)
C8—N1—C5—C4	-177.1 (2)	C46—C41—C42—C43	-1.5 (5)
C6—C4—C5—O2	-2.3 (4)	P2—C41—C42—C43	-176.7 (2)
C3—C4—C5—O2	177.4 (3)	C41—C42—C43—C44	1.3 (5)
C6—C4—C5—N1	175.9 (3)	C42—C43—C44—C45	-0.5 (5)
C3—C4—C5—N1	-4.4 (4)	C43—C44—C45—C46	0.0 (5)
C3—C4—C6—C7^{i}	-0.8 (4)	C44—C45—C46—C41	-0.2 (5)
C5—C4—C6—C7^{i}	179.0 (3)	C42—C41—C46—C45	1.0 (5)
C3—C2—C7—C6^{i}	-1.8 (5)	P2—C41—C46—C45	175.9 (2)
C1—C2—C7—C6^{i}	177.8 (3)	C41—P2—C47—C52	-109.7 (3)
C5—N1—C8—C9	-102.5 (3)	C35—P2—C47—C52	141.4 (3)
C1—N1—C8—C9	76.1 (3)	Cu1—P2—C47—C52	16.2 (3)
P5—O3—C9—C8	-135.9 (2)	C41—P2—C47—C48	68.5 (3)
N1—C8—C9—O3	57.7 (3)	C35—P2—C47—C48	-40.5 (3)
O3—P5—C10—C11	78.5 (3)	Cu1—P2—C47—C48	-165.6 (2)
S2—P5—C10—C11	-161.3 (2)	C52—C47—C48—C49	0.3 (5)

S1—P5—C10—C11	-33.9 (3)	P2—C47—C48—C49	-177.9 (2)
Cu1—P5—C10—C11	-91.2 (3)	C47—C48—C49—C50	-1.2 (5)
O3—P5—C10—C15	-100.1 (3)	C48—C49—C50—C51	1.3 (5)
S2—P5—C10—C15	20.1 (3)	C49—C50—C51—C52	-0.4 (6)
S1—P5—C10—C15	147.5 (2)	C48—C47—C52—C51	0.5 (5)
Cu1—P5—C10—C15	90.1 (3)	P2—C47—C52—C51	178.7 (3)
C15—C10—C11—C12	1.4 (5)	C50—C51—C52—C47	-0.5 (6)
Symmetry code: (i) -*x*+1, -*y*+1, -*z*.			

Table A7: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2(SnPh_3)_2]_2$

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	-0.25941 (3)	0.93483 (4)	-0.020622 (17)	0.02446 (10)
Sn2	0.43724 (2)	1.59568 (4)	0.815321 (17)	0.02317 (10)
S1	-0.29717 (13)	0.97351 (18)	0.12648 (8)	0.0361 (4)
S5	0.31298 (12)	1.48581 (16)	0.74897 (7)	0.0286 (4)
S7	-0.12888 (14)	1.05180 (19)	0.03851 (8)	0.0357 (4)
S8	0.50110 (13)	1.57029 (16)	0.67655 (8)	0.0311 (4)
P1	0.37359 (12)	1.48971 (15)	0.67147 (7)	0.0230 (3)
P2	-0.17095 (13)	1.04961 (16)	0.12101 (7)	0.0263 (4)
O1	0.0247 (4)	1.3662 (5)	0.5527 (2)	0.0362 (12)
O2	0.1905 (4)	0.8398 (4)	0.4054 (2)	0.0370 (12)
O3	0.1593 (4)	1.0695 (4)	0.2380 (2)	0.0332 (12)
O4	-0.0062 (4)	1.5957 (4)	0.3859 (2)	0.0358 (12)
O5	0.0248 (3)	0.8124 (4)	0.2445 (2)	0.0278 (10)
O6	-0.0795 (4)	0.9832 (4)	0.1588 (2)	0.0302 (11)
O7	0.1200 (3)	1.6440 (4)	0.5633 (2)	0.0308 (11)
O8	0.2889 (4)	1.5523 (4)	0.62656 (19)	0.0258 (10)
O9	-0.1057 (4)	1.5718 (5)	0.2144 (2)	0.0414 (13)
O10	0.3547 (4)	0.9521 (4)	0.5951 (2)	0.0358 (12)
N1	0.0109 (4)	1.4823 (5)	0.4689 (3)	0.0269 (12)
N2	0.1726 (4)	0.9538 (5)	0.3214 (3)	0.0301 (13)
C1	0.0331 (5)	1.3698 (7)	0.5012 (3)	0.0264 (15)
C2	0.0674 (5)	1.2605 (6)	0.4694 (3)	0.0269 (15)
C3	0.0898 (5)	1.1479 (6)	0.4988 (3)	0.0311 (16)
H3	0.0818	1.1406	0.5386	0.037*
C4	0.1244 (5)	1.0445 (7)	0.4693 (3)	0.0326 (17)
H4	0.1402	0.9673	0.4897	0.039*
C5	0.1360 (5)	1.0526 (6)	0.4116 (3)	0.0282 (16)
C6	0.1691 (5)	0.9404 (7)	0.3810 (3)	0.0319 (17)
C7	0.1515 (5)	1.0656 (6)	0.2891 (3)	0.0298 (17)
C8	0.1216 (5)	1.1767 (6)	0.3217 (3)	0.0272 (15)

C9	0.1005 (6)	1.2902 (7)	0.2930 (3)	0.0348 (17)
H9	0.1095	1.2973	0.2534	0.042*
C10	0.0660 (6)	1.3954 (6)	0.3212 (3)	0.0311 (17)
H10	0.0498	1.4721	0.3005	0.037*
C11	0.0555 (5)	1.3870 (6)	0.3794 (3)	0.0271 (15)
C12	0.0186 (5)	1.4979 (6)	0.4099 (3)	0.0293 (16)
C13	0.0772 (5)	1.2729 (6)	0.4103 (2)	0.0248 (15)
C14	0.1117 (5)	1.1658 (6)	0.3810 (3)	0.0278 (15)
C15	0.1955 (5)	0.8396 (6)	0.2903 (3)	0.0324 (16)
H15A	0.2498	0.7930	0.3135	0.039*
H15B	0.2174	0.8640	0.2530	0.039*
C16	0.1058 (5)	0.7533 (6)	0.2788 (3)	0.0330 (16)
H16A	0.1240	0.6755	0.2588	0.040*
H16B	0.0856	0.7273	0.3163	0.040*
C17	0.0323 (5)	0.8103 (6)	0.1843 (3)	0.0317 (16)
H17A	0.0501	0.7235	0.1728	0.038*
H17B	0.0850	0.8691	0.1761	0.038*
C18	-0.0623 (6)	0.8488 (6)	0.1496 (3)	0.0345 (17)
H18A	-0.0596	0.8327	0.1079	0.041*
H18B	-0.1169	0.7980	0.1616	0.041*
C19	-0.0230 (5)	1.5941 (7)	0.4986 (3)	0.0303 (16)
H19A	-0.0492	1.5655	0.5340	0.036*
H19B	-0.0775	1.6347	0.4728	0.036*
C20	0.0553 (5)	1.6908 (6)	0.5151 (3)	0.0294 (15)
H20A	0.0922	1.7068	0.4820	0.035*
H20B	0.0254	1.7720	0.5254	0.035*
C21	0.1986 (5)	1.7269 (6)	0.5808 (3)	0.0302 (15)
H21A	0.1734	1.8137	0.5862	0.036*
H21B	0.2430	1.7305	0.5506	0.036*
C22	0.2537 (5)	1.6788 (7)	0.6369 (3)	0.0275 (15)
H22A	0.3097	1.7357	0.6500	0.033*
H22B	0.2098	1.6764	0.6673	0.033*
C23	-0.1554 (5)	1.2086 (6)	0.1475 (3)	0.0276 (15)
C24	-0.0678 (5)	1.2731 (7)	0.1464 (3)	0.0315 (16)
H24	-0.0158	1.2325	0.1303	0.038*
C25	-0.0542 (6)	1.3943 (6)	0.1680 (3)	0.0340 (16)
H25	0.0062	1.4372	0.1662	0.041*
C26	-0.1294 (6)	1.4544 (6)	0.1925 (3)	0.0305 (16)
C27	-0.2177 (6)	1.3921 (6)	0.1932 (3)	0.0328 (16)
H27	-0.2692	1.4324	0.2098	0.039*
C28	-0.2315 (6)	1.2714 (7)	0.1698 (3)	0.0341 (16)
H28	-0.2935	1.2308	0.1690	0.041*
C29	-0.1757 (7)	1.6306 (7)	0.2463 (4)	0.052 (2)

H29A	-0.1903	1.5732	0.2772	0.078*
H29B	-0.2362	1.6484	0.2201	0.078*
H29C	-0.1485	1.7103	0.2634	0.078*
C30	0.3681 (5)	1.3273 (6)	0.6461 (3)	0.0226 (13)
C31	0.4537 (5)	1.2666 (6)	0.6347 (3)	0.0277 (14)
H31	0.5141	1.3119	0.6396	0.033*
C32	0.4519 (5)	1.1432 (6)	0.6165 (3)	0.0294 (15)
H32	0.5103	1.1040	0.6074	0.035*
C33	0.3645 (6)	1.0749 (6)	0.6114 (3)	0.0276 (15)
C34	0.2780 (5)	1.1360 (7)	0.6220 (3)	0.0278 (14)
H34	0.2178	1.0903	0.6173	0.033*
C35	0.2792 (6)	1.2603 (6)	0.6389 (3)	0.0297 (15)
H35	0.2201	1.3011	0.6458	0.036*
C36	0.4429 (6)	0.8860 (7)	0.5854 (4)	0.049 (2)
H36A	0.4873	0.8802	0.6220	0.073*
H36B	0.4754	0.9327	0.5569	0.073*
H36C	0.4261	0.8002	0.5709	0.073*
C37	-0.3835 (6)	1.0538 (7)	-0.0385 (4)	0.0364 (19)
C38	-0.4626 (6)	1.0078 (7)	-0.0773 (3)	0.0377 (18)
H38	-0.4586	0.9262	-0.0944	0.045*
C39	-0.5480 (7)	1.0821 (8)	-0.0910 (4)	0.051 (2)
H39	-0.6023	1.0496	-0.1164	0.061*
C40	-0.5527 (7)	1.1992 (8)	-0.0679 (4)	0.049 (2)
H40	-0.6119	1.2467	-0.0752	0.058*
C41	-0.4729 (7)	1.2508 (7)	-0.0341 (4)	0.045 (2)
H41	-0.4746	1.3365	-0.0213	0.054*
C42	-0.3887 (6)	1.1761 (7)	-0.0184 (4)	0.0365 (18)
H42	-0.3346	1.2106	0.0065	0.044*
C43	-0.2936 (5)	0.7535 (6)	0.0104 (3)	0.0263 (14)
C44	-0.2226 (5)	0.6652 (7)	0.0325 (3)	0.0310 (16)
H44	-0.1550	0.6845	0.0328	0.037*
C45	-0.2501 (6)	0.5481 (7)	0.0545 (3)	0.0386 (19)
H45	-0.2006	0.4901	0.0705	0.046*
C46	-0.3450 (6)	0.5169 (7)	0.0534 (3)	0.0376 (18)
H46	-0.3622	0.4360	0.0671	0.045*
C47	-0.4191 (6)	0.6035 (7)	0.0319 (4)	0.0327 (17)
H47	-0.4864	0.5819	0.0313	0.039*
C48	-0.3926 (5)	0.7206 (6)	0.0116 (3)	0.0283 (15)
H48	-0.4426	0.7803	-0.0018	0.034*
C49	-0.1847 (6)	0.9179 (7)	-0.0954 (3)	0.0295 (17)
C50	-0.1399 (6)	1.0239 (8)	-0.1159 (4)	0.044 (2)
H50	-0.1359	1.0998	-0.0935	0.052*
C51	-0.1016 (7)	1.0234 (11)	-0.1667 (5)	0.059 (3)

H51	-0.0717	1.0976	-0.1798	0.071*
C52	-0.1067 (9)	0.9145 (16)	-0.1988 (5)	0.097 (6)
H52	-0.0831	0.9138	-0.2353	0.116*
C53	-0.1465 (6)	0.8036 (12)	-0.1782 (4)	0.067 (3)
H53	-0.1470	0.7270	-0.1999	0.080*
C54	-0.1852 (6)	0.8055 (8)	-0.1258 (4)	0.045 (2)
H54	-0.2117	0.7303	-0.1114	0.054*
C55	0.5634 (5)	1.4776 (7)	0.8378 (3)	0.0291 (15)
C56	0.5738 (6)	1.3573 (7)	0.8162 (4)	0.0364 (18)
H56	0.5240	1.3228	0.7882	0.044*
C57	0.6574 (6)	1.2860 (7)	0.8353 (4)	0.0413 (19)
H57	0.6652	1.2033	0.8200	0.050*
C58	0.7283 (6)	1.3356 (7)	0.8762 (4)	0.046 (2)
H58	0.7854	1.2871	0.8892	0.055*
C59	0.7178 (7)	1.4530 (8)	0.8985 (4)	0.043 (2)
H59	0.7678	1.4865	0.9266	0.052*
C60	0.6349 (6)	1.5246 (7)	0.8805 (3)	0.0359 (17)
H60	0.6267	1.6057	0.8973	0.043*
C61	0.4758 (5)	1.7806 (6)	0.7894 (3)	0.0241 (14)
C62	0.4071 (6)	1.8726 (7)	0.7725 (3)	0.0380 (18)
H62	0.3393	1.8554	0.7729	0.046*
C63	0.4369 (6)	1.9910 (7)	0.7547 (3)	0.0385 (18)
H63	0.3889	2.0547	0.7438	0.046*
C64	0.5323 (6)	2.0174 (7)	0.7526 (3)	0.0396 (18)
H64	0.5508	2.0980	0.7392	0.047*
C65	0.6038 (6)	1.9264 (6)	0.7702 (4)	0.0368 (19)
H65	0.6714	1.9451	0.7699	0.044*
C66	0.5749 (5)	1.8079 (6)	0.7882 (3)	0.0285 (15)
H66	0.6232	1.7449	0.7999	0.034*
C67	0.3571 (6)	1.5997 (6)	0.8889 (3)	0.0283 (16)
C68	0.3090 (6)	1.4929 (7)	0.9032 (3)	0.0351 (17)
H68	0.3019	1.4225	0.8774	0.042*
C69	0.2703 (6)	1.4867 (7)	0.9556 (3)	0.0390 (18)
H69	0.2372	1.4117	0.9650	0.047*
C70	0.2790 (6)	1.5860 (8)	0.9934 (4)	0.0374 (19)
H70	0.2558	1.5785	1.0299	0.045*
C71	0.3216 (6)	1.6969 (8)	0.9785 (3)	0.040 (2)
H71	0.3239	1.7685	1.0036	0.049*
C72	0.3622 (5)	1.7052 (7)	0.9258 (3)	0.0362 (18)
H72	0.3927	1.7817	0.9157	0.043*

Table A8: Atomic displacement parameters ($Å^2$) for NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0237 (2)	0.0290 (2)	0.0206 (2)	-0.00518 (17)	0.00250 (16)	-0.00310 (17)
Sn2	0.0209 (2)	0.0301 (2)	0.01811 (19)	-0.00336 (17)	0.00108 (15)	-0.00226 (17)
S1	0.0283 (9)	0.0461 (10)	0.0354 (9)	-0.0103 (8)	0.0090 (7)	-0.0085 (8)
S5	0.0256 (8)	0.0406 (9)	0.0197 (8)	-0.0120 (7)	0.0033 (6)	-0.0046 (6)
S7	0.0352 (10)	0.0485 (11)	0.0237 (9)	-0.0189 (8)	0.0051 (7)	-0.0085 (7)
S8	0.0273 (9)	0.0378 (9)	0.0297 (9)	-0.0074 (7)	0.0086 (7)	-0.0054 (7)
P1	0.0233 (8)	0.0284 (8)	0.0171 (7)	-0.0036 (6)	0.0016 (6)	-0.0015 (6)
P2	0.0259 (9)	0.0312 (9)	0.0219 (8)	-0.0041 (7)	0.0031 (7)	-0.0055 (7)
O1	0.033 (3)	0.052 (3)	0.023 (3)	-0.007 (2)	0.004 (2)	-0.001 (2)
O2	0.040 (3)	0.033 (3)	0.037 (3)	0.006 (2)	0.000 (2)	0.009 (2)
O3	0.035 (3)	0.040 (3)	0.026 (3)	-0.006 (2)	0.010 (2)	-0.006 (2)
O4	0.041 (3)	0.035 (3)	0.030 (3)	0.003 (2)	0.000 (2)	0.003 (2)
O5	0.027 (3)	0.026 (2)	0.031 (3)	-0.0010 (18)	0.008 (2)	-0.0059 (19)
O6	0.032 (3)	0.029 (2)	0.028 (3)	0.001 (2)	0.001 (2)	-0.008 (2)
O7	0.032 (3)	0.028 (2)	0.030 (3)	0.004 (2)	-0.004 (2)	-0.003 (2)
O8	0.038 (3)	0.022 (2)	0.017 (2)	-0.0004 (19)	0.001 (2)	-0.0018 (17)
O9	0.056 (4)	0.032 (3)	0.039 (3)	-0.002 (2)	0.014 (3)	-0.006 (2)
O10	0.033 (3)	0.028 (2)	0.049 (3)	0.001 (2)	0.014 (2)	-0.006 (2)
N1	0.019 (3)	0.033 (3)	0.028 (3)	-0.001 (2)	0.001 (2)	-0.005 (2)
N2	0.025 (3)	0.036 (3)	0.028 (3)	-0.002 (2)	-0.002 (2)	0.000 (2)
C1	0.018 (3)	0.036 (4)	0.024 (4)	-0.010 (3)	-0.002 (3)	0.003 (3)
C2	0.021 (3)	0.032 (4)	0.027 (4)	-0.006 (3)	0.001 (3)	0.001 (3)
C3	0.029 (4)	0.036 (4)	0.026 (4)	-0.012 (3)	-0.003 (3)	0.008 (3)
C4	0.029 (4)	0.033 (4)	0.033 (4)	-0.009 (3)	-0.004 (3)	0.008 (3)
C5	0.029 (4)	0.025 (3)	0.027 (4)	-0.005 (3)	-0.008 (3)	0.001 (3)
C6	0.023 (4)	0.041 (4)	0.029 (4)	-0.003 (3)	-0.006 (3)	-0.002 (3)
C7	0.021 (3)	0.036 (4)	0.031 (4)	-0.007 (3)	-0.001 (3)	0.001 (3)
C8	0.024 (4)	0.031 (4)	0.025 (3)	-0.009 (3)	0.001 (3)	-0.002 (3)
C9	0.046 (5)	0.036 (4)	0.021 (3)	-0.010 (3)	-0.002 (3)	0.002 (3)
C10	0.039 (4)	0.027 (4)	0.024 (4)	-0.009 (3)	-0.005 (3)	0.002 (3)
C11	0.019 (3)	0.034 (4)	0.027 (4)	-0.007 (3)	-0.001 (3)	-0.004 (3)
C12	0.030 (4)	0.032 (4)	0.023 (3)	-0.007 (3)	-0.006 (3)	0.002 (3)
C13	0.024 (3)	0.031 (3)	0.017 (4)	-0.009 (3)	-0.007 (3)	0.002 (3)
C14	0.024 (4)	0.032 (4)	0.026 (3)	-0.009 (3)	-0.002 (3)	-0.002 (3)
C15	0.025 (4)	0.039 (4)	0.033 (4)	0.006 (3)	0.005 (3)	-0.005 (3)
C16	0.034 (4)	0.027 (4)	0.038 (4)	0.004 (3)	0.006 (3)	-0.001 (3)
C17	0.039 (4)	0.026 (3)	0.029 (4)	0.003 (3)	0.003 (3)	-0.008 (3)
C18	0.033 (4)	0.029 (4)	0.041 (4)	-0.005 (3)	0.001 (3)	-0.013 (3)
C19	0.018 (3)	0.043 (4)	0.030 (4)	0.003 (3)	0.002 (3)	-0.001 (3)
C20	0.033 (4)	0.029 (3)	0.026 (3)	0.010 (3)	0.003 (3)	0.000 (3)

C21	0.030 (4)	0.026 (3)	0.034 (4)	0.001 (3)	0.000 (3)	0.002 (3)
C22	0.027 (4)	0.032 (4)	0.025 (4)	0.000 (3)	0.009 (3)	0.001 (3)
C23	0.034 (4)	0.027 (3)	0.021 (3)	-0.002 (3)	0.000 (3)	-0.002 (3)
C24	0.033 (4)	0.037 (4)	0.023 (3)	0.005 (3)	-0.003 (3)	-0.003 (3)
C25	0.041 (4)	0.031 (4)	0.029 (4)	-0.005 (3)	-0.001 (3)	-0.001 (3)
C26	0.046 (5)	0.026 (3)	0.019 (3)	0.003 (3)	0.004 (3)	0.004 (3)
C27	0.040 (4)	0.032 (4)	0.028 (4)	0.006 (3)	0.009 (3)	0.002 (3)
C28	0.037 (4)	0.036 (4)	0.028 (4)	-0.006 (3)	0.004 (3)	0.005 (3)
C29	0.061 (6)	0.032 (4)	0.067 (6)	-0.004 (4)	0.026 (5)	-0.012 (4)
C30	0.024 (3)	0.029 (3)	0.016 (3)	-0.004 (3)	0.007 (3)	-0.001 (2)
C31	0.022 (3)	0.039 (4)	0.025 (3)	-0.007 (3)	0.013 (3)	0.000 (3)
C32	0.027 (4)	0.031 (3)	0.032 (4)	0.001 (3)	0.008 (3)	0.003 (3)
C33	0.032 (4)	0.031 (4)	0.021 (3)	0.002 (3)	0.011 (3)	0.001 (3)
C34	0.025 (4)	0.034 (4)	0.024 (3)	-0.005 (3)	0.004 (3)	0.002 (3)
C35	0.032 (4)	0.034 (4)	0.023 (3)	0.000 (3)	0.004 (3)	0.000 (3)
C36	0.041 (5)	0.031 (4)	0.077 (6)	0.002 (3)	0.015 (4)	-0.013 (4)
C37	0.030 (4)	0.040 (4)	0.038 (5)	0.000 (3)	0.000 (3)	0.006 (3)
C38	0.041 (4)	0.037 (4)	0.034 (4)	-0.003 (3)	0.000 (3)	-0.009 (3)
C39	0.048 (6)	0.058 (5)	0.039 (5)	0.003 (4)	-0.018 (4)	0.005 (4)
C40	0.053 (5)	0.047 (5)	0.047 (5)	0.013 (4)	0.007 (4)	0.006 (4)
C41	0.052 (5)	0.036 (4)	0.048 (5)	0.013 (4)	0.011 (4)	0.007 (4)
C42	0.042 (5)	0.031 (4)	0.038 (4)	-0.006 (3)	0.010 (4)	0.002 (3)
C43	0.024 (3)	0.026 (3)	0.028 (4)	-0.001 (3)	0.001 (3)	-0.001 (3)
C44	0.024 (4)	0.041 (4)	0.028 (4)	0.004 (3)	0.004 (3)	-0.003 (3)
C45	0.042 (5)	0.042 (4)	0.028 (4)	0.009 (3)	-0.005 (3)	0.003 (3)
C46	0.050 (5)	0.034 (4)	0.029 (4)	0.003 (3)	0.009 (3)	0.007 (3)
C47	0.032 (4)	0.041 (4)	0.028 (4)	0.001 (3)	0.016 (3)	0.000 (3)
C48	0.030 (4)	0.027 (3)	0.028 (4)	0.001 (3)	0.003 (3)	-0.007 (3)
C49	0.029 (4)	0.043 (4)	0.020 (4)	0.003 (3)	0.014 (3)	0.004 (3)
C50	0.036 (5)	0.051 (5)	0.047 (5)	0.007 (4)	0.016 (4)	0.013 (4)
C51	0.037 (5)	0.095 (7)	0.050 (6)	0.023 (5)	0.020 (5)	0.046 (6)
C52	0.031 (6)	0.232 (19)	0.026 (6)	0.031 (8)	0.002 (5)	0.022 (8)
C53	0.025 (5)	0.138 (10)	0.032 (5)	0.022 (5)	-0.011 (4)	-0.040 (6)
C54	0.021 (4)	0.071 (6)	0.039 (5)	0.008 (4)	-0.006 (3)	-0.016 (4)
C55	0.029 (4)	0.033 (4)	0.023 (4)	0.001 (3)	-0.003 (3)	-0.001 (3)
C56	0.029 (4)	0.031 (4)	0.047 (5)	-0.003 (3)	-0.001 (3)	0.002 (3)
C57	0.046 (5)	0.029 (4)	0.048 (5)	0.004 (3)	0.008 (4)	-0.002 (3)
C58	0.035 (4)	0.043 (5)	0.056 (5)	0.009 (4)	-0.007 (4)	0.006 (4)
C59	0.040 (5)	0.051 (5)	0.035 (4)	0.006 (4)	-0.005 (4)	0.007 (4)
C60	0.035 (4)	0.037 (4)	0.032 (4)	0.000 (3)	-0.010 (3)	-0.006 (3)
C61	0.029 (4)	0.028 (3)	0.016 (3)	-0.003 (3)	0.003 (3)	-0.001 (2)
C62	0.036 (4)	0.042 (4)	0.034 (4)	0.002 (3)	-0.001 (3)	-0.004 (3)
C63	0.046 (5)	0.045 (4)	0.025 (4)	0.015 (4)	0.005 (3)	0.004 (3)

C64	0.044 (5)	0.036 (4)	0.038 (4)	0.000 (3)	0.002 (4)	0.006 (3)
C65	0.033 (4)	0.037 (4)	0.037 (5)	-0.004 (3)	-0.005 (4)	-0.002 (3)
C66	0.026 (4)	0.034 (4)	0.024 (3)	0.006 (3)	-0.003 (3)	-0.002 (3)
C67	0.026 (4)	0.037 (4)	0.021 (4)	0.000 (3)	0.001 (3)	-0.004 (3)
C68	0.042 (4)	0.034 (4)	0.031 (4)	0.003 (3)	0.011 (3)	-0.004 (3)
C69	0.044 (5)	0.041 (4)	0.033 (4)	0.003 (3)	0.007 (3)	0.019 (3)
C70	0.024 (4)	0.067 (5)	0.023 (4)	0.008 (3)	0.009 (3)	0.006 (3)
C71	0.032 (4)	0.060 (5)	0.027 (4)	0.014 (4)	-0.006 (3)	-0.016 (4)
C72	0.026 (4)	0.049 (4)	0.032 (4)	-0.001 (3)	-0.002 (3)	-0.005 (3)

Table A9: Geometric parameters (Å, °) for NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$

Sn1—C37	2.110 (8)	C28—H28	0.9500
Sn1—C43	2.113 (6)	C29—H29A	0.9800
Sn1—C49	2.143 (7)	C29—H29B	0.9800
Sn1—S7	2.4397 (17)	C29—H29C	0.9800
Sn2—C61	2.123 (6)	C30—C31	1.393 (9)
Sn2—C55	2.138 (7)	C30—C35	1.401 (9)
Sn2—C67	2.157 (8)	C31—C32	1.364 (9)
Sn2—S5	2.4327 (16)	C31—H31	0.9500
S1—P2	1.929 (2)	C32—C33	1.390 (10)
S5—P1	2.085 (2)	C32—H32	0.9500
S7—P2	2.077 (3)	C33—C34	1.401 (10)
S8—P1	1.934 (2)	C34—C35	1.364 (9)
P1—O8	1.597 (5)	C34—H34	0.9500
P1—C30	1.804 (6)	C35—H35	0.9500
P2—O6	1.594 (5)	C36—H36A	0.9800
P2—C23	1.784 (6)	C36—H36B	0.9800
O1—C1	1.220 (8)	C36—H36C	0.9800
O2—C6	1.218 (8)	C37—C42	1.373 (10)
O3—C7	1.209 (9)	C37—C38	1.401 (11)
O4—C12	1.196 (8)	C38—C39	1.410 (12)
O5—C17	1.418 (8)	C38—H38	0.9500
O5—C16	1.422 (8)	C39—C40	1.348 (12)
O6—C18	1.453 (8)	C39—H39	0.9500
O7—C21	1.403 (8)	C40—C41	1.371 (12)
O7—C20	1.422 (8)	C40—H40	0.9500
O8—C22	1.446 (8)	C41—C42	1.405 (11)
O9—C26	1.358 (8)	C41—H41	0.9500
O9—C29	1.432 (9)	C42—H42	0.9500
O10—C33	1.347 (8)	C43—C44	1.393 (9)
O10—C36	1.441 (9)	C43—C48	1.407 (10)
N1—C12	1.402 (9)	C44—C45	1.404 (11)

N1—C1	1.412 (9)	C44—H44	0.9500
N1—C19	1.469 (9)	C45—C46	1.341 (11)
N2—C6	1.400 (10)	C45—H45	0.9500
N2—C7	1.403 (9)	C46—C47	1.406 (11)
N2—C15	1.457 (9)	C46—H46	0.9500
C1—C2	1.477 (10)	C47—C48	1.384 (10)
C2—C3	1.380 (9)	C47—H47	0.9500
C2—C13	1.407 (9)	C48—H48	0.9500
C3—C4	1.401 (11)	C49—C54	1.376 (10)
C3—H3	0.9500	C49—C50	1.388 (10)
C4—C5	1.376 (10)	C50—C51	1.358 (12)
C4—H4	0.9500	C50—H50	0.9500
C5—C14	1.403 (9)	C51—C52	1.362 (16)
C5—C6	1.481 (10)	C51—H51	0.9500
C7—C8	1.479 (10)	C52—C53	1.398 (17)
C8—C9	1.378 (10)	C52—H52	0.9500
C8—C14	1.411 (10)	C53—C54	1.394 (13)
C9—C10	1.400 (10)	C53—H53	0.9500
C9—H9	0.9500	C54—H54	0.9500
C10—C11	1.382 (10)	C55—C56	1.375 (10)
C10—H10	0.9500	C55—C60	1.391 (9)
C11—C13	1.408 (9)	C56—C57	1.393 (11)
C11—C12	1.489 (10)	C56—H56	0.9500
C13—C14	1.429 (9)	C57—C58	1.370 (11)
C15—C16	1.524 (9)	C57—H57	0.9500
C15—H15A	0.9900	C58—C59	1.354 (11)
C15—H15B	0.9900	C58—H58	0.9500
C16—H16A	0.9900	C59—C60	1.382 (10)
C16—H16B	0.9900	C59—H59	0.9500
C17—C18	1.490 (10)	C60—H60	0.9500
C17—H17A	0.9900	C61—C62	1.371 (10)
C17—H17B	0.9900	C61—C66	1.395 (10)
C18—H18A	0.9900	C62—C63	1.390 (11)
C18—H18B	0.9900	C62—H62	0.9500
C19—C20	1.492 (9)	C63—C64	1.346 (11)
C19—H19A	0.9900	C63—H63	0.9500
C19—H19B	0.9900	C64—C65	1.392 (11)
C20—H20A	0.9900	C64—H64	0.9500
C20—H20B	0.9900	C65—C66	1.389 (10)
C21—C22	1.505 (9)	C65—H65	0.9500
C21—H21A	0.9900	C66—H66	0.9500
C21—H21B	0.9900	C67—C68	1.366 (10)
C22—H22A	0.9900	C67—C72	1.399 (10)

C22—H22B	0.9900	C68—C69	1.394 (11)
C23—C24	1.384 (10)	C68—H68	0.9500
C23—C28	1.395 (10)	C69—C70	1.360 (12)
C24—C25	1.373 (9)	C69—H69	0.9500
C24—H24	0.9500	C70—C71	1.369 (11)
C25—C26	1.395 (11)	C70—H70	0.9500
C25—H25	0.9500	C71—C72	1.416 (11)
C26—C27	1.380 (11)	C71—H71	0.9500
C27—C28	1.383 (9)	C72—H72	0.9500
C27—H27	0.9500		
C37—Sn1—C43	113.0 (3)	C28—C27—H27	119.8
C37—Sn1—C49	110.6 (3)	C27—C28—C23	120.7 (7)
C43—Sn1—C49	110.8 (3)	C27—C28—H28	119.7
C37—Sn1—S7	109.0 (2)	C23—C28—H28	119.7
C43—Sn1—S7	116.26 (18)	O9—C29—H29A	109.5
C49—Sn1—S7	96.0 (2)	O9—C29—H29B	109.5
C61—Sn2—C55	112.1 (3)	H29A—C29—H29B	109.5
C61—Sn2—C67	112.4 (3)	O9—C29—H29C	109.5
C55—Sn2—C67	107.5 (3)	H29A—C29—H29C	109.5
C61—Sn2—S5	115.77 (18)	H29B—C29—H29C	109.5
C55—Sn2—S5	110.82 (19)	C31—C30—C35	119.4 (6)
C67—Sn2—S5	97.10 (19)	C31—C30—P1	119.8 (5)
P1—S5—Sn2	102.21 (8)	C35—C30—P1	120.8 (5)
P2—S7—Sn1	103.92 (8)	C32—C31—C30	121.0 (6)
O8—P1—C30	100.5 (3)	C32—C31—H31	119.5
O8—P1—S8	115.7 (2)	C30—C31—H31	119.5
C30—P1—S8	115.6 (2)	C31—C32—C33	119.8 (6)
O8—P1—S5	103.5 (2)	C31—C32—H32	120.1
C30—P1—S5	105.1 (2)	C33—C32—H32	120.1
S8—P1—S5	114.79 (10)	O10—C33—C32	124.9 (7)
O6—P2—C23	99.8 (3)	O10—C33—C34	115.7 (6)
O6—P2—S1	115.5 (2)	C32—C33—C34	119.4 (6)
C23—P2—S1	115.6 (3)	C35—C34—C33	120.8 (6)
O6—P2—S7	102.6 (2)	C35—C34—H34	119.6
C23—P2—S7	105.9 (2)	C33—C34—H34	119.6
S1—P2—S7	115.45 (11)	C34—C35—C30	119.5 (7)
C17—O5—C16	113.1 (5)	C34—C35—H35	120.2
C18—O6—P2	118.4 (4)	C30—C35—H35	120.2
C21—O7—C20	112.8 (5)	O10—C36—H36A	109.5
C22—O8—P1	120.1 (4)	O10—C36—H36B	109.5
C26—O9—C29	116.3 (6)	H36A—C36—H36B	109.5
C33—O10—C36	116.8 (6)	O10—C36—H36C	109.5
C12—N1—C1	125.4 (6)	H36A—C36—H36C	109.5

C12—N1—C19	115.9 (6)	H36B—C36—H36C	109.5
C1—N1—C19	118.6 (6)	C42—C37—C38	118.2 (7)
C6—N2—C7	125.5 (6)	C42—C37—Sn1	124.4 (6)
C6—N2—C15	116.5 (6)	C38—C37—Sn1	117.2 (6)
C7—N2—C15	117.8 (6)	C37—C38—C39	120.2 (7)
O1—C1—N1	120.4 (7)	C37—C38—H38	119.9
O1—C1—C2	123.1 (7)	C39—C38—H38	119.9
N1—C1—C2	116.5 (6)	C40—C39—C38	119.9 (8)
C3—C2—C13	121.3 (6)	C40—C39—H39	120.0
C3—C2—C1	119.0 (6)	C38—C39—H39	120.0
C13—C2—C1	119.8 (6)	C39—C40—C41	120.8 (8)
C2—C3—C4	119.4 (7)	C39—C40—H40	119.6
C2—C3—H3	120.3	C41—C40—H40	119.6
C4—C3—H3	120.3	C40—C41—C42	119.6 (7)
C5—C4—C3	121.3 (7)	C40—C41—H41	120.2
C5—C4—H4	119.3	C42—C41—H41	120.2
C3—C4—H4	119.3	C37—C42—C41	120.9 (8)
C4—C5—C14	119.8 (7)	C37—C42—H42	119.6
C4—C5—C6	120.3 (6)	C41—C42—H42	119.6
C14—C5—C6	119.9 (7)	C44—C43—C48	117.3 (6)
O2—C6—N2	120.8 (7)	C44—C43—Sn1	123.4 (5)
O2—C6—C5	122.5 (7)	C48—C43—Sn1	119.2 (5)
N2—C6—C5	116.7 (6)	C43—C44—C45	120.7 (7)
O3—C7—N2	121.0 (7)	C43—C44—H44	119.7
O3—C7—C8	123.0 (6)	C45—C44—H44	119.7
N2—C7—C8	116.1 (7)	C46—C45—C44	121.0 (7)
C9—C8—C14	120.1 (7)	C46—C45—H45	119.5
C9—C8—C7	119.4 (7)	C44—C45—H45	119.5
C14—C8—C7	120.4 (6)	C45—C46—C47	120.3 (7)
C8—C9—C10	121.3 (7)	C45—C46—H46	119.9
C8—C9—H9	119.3	C47—C46—H46	119.9
C10—C9—H9	119.3	C48—C47—C46	119.1 (8)
C11—C10—C9	119.6 (6)	C48—C47—H47	120.4
C11—C10—H10	120.2	C46—C47—H47	120.4
C9—C10—H10	120.2	C47—C48—C43	121.6 (7)
C10—C11—C13	120.7 (6)	C47—C48—H48	119.2
C10—C11—C12	120.1 (6)	C43—C48—H48	119.2
C13—C11—C12	119.1 (6)	C54—C49—C50	119.0 (8)
O4—C12—N1	120.1 (7)	C54—C49—Sn1	121.2 (6)
O4—C12—C11	123.1 (7)	C50—C49—Sn1	119.6 (6)
N1—C12—C11	116.8 (6)	C51—C50—C49	122.5 (9)
C2—C13—C11	122.4 (6)	C51—C50—H50	118.8
C2—C13—C14	118.3 (6)	C49—C50—H50	118.8

C11—C13—C14	119.3 (5)	C50—C51—C52	118.8 (10)
C5—C14—C8	121.2 (6)	C50—C51—H51	120.6
C5—C14—C13	119.9 (6)	C52—C51—H51	120.6
C8—C14—C13	118.9 (6)	C51—C52—C53	120.5 (11)
N2—C15—C16	110.8 (6)	C51—C52—H52	119.8
N2—C15—H15A	109.5	C53—C52—H52	119.8
C16—C15—H15A	109.5	C54—C53—C52	120.0 (10)
N2—C15—H15B	109.5	C54—C53—H53	120.0
C16—C15—H15B	109.5	C52—C53—H53	120.0
H15A—C15—H15B	108.1	C49—C54—C53	119.0 (9)
O5—C16—C15	113.0 (5)	C49—C54—H54	120.5
O5—C16—H16A	109.0	C53—C54—H54	120.5
C15—C16—H16A	109.0	C56—C55—C60	119.3 (7)
O5—C16—H16B	109.0	C56—C55—Sn2	124.5 (5)
C15—C16—H16B	109.0	C60—C55—Sn2	116.0 (5)
H16A—C16—H16B	107.8	C55—C56—C57	120.0 (7)
O5—C17—C18	110.9 (6)	C55—C56—H56	120.0
O5—C17—H17A	109.5	C57—C56—H56	120.0
C18—C17—H17A	109.5	C58—C57—C56	119.7 (7)
O5—C17—H17B	109.5	C58—C57—H57	120.2
C18—C17—H17B	109.5	C56—C57—H57	120.2
H17A—C17—H17B	108.1	C59—C58—C57	120.7 (7)
O6—C18—C17	109.3 (5)	C59—C58—H58	119.7
O6—C18—H18A	109.8	C57—C58—H58	119.7
C17—C18—H18A	109.8	C58—C59—C60	120.5 (8)
O6—C18—H18B	109.8	C58—C59—H59	119.8
C17—C18—H18B	109.8	C60—C59—H59	119.8
H18A—C18—H18B	108.3	C59—C60—C55	119.7 (7)
N1—C19—C20	113.8 (6)	C59—C60—H60	120.1
N1—C19—H19A	108.8	C55—C60—H60	120.1
C20—C19—H19A	108.8	C62—C61—C66	119.0 (6)
N1—C19—H19B	108.8	C62—C61—Sn2	122.6 (6)
C20—C19—H19B	108.8	C66—C61—Sn2	118.4 (5)
H19A—C19—H19B	107.7	C61—C62—C63	119.8 (8)
O7—C20—C19	108.6 (5)	C61—C62—H62	120.1
O7—C20—H20A	110.0	C63—C62—H62	120.1
C19—C20—H20A	110.0	C64—C63—C62	121.5 (7)
O7—C20—H20B	110.0	C64—C63—H63	119.3
C19—C20—H20B	110.0	C62—C63—H63	119.3
H20A—C20—H20B	108.3	C63—C64—C65	120.0 (7)
O7—C21—C22	108.6 (5)	C63—C64—H64	120.0
O7—C21—H21A	110.0	C65—C64—H64	120.0
C22—C21—H21A	110.0	C66—C65—C64	119.0 (8)

O7—C21—H21B	110.0	C66—C65—H65	120.5
C22—C21—H21B	110.0	C64—C65—H65	120.5
H21A—C21—H21B	108.3	C65—C66—C61	120.6 (7)
O8—C22—C21	107.8 (5)	C65—C66—H66	119.7
O8—C22—H22A	110.1	C61—C66—H66	119.7
C21—C22—H22A	110.1	C68—C67—C72	119.2 (7)
O8—C22—H22B	110.1	C68—C67—Sn2	119.5 (5)
C21—C22—H22B	110.1	C72—C67—Sn2	120.9 (6)
H22A—C22—H22B	108.5	C67—C68—C69	120.3 (7)
C24—C23—C28	118.2 (6)	C67—C68—H68	119.8
C24—C23—P2	121.1 (6)	C69—C68—H68	119.8
C28—C23—P2	120.7 (5)	C70—C69—C68	121.2 (7)
C25—C24—C23	121.5 (7)	C70—C69—H69	119.4
C25—C24—H24	119.2	C68—C69—H69	119.4
C23—C24—H24	119.2	C69—C70—C71	119.6 (8)
C24—C25—C26	119.8 (7)	C69—C70—H70	120.2
C24—C25—H25	120.1	C71—C70—H70	120.2
C26—C25—H25	120.1	C70—C71—C72	120.2 (7)
O9—C26—C27	126.4 (7)	C70—C71—H71	119.9
O9—C26—C25	114.3 (7)	C72—C71—H71	119.9
C27—C26—C25	119.3 (6)	C67—C72—C71	119.3 (7)
C26—C27—C28	120.3 (7)	C67—C72—H72	120.4
C26—C27—H27	119.8	C71—C72—H72	120.4
C61—Sn2—S5—P1	55.4 (2)	O9—C26—C27—C28	-179.1 (7)
C55—Sn2—S5—P1	-73.6 (2)	C25—C26—C27—C28	0.0 (11)
C67—Sn2—S5—P1	174.56 (19)	C26—C27—C28—C23	2.7 (11)
C37—Sn1—S7—P2	77.0 (3)	C24—C23—C28—C27	-3.6 (10)
C43—Sn1—S7—P2	-52.2 (2)	P2—C23—C28—C27	176.6 (6)
C49—Sn1—S7—P2	-168.9 (2)	O8—P1—C30—C31	128.6 (5)
Sn2—S5—P1—O8	-125.89 (18)	S8—P1—C30—C31	3.3 (6)
Sn2—S5—P1—C30	129.2 (2)	S5—P1—C30—C31	-124.3 (5)
Sn2—S5—P1—S8	1.09 (13)	O8—P1—C30—C35	-52.8 (6)
Sn1—S7—P2—O6	122.04 (19)	S8—P1—C30—C35	-178.0 (5)
Sn1—S7—P2—C23	-133.8 (2)	S5—P1—C30—C35	54.4 (6)
Sn1—S7—P2—S1	-4.46 (14)	C35—C30—C31—C32	0.1 (10)
C23—P2—O6—C18	-178.4 (5)	P1—C30—C31—C32	178.8 (5)
S1—P2—O6—C18	56.9 (5)	C30—C31—C32—C33	-2.5 (10)
S7—P2—O6—C18	-69.5 (5)	C36—O10—C33—C32	3.5 (11)
C30—P1—O8—C22	168.2 (5)	C36—O10—C33—C34	-178.3 (7)
S8—P1—O8—C22	-66.6 (5)	C31—C32—C33—O10	-178.5 (7)
S5—P1—O8—C22	59.8 (5)	C31—C32—C33—C34	3.4 (10)
C12—N1—C1—O1	179.5 (6)	O10—C33—C34—C35	179.8 (6)
C19—N1—C1—O1	-0.3 (9)	C32—C33—C34—C35	-2.0 (10)

C12—N1—C1—C2	0.1 (9)	C33—C34—C35—C30	-0.4 (10)
C19—N1—C1—C2	-179.7 (5)	C31—C30—C35—C34	1.3 (10)
O1—C1—C2—C3	0.9 (10)	P1—C30—C35—C34	-177.3 (5)
N1—C1—C2—C3	-179.7 (6)	C43—Sn1—C37—C42	129.5 (7)
O1—C1—C2—C13	-178.6 (6)	C49—Sn1—C37—C42	-105.7 (7)
N1—C1—C2—C13	0.7 (9)	S7—Sn1—C37—C42	-1.4 (8)
C13—C2—C3—C4	0.9 (10)	C43—Sn1—C37—C38	-55.8 (7)
C1—C2—C3—C4	-178.6 (6)	C49—Sn1—C37—C38	69.0 (7)
C2—C3—C4—C5	-0.4 (11)	S7—Sn1—C37—C38	173.3 (6)
C3—C4—C5—C14	-0.8 (11)	C42—C37—C38—C39	-5.3 (13)
C3—C4—C5—C6	-177.7 (6)	Sn1—C37—C38—C39	179.7 (7)
C7—N2—C6—O2	-178.7 (6)	C37—C38—C39—C40	1.8 (14)
C15—N2—C6—O2	4.5 (10)	C38—C39—C40—C41	4.2 (15)
C7—N2—C6—C5	2.9 (10)	C39—C40—C41—C42	-6.5 (14)
C15—N2—C6—C5	-173.9 (6)	C38—C37—C42—C41	3.0 (12)
C4—C5—C6—O2	-2.7 (11)	Sn1—C37—C42—C41	177.6 (6)
C14—C5—C6—O2	-179.5 (7)	C40—C41—C42—C37	2.8 (13)
C4—C5—C6—N2	175.7 (6)	C37—Sn1—C43—C44	-170.9 (6)
C14—C5—C6—N2	-1.1 (10)	C49—Sn1—C43—C44	64.4 (6)
C6—N2—C7—O3	177.8 (7)	S7—Sn1—C43—C44	-43.7 (6)
C15—N2—C7—O3	-5.5 (10)	C37—Sn1—C43—C48	6.0 (6)
C6—N2—C7—C8	-1.1 (10)	C49—Sn1—C43—C48	-118.8 (5)
C15—N2—C7—C8	175.7 (6)	S7—Sn1—C43—C48	133.1 (5)
O3—C7—C8—C9	0.6 (11)	C48—C43—C44—C45	0.6 (10)
N2—C7—C8—C9	179.5 (6)	Sn1—C43—C44—C45	177.5 (5)
O3—C7—C8—C14	178.6 (7)	C43—C44—C45—C46	1.8 (11)
N2—C7—C8—C14	-2.5 (9)	C44—C45—C46—C47	-2.3 (12)
C14—C8—C9—C10	-2.1 (11)	C45—C46—C47—C48	0.5 (12)
C7—C8—C9—C10	175.9 (7)	C46—C47—C48—C43	1.9 (11)
C8—C9—C10—C11	2.0 (11)	C44—C43—C48—C47	-2.4 (10)
C9—C10—C11—C13	-1.4 (11)	Sn1—C43—C48—C47	-179.5 (6)
C9—C10—C11—C12	-179.8 (7)	C37—Sn1—C49—C54	-110.2 (7)
C1—N1—C12—O4	176.7 (6)	C43—Sn1—C49—C54	15.9 (7)
C19—N1—C12—O4	-3.5 (9)	S7—Sn1—C49—C54	136.9 (6)
C1—N1—C12—C11	-1.5 (9)	C37—Sn1—C49—C50	65.8 (7)
C19—N1—C12—C11	178.3 (5)	C43—Sn1—C49—C50	-168.1 (6)
C10—C11—C12—O4	2.4 (11)	S7—Sn1—C49—C50	-47.1 (6)
C13—C11—C12—O4	-176.0 (7)	C54—C49—C50—C51	4.0 (13)
C10—C11—C12—N1	-179.4 (6)	Sn1—C49—C50—C51	-172.0 (6)
C13—C11—C12—N1	2.1 (9)	C49—C50—C51—C52	-0.4 (14)
C3—C2—C13—C11	-179.6 (6)	C50—C51—C52—C53	-3.1 (15)
C1—C2—C13—C11	0.0 (10)	C51—C52—C53—C54	2.9 (15)
C3—C2—C13—C14	-0.3 (9)	C50—C49—C54—C53	-4.1 (11)

C1—C2—C13—C14	179.2 (6)	Sn1—C49—C54—C53	171.9 (5)
C10—C11—C13—C2	-179.8 (6)	C52—C53—C54—C49	0.8 (12)
C12—C11—C13—C2	-1.4 (10)	C61—Sn2—C55—C56	-129.2 (7)
C10—C11—C13—C14	0.9 (10)	C67—Sn2—C55—C56	106.8 (7)
C12—C11—C13—C14	179.3 (6)	S5—Sn2—C55—C56	1.8 (7)
C4—C5—C14—C8	-179.2 (6)	C61—Sn2—C55—C60	55.9 (7)
C6—C5—C14—C8	-2.4 (10)	C67—Sn2—C55—C60	-68.1 (6)
C4—C5—C14—C13	1.5 (10)	S5—Sn2—C55—C60	-173.1 (5)
C6—C5—C14—C13	178.3 (6)	C60—C55—C56—C57	-2.8 (12)
C9—C8—C14—C5	-177.8 (7)	Sn2—C55—C56—C57	-177.5 (6)
C7—C8—C14—C5	4.3 (10)	C55—C56—C57—C58	1.0 (13)
C9—C8—C14—C13	1.5 (9)	C56—C57—C58—C59	0.2 (14)
C7—C8—C14—C13	-176.4 (6)	C57—C58—C59—C60	0.5 (14)
C2—C13—C14—C5	-0.9 (9)	C58—C59—C60—C55	-2.4 (14)
C11—C13—C14—C5	178.4 (7)	C56—C55—C60—C59	3.5 (13)
C2—C13—C14—C8	179.8 (6)	Sn2—C55—C60—C59	178.6 (6)
C11—C13—C14—C8	-0.9 (9)	C55—Sn2—C61—C62	179.4 (6)
C6—N2—C15—C16	77.7 (8)	C67—Sn2—C61—C62	-59.4 (6)
C7—N2—C15—C16	-99.4 (7)	S5—Sn2—C61—C62	50.9 (6)
C17—O5—C16—C15	80.8 (7)	C55—Sn2—C61—C66	1.0 (6)
N2—C15—C16—O5	60.4 (8)	C67—Sn2—C61—C66	122.2 (5)
C16—O5—C17—C18	168.4 (5)	S5—Sn2—C61—C66	-127.5 (5)
P2—O6—C18—C17	173.7 (5)	C66—C61—C62—C63	-0.2 (11)
O5—C17—C18—O6	69.2 (7)	Sn2—C61—C62—C63	-178.6 (5)
C12—N1—C19—C20	-79.5 (7)	C61—C62—C63—C64	1.3 (12)
C1—N1—C19—C20	100.3 (7)	C62—C63—C64—C65	-2.1 (12)
C21—O7—C20—C19	177.8 (6)	C63—C64—C65—C66	1.7 (12)
N1—C19—C20—O7	-74.0 (7)	C64—C65—C66—C61	-0.7 (12)
C20—O7—C21—C22	171.7 (6)	C62—C61—C66—C65	-0.1 (10)
P1—O8—C22—C21	163.3 (4)	Sn2—C61—C66—C65	178.4 (6)
O7—C21—C22—O8	59.7 (7)	C61—Sn2—C67—C68	166.1 (6)
O6—P2—C23—C24	54.9 (6)	C55—Sn2—C67—C68	-70.1 (6)
S1—P2—C23—C24	179.5 (5)	S5—Sn2—C67—C68	44.4 (6)
S7—P2—C23—C24	-51.3 (6)	C61—Sn2—C67—C72	-20.8 (7)
O6—P2—C23—C28	-125.3 (6)	C55—Sn2—C67—C72	103.0 (6)
S1—P2—C23—C28	-0.7 (6)	S5—Sn2—C67—C72	-142.5 (6)
S7—P2—C23—C28	128.5 (5)	C72—C67—C68—C69	-3.6 (11)
C28—C23—C24—C25	1.7 (10)	Sn2—C67—C68—C69	169.7 (6)
P2—C23—C24—C25	-178.4 (5)	C67—C68—C69—C70	0.2 (12)
C23—C24—C25—C26	0.9 (10)	C68—C69—C70—C71	3.8 (12)
C29—O9—C26—C27	6.7 (11)	C69—C70—C71—C72	-4.3 (12)
C29—O9—C26—C25	-172.5 (7)	C68—C67—C72—C71	3.0 (11)
C24—C25—C26—O9	177.4 (6)	Sn2—C67—C72—C71	-170.1 (5)

C24—C25—C26—C27	-1.8 (10)	C70—C71—C72—C67	0.9 (11)

Table A10: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2(SnPh_3)_2]_2$⊂15DN38C10

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1A	0.55437 (3)	0.90708 (2)	-0.335923 (13)	0.03600 (10)	
Sn1B	0.29242 (3)	0.42871 (2)	-0.185473 (13)	0.03841 (10)	
S1A	0.38084 (11)	0.99968 (8)	-0.28392 (5)	0.0381 (3)	
S1B	0.26945 (11)	0.35360 (8)	-0.10650 (5)	0.0397 (3)	
S2A	0.28052 (18)	0.95847 (11)	-0.38807 (6)	0.0672 (5)	
S2B	0.54990 (12)	0.40517 (8)	-0.13233 (5)	0.0403 (3)	
P1A	0.29245 (12)	1.03923 (9)	-0.33912 (5)	0.0409 (3)	
P1B	0.44384 (12)	0.32940 (8)	-0.09796 (5)	0.0355 (3)	
O1A	0.1767 (3)	1.5313 (2)	-0.38439 (14)	0.0447 (9)	
O1B	0.3271 (3)	0.0801 (2)	0.00503 (14)	0.0434 (9)	
O2A	0.3115 (3)	1.3393 (2)	-0.50691 (13)	0.0461 (9)	
O2B	0.2939 (3)	-0.1464 (2)	-0.08203 (15)	0.0508 (10)	
O3A	0.3043 (3)	1.2825 (2)	-0.38968 (13)	0.0413 (8)	
O3B	0.4487 (3)	0.0732 (2)	-0.11511 (13)	0.0414 (9)	
O4A	0.3643 (3)	1.1138 (2)	-0.36251 (12)	0.0388 (8)	
O4B	0.4837 (3)	0.2347 (2)	-0.11171 (13)	0.0412 (8)	
O5A	-0.1897 (6)	1.1854 (4)	-0.2484 (3)	0.068 (2)	0.730 (7)
O5B	0.3645 (3)	0.3206 (2)	0.12214 (13)	0.0449 (9)	
O5C	-0.1313 (19)	1.2507 (11)	-0.2201 (7)	0.072 (6)	0.270 (7)
O6A	-0.2684 (4)	1.4993 (2)	-0.36813 (14)	0.0500 (10)	
O6B	0.0174 (3)	-0.0462 (2)	-0.16015 (14)	0.0433 (9)	
O7A	-0.2821 (5)	1.6673 (3)	-0.32124 (17)	0.0750 (14)	
O7B	0.0207 (3)	-0.2183 (2)	-0.15628 (13)	0.0427 (9)	
O8A	-0.0678 (4)	1.7367 (3)	-0.34420 (16)	0.0605 (11)	
O8B	-0.0034 (3)	-0.3377 (2)	-0.08200 (14)	0.0478 (9)	
O9A	-0.0642 (3)	1.8747 (3)	-0.41028 (18)	0.0618 (12)	
O9B	0.1276 (3)	-0.4137 (2)	-0.01328 (14)	0.0467 (9)	
O10A	0.0411 (3)	1.7962 (2)	-0.50818 (17)	0.0558 (11)	
O10B	0.1377 (3)	-0.2795 (2)	0.05797 (14)	0.0444 (9)	
O11A	0.7233 (3)	0.8132 (2)	-0.37968 (14)	0.0431 (9)	
N1A	0.2456 (4)	1.4363 (2)	-0.44604 (15)	0.0353 (9)	
N1B	0.3096 (4)	-0.0291 (2)	-0.04235 (17)	0.0380 (10)	
C1A	-0.0124 (4)	1.5978 (3)	-0.42905 (18)	0.0345 (11)	
H1A	-0.0011	1.6264	-0.4017	0.041*	
C1B	0.0778 (5)	0.1207 (3)	0.03268 (19)	0.0395 (12)	
H1B	0.1238	0.1591	0.0412	0.047*	
C2A	0.0654 (4)	1.5293 (3)	-0.44696 (18)	0.0323 (11)	

C2B	0.1323 (4)	0.0521 (3)	0.00483 (18)	0.0332 (11)	
C3A	0.1649 (4)	1.5002 (3)	-0.42232 (19)	0.0351 (11)	
C3B	0.2610 (5)	0.0375 (3)	-0.0098 (2)	0.0389 (12)	
C4A	0.0482 (4)	1.4866 (3)	-0.48895 (17)	0.0272 (10)	
C4B	0.0614 (4)	-0.0063 (3)	-0.00799 (19)	0.0340 (11)	
C5A	0.1268 (4)	1.4178 (3)	-0.50865 (17)	0.0301 (10)	
C5B	0.1135 (5)	-0.0768 (3)	-0.03667 (19)	0.0359 (11)	
C6A	0.2341 (4)	1.3939 (3)	-0.48789 (19)	0.0352 (11)	
C6B	0.2440 (5)	-0.0881 (3)	-0.0560 (2)	0.0404 (12)	
C7A	0.1082 (4)	1.3754 (3)	-0.54843 (18)	0.0348 (11)	
H7A	0.1592	1.3288	-0.5605	0.042*	
C7B	0.0447 (4)	-0.1334 (3)	-0.0482 (2)	0.0377 (12)	
H7B	0.0800	-0.1804	-0.0665	0.045*	
C8A	0.3545 (5)	1.4167 (3)	-0.4259 (2)	0.0451 (13)	
H8A1	0.3806	1.4676	-0.4168	0.054*	
H8A2	0.4167	1.3898	-0.4517	0.054*	
C8B	0.4385 (5)	-0.0425 (3)	-0.0604 (2)	0.0458 (14)	
H8B1	0.4649	-0.1010	-0.0587	0.055*	
H8B2	0.4765	-0.0137	-0.0386	0.055*	
C9A	0.3357 (5)	1.3608 (3)	-0.3803 (2)	0.0459 (14)	
H9A1	0.4081	1.3533	-0.3673	0.055*	
H9A2	0.2739	1.3883	-0.3546	0.055*	
C9B	0.4767 (5)	-0.0132 (3)	-0.1132 (2)	0.0476 (14)	
H9B1	0.5614	-0.0276	-0.1244	0.057*	
H9B2	0.4366	-0.0399	-0.1351	0.057*	
C10A	0.3998 (5)	1.2282 (3)	-0.4176 (2)	0.0413 (12)	
H10A	0.4712	1.2304	-0.4046	0.050*	
H10B	0.4156	1.2445	-0.4524	0.050*	
C10B	0.5106 (5)	0.1092 (3)	-0.1585 (2)	0.0435 (13)	
H10C	0.4956	0.0838	-0.1879	0.052*	
H10D	0.5952	0.1003	-0.1593	0.052*	
C11A	0.3645 (5)	1.1428 (3)	-0.41285 (19)	0.0405 (12)	
H11A	0.2861	1.1428	-0.4201	0.049*	
H11B	0.4198	1.1064	-0.4365	0.049*	
C11B	0.4705 (5)	0.1996 (3)	-0.15817 (19)	0.0425 (13)	
H11C	0.5177	0.2259	-0.1862	0.051*	
H11D	0.3882	0.2086	-0.1613	0.051*	
C12A	0.1455 (7)	1.0817 (6)	-0.3093 (5)	0.038 (3)	0.730 (7)
C12B	0.4294 (4)	0.3254 (3)	-0.03197 (18)	0.0333 (11)	
C12C	0.1678 (19)	1.1050 (18)	-0.3043 (13)	0.047 (8)	0.270 (7)
C13A	0.1285 (8)	1.1232 (5)	-0.2659 (4)	0.054 (2)	0.730 (7)

H13A	0.1924	1.1264	-0.2507	0.065*	0.730 (7)
C13B	0.4405 (5)	0.3953 (3)	-0.00565 (19)	0.0364 (11)	
H13B	0.4609	0.4427	-0.0232	0.044*	
C13C	0.1610 (19)	1.1869 (13)	-0.2893 (8)	0.047 (5)	0.270 (7)
H13C	0.2292	1.2128	-0.2994	0.056*	0.270 (7)
C14A	0.0151 (8)	1.1622 (7)	-0.2430 (4)	0.055 (2)	0.730 (7)
H14A	0.0030	1.1930	-0.2138	0.066*	0.730 (7)
C14B	0.4220 (4)	0.3959 (3)	0.04560 (19)	0.0379 (12)	
H14B	0.4312	0.4428	0.0625	0.045*	
C14C	0.063 (2)	1.2346 (14)	-0.2608 (8)	0.056 (6)	0.270 (7)
H14C	0.0682	1.2884	-0.2515	0.068*	0.270 (7)
C15A	-0.0763 (9)	1.1517 (8)	-0.2668 (4)	0.047 (2)	0.730 (7)
C15B	0.3896 (4)	0.3258 (3)	0.07186 (19)	0.0376 (12)	
C15C	-0.042 (2)	1.1980 (16)	-0.2468 (8)	0.044 (6)	0.270 (7)
C16A	-0.0593 (7)	1.1100 (6)	-0.3109 (4)	0.061 (3)	0.730 (7)
H16A	-0.1228	1.1073	-0.3265	0.073*	0.730 (7)
C16B	0.3780 (5)	0.2555 (3)	0.0463 (2)	0.0402 (12)	
H16B	0.3564	0.2085	0.0640	0.048*	
C16C	-0.040 (3)	1.1198 (18)	-0.2599 (12)	0.053 (8)	0.270 (7)
H16C	-0.1083	1.0946	-0.2479	0.064*	0.270 (7)
C17A	0.0503 (7)	1.0720 (6)	-0.3322 (3)	0.057 (2)	0.730 (7)
H17A	0.0615	1.0407	-0.3612	0.068*	0.730 (7)
C17B	0.3981 (4)	0.2550 (3)	-0.0051 (2)	0.0377 (12)	
H17B	0.3908	0.2076	-0.0220	0.045*	
C17C	0.053 (2)	1.0728 (15)	-0.2892 (9)	0.053 (6)	0.270 (7)
H17C	0.0428	1.0205	-0.2995	0.064*	0.270 (7)
C18C	-0.229 (7)	1.205 (4)	-0.206 (3)	0.16 (3)	0.270 (7)
H18A	-0.2661	1.2010	-0.2343	0.247*	0.270 (7)
H18B	-0.2843	1.2314	-0.1790	0.247*	0.270 (7)
H18C	-0.2012	1.1502	-0.1966	0.247*	0.270 (7)
C18B	0.3626 (6)	0.3928 (4)	0.1506 (2)	0.0523 (15)	
H18D	0.4403	0.4107	0.1441	0.078*	
H18E	0.3393	0.3808	0.1855	0.078*	
H18F	0.3071	0.4356	0.1413	0.078*	
C18A	-0.2147 (13)	1.2314 (9)	-0.2022 (7)	0.059 (3)	0.730 (7)
H18G	-0.2125	1.1939	-0.1748	0.089*	0.730 (7)
H18H	-0.2920	1.2620	-0.1979	0.089*	0.730 (7)
H18I	-0.1564	1.2689	-0.2031	0.089*	0.730 (7)
C19A	0.6182 (5)	0.9887 (3)	-0.39454 (19)	0.0392 (12)	
C19B	0.1186 (5)	0.4316 (3)	-0.2005 (2)	0.0440 (13)	
C20A	0.6623 (4)	1.0603 (3)	-0.3853 (2)	0.0374 (12)	
H20A	0.6633	1.0742	-0.3526	0.045*	
C20B	0.0220 (5)	0.4084 (4)	-0.1668 (2)	0.0498 (14)	

H20B	0.0327	0.3869	-0.1361	0.060*	
C21A	0.7058 (5)	1.1127 (3)	-0.4242 (2)	0.0434 (13)	
H21A	0.7359	1.1607	-0.4175	0.052*	
C21B	-0.0898 (6)	0.4163 (4)	-0.1775 (3)	0.0655 (18)	
H21B	-0.1539	0.4018	-0.1538	0.079*	
C22A	0.7034 (5)	1.0926 (4)	-0.4723 (2)	0.0522 (15)	
H22A	0.7313	1.1273	-0.4984	0.063*	
C22B	-0.1060 (7)	0.4460 (5)	-0.2238 (3)	0.074 (2)	
H22B	-0.1808	0.4505	-0.2317	0.089*	
C23A	0.6598 (6)	1.0214 (4)	-0.4820 (2)	0.0592 (17)	
H23A	0.6580	1.0082	-0.5148	0.071*	
C23B	-0.0120 (8)	0.4686 (5)	-0.2577 (3)	0.075 (2)	
H23B	-0.0230	0.4883	-0.2887	0.090*	
C24A	0.6185 (5)	0.9687 (4)	-0.4435 (2)	0.0515 (15)	
H24A	0.5909	0.9199	-0.4507	0.062*	
C24B	0.1016 (7)	0.4625 (4)	-0.2465 (2)	0.0639 (18)	
H24B	0.1650	0.4791	-0.2697	0.077*	
C25A	0.6440 (4)	0.8981 (3)	-0.27467 (18)	0.0360 (11)	
C25B	0.3274 (5)	0.5505 (3)	-0.1740 (2)	0.0396 (12)	
C26A	0.6064 (5)	0.8491 (4)	-0.2344 (2)	0.0520 (15)	
H26A	0.5390	0.8227	-0.2332	0.062*	
C26B	0.2916 (5)	0.5870 (3)	-0.1272 (2)	0.0450 (13)	
H26B	0.2560	0.5573	-0.1000	0.054*	
C27A	0.6666 (6)	0.8384 (4)	-0.1957 (2)	0.0545 (16)	
H27A	0.6412	0.8034	-0.1695	0.065*	
C27B	0.3101 (5)	0.6696 (4)	-0.1216 (2)	0.0507 (14)	
H27B	0.2850	0.6948	-0.0904	0.061*	
C28A	0.7630 (5)	0.8789 (3)	-0.1957 (2)	0.0468 (14)	
H28A	0.8039	0.8716	-0.1697	0.056*	
C28B	0.3639 (5)	0.7133 (3)	-0.1608 (2)	0.0509 (15)	
H28B	0.3776	0.7674	-0.1563	0.061*	
C29A	0.7981 (6)	0.9303 (4)	-0.2345 (2)	0.0575 (16)	
H29A	0.8622	0.9597	-0.2344	0.069*	
C29B	0.3978 (5)	0.6770 (3)	-0.2072 (2)	0.0507 (15)	
H29B	0.4340	0.7069	-0.2342	0.061*	
C30A	0.7395 (5)	0.9391 (4)	-0.2738 (2)	0.0547 (16)	
H30A	0.7656	0.9737	-0.3002	0.066*	
C30B	0.3785 (5)	0.5956 (3)	-0.2140 (2)	0.0463 (13)	
H30B	0.4002	0.5718	-0.2457	0.056*	
C31A	0.4617 (5)	0.8071 (3)	-0.3497 (2)	0.0456 (13)	
C31B	0.4188 (5)	0.3624 (3)	-0.24265 (18)	0.0387 (12)	
C32A	0.3654 (5)	0.7865 (4)	-0.3141 (2)	0.0492 (14)	
H32A	0.3417	0.8167	-0.2846	0.059*	

C32B	0.5319 (5)	0.3864 (3)	-0.25907 (19)	0.0428 (13)	
H32B	0.5502	0.4350	-0.2468	0.051*	
C33A	0.3042 (5)	0.7211 (4)	-0.3222 (3)	0.0592 (17)	
H33A	0.2425	0.7058	-0.2976	0.071*	
C33B	0.6170 (5)	0.3395 (4)	-0.2931 (2)	0.0471 (14)	
H33B	0.6914	0.3571	-0.3042	0.056*	
C34A	0.3364 (6)	0.6794 (4)	-0.3672 (3)	0.0655 (19)	
H34A	0.2953	0.6363	-0.3731	0.079*	
C34B	0.5912 (6)	0.2669 (4)	-0.3103 (2)	0.0510 (15)	
H34B	0.6490	0.2344	-0.3327	0.061*	
C35A	0.4277 (6)	0.7009 (4)	-0.4028 (3)	0.0669 (19)	
H35A	0.4464	0.6739	-0.4335	0.080*	
C35B	0.4804 (6)	0.2415 (4)	-0.2949 (2)	0.0538 (16)	
H35B	0.4636	0.1922	-0.3068	0.065*	
C36A	0.4935 (5)	0.7626 (4)	-0.3939 (2)	0.0502 (15)	
H36A	0.5592	0.7741	-0.4176	0.060*	
C36B	0.3935 (5)	0.2897 (3)	-0.2615 (2)	0.0464 (13)	
H36B	0.3181	0.2732	-0.2518	0.056*	
C37A	-0.2590 (5)	1.4442 (3)	-0.4062 (2)	0.0430 (13)	
C37B	0.0372 (5)	0.0265 (3)	-0.1410 (2)	0.0400 (12)	
C38A	-0.3323 (5)	1.4485 (3)	-0.4389 (2)	0.0418 (13)	
H38A	-0.3938	1.4912	-0.4363	0.050*	
C38B	0.1468 (5)	0.0530 (3)	-0.1452 (2)	0.0500 (15)	
H38B	0.2143	0.0206	-0.1616	0.060*	
C39A	-0.3164 (4)	1.3893 (3)	-0.4765 (2)	0.0396 (12)	
H39A	-0.3685	1.3927	-0.4984	0.047*	
C39B	0.1564 (5)	0.1290 (3)	-0.1246 (3)	0.0553 (16)	
H39B	0.2313	0.1453	-0.1263	0.066*	
C40A	-0.2270 (4)	1.3272 (3)	-0.4818 (2)	0.0409 (12)	
H40A	-0.2178	1.2883	-0.5070	0.049*	
C40B	0.0590 (5)	0.1801 (3)	-0.1020 (2)	0.0464 (14)	
H40B	0.0673	0.2317	-0.0902	0.056*	
C41A	-0.1474 (4)	1.3216 (3)	-0.4487 (2)	0.0380 (12)	
C41B	-0.0544 (4)	0.1533 (3)	-0.0968 (2)	0.0386 (12)	
C42A	-0.0491 (5)	1.2577 (3)	-0.4531 (2)	0.0467 (14)	
C42B	-0.1586 (5)	0.2031 (3)	-0.0719 (2)	0.0387 (12)	
C43A	0.0272 (5)	1.2550 (4)	-0.4212 (3)	0.0572 (17)	
H43A	0.0920	1.2147	-0.4249	0.069*	
C43B	-0.2668 (5)	0.1752 (3)	-0.06395 (19)	0.0395 (12)	
H43B	-0.3335	0.2078	-0.0470	0.047*	
C44A	0.0072 (6)	1.3133 (4)	-0.3827 (2)	0.0586 (17)	
H44A	0.0578	1.3097	-0.3603	0.070*	
C44B	-0.2773 (5)	0.0964 (3)	-0.0816 (2)	0.0416 (12)	

H44B	-0.3512	0.0771	-0.0755	0.050*	
C45A	-0.0829 (5)	1.3746 (4)	-0.3771 (2)	0.0498 (14)	
H45A	-0.0927	1.4130	-0.3516	0.060*	
C45B	-0.1818 (4)	0.0479 (3)	-0.10736 (19)	0.0357 (11)	
H45B	-0.1914	-0.0031	-0.1195	0.043*	
C46A	-0.1633 (5)	1.3804 (3)	-0.4105 (2)	0.0394 (12)	
C46B	-0.0679 (5)	0.0748 (3)	-0.11572 (19)	0.0384 (12)	
C47A	-0.3638 (6)	1.5650 (4)	-0.3626 (2)	0.0587 (17)	
H47A	-0.4381	1.5420	-0.3605	0.070*	
H47B	-0.3523	1.6004	-0.3918	0.070*	
C47B	0.1209 (5)	-0.1009 (3)	-0.1821 (2)	0.0463 (14)	
H47C	0.1710	-0.1134	-0.1579	0.056*	
H47D	0.1662	-0.0747	-0.2107	0.056*	
C48A	-0.3698 (7)	1.6144 (4)	-0.3172 (3)	0.076 (2)	
H48A	-0.4467	1.6470	-0.3093	0.092*	
H48B	-0.3637	1.5771	-0.2896	0.092*	
C48B	0.0822 (5)	-0.1780 (3)	-0.1979 (2)	0.0452 (13)	
H48C	0.0312	-0.1650	-0.2216	0.054*	
H48D	0.1510	-0.2142	-0.2143	0.054*	
C49A	-0.1853 (6)	1.6338 (4)	-0.3074 (3)	0.071 (2)	
H49A	-0.1404	1.5965	-0.3334	0.085*	
H49B	-0.2072	1.6016	-0.2774	0.085*	
C49B	0.0107 (6)	-0.3017 (3)	-0.1666 (2)	0.0480 (14)	
H49C	0.0890	-0.3322	-0.1752	0.058*	
H49D	-0.0274	-0.3042	-0.1949	0.058*	
C50A	-0.1063 (8)	1.6985 (5)	-0.2971 (3)	0.090 (3)	
H50A	-0.1510	1.7390	-0.2728	0.108*	
H50B	-0.0390	1.6723	-0.2843	0.108*	
C50B	-0.0601 (6)	-0.3393 (4)	-0.1222 (2)	0.0537 (15)	
H50C	-0.1385	-0.3088	-0.1137	0.064*	
H50D	-0.0690	-0.3958	-0.1296	0.064*	
C51A	0.0064 (7)	1.8001 (5)	-0.3452 (3)	0.083 (3)	
H51A	0.0773	1.7788	-0.3333	0.099*	
H51B	-0.0349	1.8448	-0.3233	0.099*	
C51B	-0.0547 (5)	-0.3865 (4)	-0.0413 (2)	0.0513 (15)	
H51C	-0.0459	-0.4439	-0.0514	0.062*	
H51D	-0.1385	-0.3681	-0.0308	0.062*	
C52A	0.0395 (6)	1.8312 (4)	-0.3970 (3)	0.076 (2)	
H52A	0.1005	1.8678	-0.3990	0.092*	
H52B	0.0704	1.7854	-0.4198	0.092*	
C52B	0.0078 (5)	-0.3775 (4)	0.0010 (2)	0.0475 (14)	
H52C	0.0056	-0.3195	0.0088	0.057*	
H52D	-0.0317	-0.4047	0.0305	0.057*	

C53A	-0.0457 (6)	1.9129 (4)	-0.4574 (3)	0.077 (2)	
H53A	0.0331	1.9303	-0.4645	0.093*	
H53B	-0.1020	1.9621	-0.4559	0.093*	
C53B	0.1943 (5)	-0.4146 (3)	0.0244 (2)	0.0479 (14)	
H53C	0.2625	-0.4559	0.0158	0.057*	
H53D	0.1462	-0.4314	0.0555	0.057*	
C54A	-0.0578 (5)	1.8601 (4)	-0.4997 (3)	0.0651 (19)	
H54A	-0.1317	1.8357	-0.4915	0.078*	
H54B	-0.0580	1.8932	-0.5296	0.078*	
C54B	0.2373 (5)	-0.3330 (3)	0.0327 (2)	0.0423 (13)	
H54C	0.2977	-0.3409	0.0527	0.051*	
H54D	0.2712	-0.3092	0.0009	0.051*	
H11F	0.7162	0.7647	-0.3610	0.06 (2)*	
H11G	0.8059	0.8295	-0.3917	0.08 (2)*	

Table A11: Atomic displacement parameters ($Å^2$) for NDI-[$CH_2CH_2OCH_2CH_2O$(An)PS_2(Sn-Ph_3)$_2$]$_2$⊂15DN38C10

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1A	0.0280 (2)	0.0410 (2)	0.0392 (2)	-0.00769 (14)	-0.00470 (14)	-0.00415 (15)
Sn1B	0.0363 (2)	0.0396 (2)	0.0377 (2)	-0.00255 (15)	-0.00437 (15)	-0.00253 (15)
S1A	0.0315 (7)	0.0433 (7)	0.0381 (7)	-0.0010 (5)	-0.0062 (5)	0.0003 (5)
S1B	0.0298 (7)	0.0474 (7)	0.0411 (7)	-0.0045 (5)	-0.0052 (5)	0.0032 (6)
S2A	0.0923 (14)	0.0703 (11)	0.0539 (10)	-0.0400 (10)	-0.0333 (9)	0.0081 (8)
S2B	0.0327 (7)	0.0475 (7)	0.0392 (7)	-0.0073 (5)	-0.0027 (5)	0.0012 (6)
P1A	0.0323 (8)	0.0515 (8)	0.0412 (8)	-0.0096 (6)	-0.0104 (6)	0.0049 (6)
P1B	0.0301 (7)	0.0383 (7)	0.0364 (7)	-0.0026 (5)	-0.0035 (5)	-0.0028 (5)
O1A	0.050 (2)	0.040 (2)	0.049 (2)	-0.0023 (17)	-0.0210 (18)	-0.0044 (17)
O1B	0.033 (2)	0.043 (2)	0.059 (2)	-0.0094 (16)	-0.0156 (17)	-0.0056 (17)
O2A	0.038 (2)	0.047 (2)	0.046 (2)	0.0181 (17)	-0.0040 (17)	-0.0010 (17)
O2B	0.039 (2)	0.039 (2)	0.072 (3)	-0.0008 (17)	-0.0068 (19)	-0.0149 (19)
O3A	0.035 (2)	0.043 (2)	0.043 (2)	0.0045 (16)	-0.0059 (16)	0.0039 (16)
O3B	0.029 (2)	0.043 (2)	0.049 (2)	-0.0005 (15)	-0.0019 (16)	-0.0034 (17)
O4A	0.038 (2)	0.047 (2)	0.0337 (19)	-0.0068 (16)	-0.0112 (15)	0.0064 (16)
O4B	0.037 (2)	0.042 (2)	0.044 (2)	0.0003 (16)	-0.0094 (16)	-0.0031 (16)
O5A	0.037 (4)	0.081 (5)	0.083 (5)	-0.001 (3)	-0.008 (3)	0.014 (4)
O5B	0.049 (2)	0.048 (2)	0.037 (2)	-0.0063 (18)	-0.0088 (17)	0.0019 (17)
O5C	0.072 (13)	0.064 (11)	0.064 (11)	-0.012 (9)	0.030 (10)	-0.005 (9)
O6A	0.053 (3)	0.047 (2)	0.046 (2)	-0.0070 (18)	0.0000 (18)	-0.0047 (18)
O6B	0.032 (2)	0.041 (2)	0.054 (2)	0.0021 (15)	-0.0033 (16)	-0.0038 (17)
O7A	0.086 (4)	0.075 (3)	0.063 (3)	-0.014 (3)	-0.009 (3)	-0.010 (3)
O7B	0.043 (2)	0.038 (2)	0.045 (2)	-0.0014 (16)	-0.0034 (17)	-0.0044 (16)

O8A	0.050 (3)	0.071 (3)	0.059 (3)	0.005 (2)	-0.014 (2)	-0.020 (2)
O8B	0.046 (2)	0.048 (2)	0.051 (2)	-0.0130 (18)	-0.0092 (18)	0.0037 (18)
O9A	0.027 (2)	0.053 (3)	0.097 (4)	-0.0013 (18)	0.004 (2)	-0.012 (2)
O9B	0.037 (2)	0.049 (2)	0.050 (2)	0.0000 (17)	-0.0017 (17)	-0.0068 (18)
O10A	0.031 (2)	0.036 (2)	0.089 (3)	0.0087 (16)	0.008 (2)	-0.003 (2)
O10B	0.028 (2)	0.040 (2)	0.062 (3)	-0.0042 (15)	-0.0021 (17)	-0.0064 (18)
O11A	0.035 (2)	0.041 (2)	0.051 (2)	-0.0052 (16)	-0.0026 (16)	-0.0075 (18)
N1A	0.024 (2)	0.037 (2)	0.044 (3)	-0.0011 (17)	-0.0086 (18)	0.0051 (19)
N1B	0.030 (2)	0.031 (2)	0.053 (3)	-0.0021 (17)	-0.0085 (19)	-0.0022 (19)
C1A	0.036 (3)	0.033 (3)	0.033 (3)	-0.003 (2)	-0.003 (2)	-0.003 (2)
C1B	0.048 (4)	0.028 (3)	0.043 (3)	-0.006 (2)	-0.011 (2)	-0.003 (2)
C2A	0.030 (3)	0.029 (2)	0.037 (3)	-0.002 (2)	-0.007 (2)	0.005 (2)
C2B	0.025 (3)	0.035 (3)	0.041 (3)	-0.004 (2)	-0.009 (2)	-0.001 (2)
C3A	0.034 (3)	0.035 (3)	0.037 (3)	-0.006 (2)	-0.008 (2)	0.002 (2)
C3B	0.034 (3)	0.037 (3)	0.047 (3)	-0.003 (2)	-0.012 (2)	0.003 (2)
C4A	0.027 (3)	0.026 (2)	0.029 (2)	-0.0043 (18)	-0.0031 (19)	0.0021 (18)
C4B	0.032 (3)	0.032 (3)	0.040 (3)	-0.006 (2)	-0.012 (2)	-0.002 (2)
C5A	0.027 (3)	0.026 (2)	0.033 (3)	-0.0001 (18)	0.0008 (19)	0.0044 (19)
C5B	0.034 (3)	0.030 (3)	0.043 (3)	-0.001 (2)	-0.008 (2)	-0.005 (2)
C6A	0.030 (3)	0.034 (3)	0.038 (3)	-0.003 (2)	0.001 (2)	0.008 (2)
C6B	0.031 (3)	0.034 (3)	0.056 (4)	-0.006 (2)	-0.008 (2)	-0.001 (2)
C7A	0.030 (3)	0.032 (3)	0.037 (3)	0.001 (2)	0.004 (2)	-0.003 (2)
C7B	0.033 (3)	0.029 (3)	0.050 (3)	-0.001 (2)	-0.006 (2)	-0.007 (2)
C8A	0.041 (3)	0.041 (3)	0.057 (4)	-0.005 (2)	-0.019 (3)	0.006 (3)
C8B	0.027 (3)	0.042 (3)	0.068 (4)	0.001 (2)	-0.011 (3)	0.001 (3)
C9A	0.040 (3)	0.049 (3)	0.051 (3)	0.005 (3)	-0.020 (3)	-0.001 (3)
C9B	0.025 (3)	0.043 (3)	0.073 (4)	0.000 (2)	-0.006 (3)	-0.010 (3)
C10A	0.032 (3)	0.047 (3)	0.042 (3)	0.001 (2)	-0.005 (2)	0.010 (2)
C10B	0.035 (3)	0.057 (3)	0.037 (3)	-0.004 (2)	-0.002 (2)	-0.004 (3)
C11A	0.035 (3)	0.045 (3)	0.042 (3)	0.001 (2)	-0.011 (2)	0.002 (2)
C11B	0.041 (3)	0.050 (3)	0.035 (3)	0.001 (2)	-0.009 (2)	-0.001 (2)
C12A	0.015 (5)	0.050 (6)	0.055 (6)	-0.013 (4)	-0.015 (5)	0.018 (5)
C12B	0.023 (3)	0.034 (3)	0.041 (3)	-0.0007 (19)	-0.004 (2)	-0.001 (2)
C12C	0.035 (14)	0.081 (19)	0.040 (15)	-0.047 (13)	-0.020 (12)	0.023 (14)
C13A	0.038 (5)	0.056 (5)	0.069 (7)	-0.001 (4)	-0.017 (4)	-0.002 (5)
C13B	0.040 (3)	0.031 (3)	0.037 (3)	-0.005 (2)	-0.004 (2)	0.003 (2)
C13C	0.039 (12)	0.048 (12)	0.049 (12)	-0.003 (9)	0.001 (9)	-0.004 (10)
C14A	0.032 (6)	0.067 (7)	0.065 (6)	-0.003 (5)	-0.011 (4)	-0.011 (5)
C14B	0.035 (3)	0.037 (3)	0.041 (3)	-0.005 (2)	-0.004 (2)	-0.008 (2)
C14C	0.085 (16)	0.042 (11)	0.045 (12)	-0.008 (11)	-0.022 (11)	0.002 (9)
C15A	0.023 (6)	0.051 (7)	0.062 (7)	0.006 (5)	-0.005 (4)	0.007 (5)
C15B	0.028 (3)	0.043 (3)	0.041 (3)	-0.001 (2)	-0.007 (2)	0.002 (2)
C15C	0.034 (13)	0.046 (12)	0.043 (11)	0.027 (11)	-0.007 (9)	0.017 (10)

C16A	0.029 (5)	0.078 (6)	0.080 (7)	-0.008 (4)	-0.020 (4)	0.011 (5)
C16B	0.037 (3)	0.037 (3)	0.047 (3)	-0.004 (2)	-0.010 (2)	0.005 (2)
C16C	0.030 (15)	0.047 (16)	0.076 (17)	0.010 (12)	-0.004 (12)	0.020 (13)
C17A	0.034 (5)	0.079 (6)	0.058 (6)	-0.003 (4)	-0.012 (4)	0.001 (5)
C17B	0.030 (3)	0.033 (3)	0.049 (3)	0.000 (2)	-0.008 (2)	-0.002 (2)
C17C	0.049 (15)	0.059 (13)	0.054 (14)	-0.006 (11)	-0.016 (11)	0.006 (11)
C18C	0.15 (5)	0.18 (6)	0.15 (5)	-0.03 (4)	0.01 (4)	0.06 (5)
C18B	0.055 (4)	0.060 (4)	0.041 (3)	-0.009 (3)	-0.006 (3)	-0.003 (3)
C18A	0.034 (7)	0.064 (7)	0.069 (8)	0.012 (5)	0.003 (5)	0.005 (6)
C19A	0.035 (3)	0.042 (3)	0.039 (3)	-0.003 (2)	-0.005 (2)	-0.005 (2)
C19B	0.044 (4)	0.041 (3)	0.048 (3)	0.003 (2)	-0.017 (3)	-0.004 (2)
C20A	0.032 (3)	0.039 (3)	0.040 (3)	-0.002 (2)	-0.004 (2)	-0.005 (2)
C20B	0.036 (4)	0.062 (4)	0.055 (4)	-0.004 (3)	-0.018 (3)	-0.005 (3)
C21A	0.040 (3)	0.039 (3)	0.048 (3)	-0.009 (2)	0.001 (2)	-0.004 (2)
C21B	0.042 (4)	0.077 (5)	0.079 (5)	-0.001 (3)	-0.018 (3)	-0.013 (4)
C22A	0.054 (4)	0.054 (4)	0.043 (3)	-0.009 (3)	0.005 (3)	0.002 (3)
C22B	0.071 (6)	0.074 (5)	0.085 (6)	0.005 (4)	-0.041 (4)	-0.014 (4)
C23A	0.067 (5)	0.074 (5)	0.036 (3)	-0.018 (3)	-0.004 (3)	-0.003 (3)
C23B	0.097 (6)	0.077 (5)	0.061 (5)	0.002 (4)	-0.048 (4)	0.001 (4)
C24A	0.053 (4)	0.053 (4)	0.046 (4)	-0.011 (3)	-0.002 (3)	-0.007 (3)
C24B	0.079 (5)	0.062 (4)	0.057 (4)	-0.008 (4)	-0.028 (4)	-0.005 (3)
C25A	0.032 (3)	0.043 (3)	0.033 (3)	-0.002 (2)	-0.007 (2)	-0.005 (2)
C25B	0.033 (3)	0.042 (3)	0.041 (3)	0.002 (2)	-0.005 (2)	-0.004 (2)
C26A	0.048 (4)	0.057 (4)	0.055 (4)	-0.021 (3)	-0.011 (3)	-0.002 (3)
C26B	0.036 (3)	0.050 (3)	0.046 (3)	-0.001 (2)	-0.003 (2)	0.001 (3)
C27A	0.074 (5)	0.044 (3)	0.044 (3)	-0.007 (3)	-0.010 (3)	0.008 (3)
C27B	0.045 (4)	0.051 (3)	0.051 (4)	0.001 (3)	-0.004 (3)	-0.011 (3)
C28A	0.052 (4)	0.049 (3)	0.039 (3)	0.006 (3)	-0.014 (3)	-0.012 (3)
C28B	0.055 (4)	0.036 (3)	0.058 (4)	-0.003 (3)	-0.005 (3)	-0.007 (3)
C29A	0.047 (4)	0.071 (4)	0.063 (4)	-0.019 (3)	-0.024 (3)	0.006 (3)
C29B	0.053 (4)	0.042 (3)	0.052 (4)	-0.007 (3)	0.002 (3)	0.006 (3)
C30A	0.051 (4)	0.070 (4)	0.051 (4)	-0.025 (3)	-0.018 (3)	0.019 (3)
C30B	0.046 (4)	0.045 (3)	0.044 (3)	-0.001 (3)	-0.005 (3)	0.000 (3)
C31A	0.032 (3)	0.049 (3)	0.055 (4)	-0.011 (2)	-0.003 (2)	-0.011 (3)
C31B	0.042 (3)	0.044 (3)	0.029 (3)	-0.002 (2)	-0.005 (2)	-0.002 (2)
C32A	0.039 (3)	0.048 (3)	0.057 (4)	-0.005 (3)	-0.001 (3)	-0.011 (3)
C32B	0.050 (4)	0.038 (3)	0.037 (3)	-0.004 (2)	-0.001 (2)	0.001 (2)
C33A	0.036 (4)	0.060 (4)	0.081 (5)	-0.013 (3)	-0.006 (3)	-0.001 (3)
C33B	0.043 (3)	0.056 (4)	0.037 (3)	0.005 (3)	-0.003 (2)	0.003 (3)
C34A	0.054 (5)	0.058 (4)	0.090 (5)	-0.014 (3)	-0.022 (4)	-0.016 (4)
C34B	0.057 (4)	0.055 (4)	0.036 (3)	0.019 (3)	-0.009 (3)	-0.015 (3)
C35A	0.053 (4)	0.075 (5)	0.077 (5)	-0.016 (3)	-0.016 (4)	-0.029 (4)
C35B	0.072 (5)	0.046 (3)	0.047 (4)	0.006 (3)	-0.026 (3)	-0.008 (3)

C36A	0.033 (3)	0.059 (4)	0.060 (4)	-0.007 (3)	-0.010 (3)	-0.014 (3)
C36B	0.050 (4)	0.051 (3)	0.038 (3)	-0.002 (3)	-0.009 (3)	-0.002 (3)
C37A	0.037 (3)	0.039 (3)	0.048 (3)	-0.008 (2)	0.008 (2)	0.001 (2)
C37B	0.034 (3)	0.035 (3)	0.049 (3)	-0.002 (2)	-0.006 (2)	0.003 (2)
C38A	0.028 (3)	0.042 (3)	0.051 (3)	0.000 (2)	0.002 (2)	0.005 (3)
C38B	0.030 (3)	0.042 (3)	0.071 (4)	-0.001 (2)	0.002 (3)	-0.001 (3)
C39A	0.020 (3)	0.051 (3)	0.046 (3)	-0.006 (2)	-0.002 (2)	0.001 (2)
C39B	0.027 (3)	0.043 (3)	0.093 (5)	-0.004 (2)	-0.006 (3)	-0.003 (3)
C40A	0.029 (3)	0.041 (3)	0.050 (3)	-0.009 (2)	0.000 (2)	-0.005 (2)
C40B	0.035 (3)	0.033 (3)	0.069 (4)	-0.007 (2)	-0.005 (3)	0.002 (3)
C41A	0.024 (3)	0.034 (3)	0.053 (3)	-0.003 (2)	-0.001 (2)	0.005 (2)
C41B	0.026 (3)	0.041 (3)	0.048 (3)	-0.004 (2)	-0.007 (2)	0.005 (2)
C42A	0.028 (3)	0.037 (3)	0.069 (4)	-0.007 (2)	0.005 (3)	0.011 (3)
C42B	0.033 (3)	0.038 (3)	0.044 (3)	-0.001 (2)	-0.007 (2)	0.001 (2)
C43A	0.032 (4)	0.055 (4)	0.080 (5)	0.004 (3)	-0.006 (3)	0.025 (3)
C43B	0.029 (3)	0.045 (3)	0.044 (3)	-0.003 (2)	-0.006 (2)	0.000 (2)
C44A	0.045 (4)	0.076 (5)	0.059 (4)	-0.014 (3)	-0.017 (3)	0.028 (4)
C44B	0.029 (3)	0.046 (3)	0.051 (3)	-0.006 (2)	-0.011 (2)	0.001 (3)
C45A	0.045 (4)	0.058 (4)	0.048 (3)	-0.015 (3)	-0.009 (3)	0.010 (3)
C45B	0.031 (3)	0.036 (3)	0.042 (3)	-0.003 (2)	-0.012 (2)	0.000 (2)
C46A	0.030 (3)	0.045 (3)	0.041 (3)	-0.009 (2)	-0.001 (2)	0.009 (2)
C46B	0.033 (3)	0.041 (3)	0.041 (3)	-0.002 (2)	-0.007 (2)	0.001 (2)
C47A	0.057 (4)	0.048 (3)	0.059 (4)	-0.006 (3)	0.019 (3)	-0.014 (3)
C47B	0.036 (3)	0.043 (3)	0.053 (4)	0.002 (2)	0.003 (3)	-0.001 (3)
C48A	0.107 (6)	0.052 (4)	0.055 (4)	-0.018 (4)	0.024 (4)	-0.007 (3)
C48B	0.038 (3)	0.051 (3)	0.041 (3)	0.001 (2)	0.000 (2)	-0.003 (3)
C49A	0.048 (4)	0.067 (5)	0.081 (5)	0.008 (3)	0.014 (4)	0.001 (4)
C49B	0.064 (4)	0.040 (3)	0.043 (3)	0.000 (3)	-0.021 (3)	-0.010 (2)
C50A	0.140 (8)	0.081 (5)	0.046 (4)	0.041 (5)	-0.039 (5)	-0.030 (4)
C50B	0.053 (4)	0.052 (4)	0.062 (4)	-0.014 (3)	-0.022 (3)	0.002 (3)
C51A	0.061 (5)	0.086 (6)	0.104 (7)	0.022 (4)	-0.035 (4)	-0.053 (5)
C51B	0.041 (4)	0.052 (4)	0.062 (4)	-0.013 (3)	-0.012 (3)	0.009 (3)
C52A	0.045 (4)	0.060 (4)	0.124 (7)	-0.009 (3)	-0.009 (4)	-0.036 (4)
C52B	0.032 (3)	0.055 (4)	0.052 (4)	-0.004 (2)	0.001 (2)	0.001 (3)
C53A	0.044 (4)	0.044 (4)	0.123 (7)	-0.003 (3)	0.031 (4)	-0.004 (4)
C53B	0.036 (3)	0.046 (3)	0.059 (4)	0.005 (2)	-0.009 (3)	-0.002 (3)
C54A	0.040 (4)	0.043 (4)	0.097 (5)	0.008 (3)	0.015 (3)	0.006 (3)
C54B	0.029 (3)	0.041 (3)	0.054 (3)	0.002 (2)	-0.005 (2)	-0.004 (3)

Table A12: Geometric parameters (Å, °) for NDI-[$CH_2CH_2OCH_2CH_2O$(An)$PS_2(SnPh_3)_2]_2$⊂15DN38C10

Sn1A—C19A	2.132 (5)	C19A—C20A	1.378 (7)
Sn1A—C31A	2.135 (5)	C19A—C24A	1.385 (8)

Sn1A—C25A	2.140 (5)	C19B—C20B	1.382 (8)
Sn1A—O11A	2.457 (3)	C19B—C24B	1.388 (8)
Sn1A—S1A	2.5625 (13)	C20A—C21A	1.401 (7)
Sn1B—C25B	2.116 (5)	C20A—H20A	0.9300
Sn1B—C31B	2.128 (5)	C20B—C21B	1.378 (8)
Sn1B—C19B	2.135 (6)	C20B—H20B	0.9300
Sn1B—S1B	2.4427 (13)	C21A—C22A	1.368 (8)
S1A—P1A	2.0461 (19)	C21A—H21A	0.9300
S1B—P1B	2.0758 (18)	C21B—C22B	1.388 (10)
S2A—P1A	1.934 (2)	C21B—H21B	0.9300
S2B—P1B	1.9386 (18)	C22A—C23A	1.372 (8)
P1A—O4A	1.603 (4)	C22A—H22A	0.9300
P1A—C12A	1.798 (8)	C22B—C23B	1.359 (10)
P1A—C12C	1.808 (18)	C22B—H22B	0.9300
P1B—O4B	1.591 (4)	C23A—C24A	1.389 (8)
P1B—C12B	1.779 (5)	C23A—H23A	0.9300
O1A—C3A	1.204 (6)	C23B—C24B	1.405 (10)
O1B—C3B	1.225 (6)	C23B—H23B	0.9300
O2A—C6A	1.230 (6)	C24A—H24A	0.9300
O2B—C6B	1.216 (6)	C24B—H24B	0.9300
O3A—C9A	1.413 (6)	C25A—C30A	1.364 (7)
O3A—C10A	1.431 (6)	C25A—C26A	1.373 (7)
O3B—C10B	1.410 (6)	C25B—C30B	1.377 (7)
O3B—C9B	1.411 (6)	C25B—C26B	1.385 (7)
O4A—C11A	1.446 (6)	C26A—C27A	1.381 (8)
O4B—C11B	1.448 (6)	C26A—H26A	0.9300
O5A—C15A	1.364 (12)	C26B—C27B	1.406 (8)
O5A—C18A	1.443 (19)	C26B—H26B	0.9300
O5B—C15B	1.349 (6)	C27A—C28A	1.364 (8)
O5B—C18B	1.420 (6)	C27A—H27A	0.9300
O5C—C15C	1.36 (3)	C27B—C28B	1.359 (8)
O5C—C18C	1.41 (7)	C27B—H27B	0.9300
O6A—C37A	1.369 (6)	C28A—C29A	1.364 (8)
O6A—C47A	1.435 (7)	C28A—H28A	0.9300
O6B—C37B	1.368 (6)	C28B—C29B	1.373 (8)
O6B—C47B	1.440 (6)	C28B—H28B	0.9300
O7A—C49A	1.314 (8)	C29A—C30A	1.384 (8)
O7A—C48A	1.396 (8)	C29A—H29A	0.9300
O7B—C48B	1.408 (6)	C29B—C30B	1.396 (8)
O7B—C49B	1.417 (6)	C29B—H29B	0.9300
O8A—C51A	1.417 (9)	C30A—H30A	0.9300
O8A—C50A	1.430 (9)	C30B—H30B	0.9300
O8B—C50B	1.394 (6)	C31A—C36A	1.383 (8)

O8B—C51B	1.423 (6)	C31A—C32A	1.392 (8)
O9A—C53A	1.408 (9)	C31B—C36B	1.388 (7)
O9A—C52A	1.433 (8)	C31B—C32B	1.395 (7)
O9B—C53B	1.408 (6)	C32A—C33A	1.394 (8)
O9B—C52B	1.424 (6)	C32A—H32A	0.9300
O10A—C42A^{i}	1.373 (7)	C32B—C33B	1.379 (7)
O10A—C54A	1.443 (6)	C32B—H32B	0.9300
O10B—C42B^{ii}	1.373 (6)	C33A—C34A	1.378 (9)
O10B—C54B	1.428 (6)	C33A—H33A	0.9300
O11A—H11F	0.9372	C33B—C34B	1.373 (8)
O11A—H11G	1.0111	C33B—H33B	0.9300
N1A—C6A	1.387 (6)	C34A—C35A	1.358 (9)
N1A—C3A	1.392 (6)	C34A—H34A	0.9300
N1A—C8A	1.479 (6)	C34B—C35B	1.377 (9)
N1B—C6B	1.395 (6)	C34B—H34B	0.9300
N1B—C3B	1.409 (7)	C35A—C36A	1.386 (8)
N1B—C8B	1.467 (6)	C35A—H35A	0.9300
C1A—C2A	1.382 (7)	C35B—C36B	1.392 (8)
C1A—C7A^{i}	1.400 (7)	C35B—H35B	0.9300
C1A—H1A	0.9300	C36A—H36A	0.9300
C1B—C2B	1.382 (7)	C36B—H36B	0.9300
C1B—C7B^{ii}	1.389 (7)	C37A—C38A	1.350 (8)
C1B—H1B	0.9300	C37A—C46A	1.419 (7)
C2A—C4A	1.415 (6)	C37B—C38B	1.373 (7)
C2A—C3A	1.480 (7)	C37B—C46B	1.428 (7)
C2B—C4B	1.421 (6)	C38A—C39A	1.394 (7)
C2B—C3B	1.457 (7)	C38A—H38A	0.9300
C4A—C4A^{i}	1.401 (9)	C38B—C39B	1.398 (8)
C4A—C5A	1.402 (6)	C38B—H38B	0.9300
C4B—C4B^{ii}	1.395 (10)	C39A—C40A	1.351 (7)
C4B—C5B	1.409 (7)	C39A—H39A	0.9300
C5A—C7A	1.368 (7)	C39B—C40B	1.367 (8)
C5A—C6A	1.480 (7)	C39B—H39B	0.9300
C5B—C7B	1.371 (7)	C40A—C41A	1.414 (7)
C5B—C6B	1.489 (7)	C40A—H40A	0.9300
C7A—C1A^{i}	1.400 (7)	C40B—C41B	1.414 (7)
C7A—H7A	0.9300	C40B—H40B	0.9300
C7B—C1B^{ii}	1.389 (7)	C41A—C46A	1.401 (7)
C7B—H7B	0.9300	C41A—C42A	1.441 (7)
C8A—C9A	1.524 (7)	C41B—C46B	1.428 (7)
C8A—H8A1	0.9700	C41B—C42B	1.429 (7)
C8A—H8A2	0.9700	C42A—C43A	1.360 (8)
C8B—C9B	1.505 (8)	C42A—O10A^{i}	1.373 (7)

C8B—H8B1	0.9700	C42B—C43B	1.360 (7)
C8B—H8B2	0.9700	C42B—O10B^{ii}	1.373 (6)
C9A—H9A1	0.9700	C43A—C44A	1.398 (9)
C9A—H9A2	0.9700	C43A—H43A	0.9300
C9B—H9B1	0.9700	C43B—C44B	1.409 (7)
C9B—H9B2	0.9700	C43B—H43B	0.9300
C10A—C11A	1.494 (7)	C44A—C45A	1.346 (8)
C10A—H10A	0.9700	C44A—H44A	0.9300
C10A—H10B	0.9700	C44B—C45B	1.360 (7)
C10B—C11B	1.493 (7)	C44B—H44B	0.9300
C10B—H10C	0.9700	C45A—C46A	1.427 (7)
C10B—H10D	0.9700	C45A—H45A	0.9300
C11A—H11A	0.9700	C45B—C46B	1.414 (7)
C11A—H11B	0.9700	C45B—H45B	0.9300
C11B—H11C	0.9700	C47A—C48A	1.481 (8)
C11B—H11D	0.9700	C47A—H47A	0.9700
C12A—C13A	1.344 (15)	C47A—H47B	0.9700
C12A—C17A	1.403 (14)	C47B—C48B	1.485 (7)
C12B—C13B	1.393 (7)	C47B—H47C	0.9700
C12B—C17B	1.394 (7)	C47B—H47D	0.9700
C12C—C13C	1.39 (3)	C48A—H48A	0.9700
C12C—C17C	1.47 (3)	C48A—H48B	0.9700
C13A—C14A	1.419 (13)	C48B—H48C	0.9700
C13A—H13A	0.9300	C48B—H48D	0.9700
C13B—C14B	1.374 (7)	C49A—C50A	1.543 (11)
C13B—H13B	0.9300	C49A—H49A	0.9700
C13C—C14C	1.40 (3)	C49A—H49B	0.9700
C13C—H13C	0.9300	C49B—C50B	1.485 (8)
C14A—C15A	1.380 (16)	C49B—H49C	0.9700
C14A—H14A	0.9300	C49B—H49D	0.9700
C14B—C15B	1.385 (7)	C50A—H50A	0.9700
C14B—H14B	0.9300	C50A—H50B	0.9700
C14C—C15C	1.41 (4)	C50B—H50C	0.9700
C14C—H14C	0.9300	C50B—H50D	0.9700
C15A—C16A	1.364 (15)	C51A—C52A	1.485 (11)
C15B—C16B	1.389 (7)	C51A—H51A	0.9700
C15C—C16C	1.33 (5)	C51A—H51B	0.9700
C16A—C17A	1.367 (12)	C51B—C52B	1.503 (8)
C16A—H16A	0.9300	C51B—H51C	0.9700
C16B—C17B	1.378 (7)	C51B—H51D	0.9700
C16B—H16B	0.9300	C52A—H52A	0.9700
C16C—C17C	1.37 (4)	C52A—H52B	0.9700
C16C—H16C	0.9300	C52B—H52C	0.9700

C17A—H17A	0.9300	C52B—H52D	0.9700
C17B—H17B	0.9300	C53A—C54A	1.495 (10)
C17C—H17C	0.9300	C53A—H53A	0.9700
C18C—H18A	0.9600	C53A—H53B	0.9700
C18C—H18B	0.9600	C53B—C54B	1.513 (7)
C18C—H18C	0.9600	C53B—H53C	0.9700
C18B—H18D	0.9600	C53B—H53D	0.9700
C18B—H18E	0.9600	C54A—H54A	0.9700
C18B—H18F	0.9600	C54A—H54B	0.9700
C18A—H18G	0.9600	C54B—H54C	0.9700
C18A—H18H	0.9600	C54B—H54D	0.9700
C18A—H18I	0.9600		
C19A—Sn1A—C31A	120.8 (2)	C22A—C23A—C24A	120.7 (6)
C19A—Sn1A—C25A	116.0 (2)	C22A—C23A—H23A	119.6
C31A—Sn1A—C25A	118.7 (2)	C24A—C23A—H23A	119.6
C19A—Sn1A—O11A	82.37 (17)	C22B—C23B—C24B	121.1 (7)
C31A—Sn1A—O11A	80.93 (17)	C22B—C23B—H23B	119.5
C25A—Sn1A—O11A	85.55 (16)	C24B—C23B—H23B	119.5
C19A—Sn1A—S1A	101.34 (14)	C19A—C24A—C23A	120.1 (6)
C31A—Sn1A—S1A	99.06 (15)	C19A—C24A—H24A	120.0
C25A—Sn1A—S1A	90.59 (14)	C23A—C24A—H24A	120.0
O11A—Sn1A—S1A	175.55 (9)	C19B—C24B—C23B	119.5 (7)
C25B—Sn1B—C31B	114.5 (2)	C19B—C24B—H24B	120.2
C25B—Sn1B—C19B	109.4 (2)	C23B—C24B—H24B	120.2
C31B—Sn1B—C19B	110.3 (2)	C30A—C25A—C26A	117.6 (5)
C25B—Sn1B—S1B	109.66 (15)	C30A—C25A—Sn1A	122.4 (4)
C31B—Sn1B—S1B	111.34 (14)	C26A—C25A—Sn1A	120.0 (4)
C19B—Sn1B—S1B	100.82 (16)	C30B—C25B—C26B	119.9 (5)
P1A—S1A—Sn1A	99.41 (6)	C30B—C25B—Sn1B	119.5 (4)
P1B—S1B—Sn1B	101.73 (6)	C26B—C25B—Sn1B	120.4 (4)
O4A—P1A—C12A	108.2 (4)	C25A—C26A—C27A	121.3 (5)
O4A—P1A—C12C	94.9 (10)	C25A—C26A—H26A	119.4
C12A—P1A—C12C	16.6 (8)	C27A—C26A—H26A	119.4
O4A—P1A—S2A	113.51 (15)	C25B—C26B—C27B	118.9 (5)
C12A—P1A—S2A	108.7 (4)	C25B—C26B—H26B	120.5
C12C—P1A—S2A	124.3 (9)	C27B—C26B—H26B	120.5
O4A—P1A—S1A	101.29 (14)	C28A—C27A—C26A	120.5 (6)
C12A—P1A—S1A	107.3 (5)	C28A—C27A—H27A	119.7
C12C—P1A—S1A	101.3 (13)	C26A—C27A—H27A	119.7
S2A—P1A—S1A	117.18 (10)	C28B—C27B—C26B	121.2 (6)
O4B—P1B—C12B	100.3 (2)	C28B—C27B—H27B	119.4
O4B—P1B—S2B	115.07 (15)	C26B—C27B—H27B	119.4
C12B—P1B—S2B	115.44 (17)	C29A—C28A—C27A	118.7 (5)

O4B—P1B—S1B	106.42 (15)	C29A—C28A—H28A	120.7
C12B—P1B—S1B	102.91 (17)	C27A—C28A—H28A	120.7
S2B—P1B—S1B	115.00 (8)	C27B—C28B—C29B	119.5 (6)
C9A—O3A—C10A	114.0 (4)	C27B—C28B—H28B	120.3
C10B—O3B—C9B	113.4 (4)	C29B—C28B—H28B	120.3
C11A—O4A—P1A	122.0 (3)	C28A—C29A—C30A	120.6 (6)
C11B—O4B—P1B	122.2 (3)	C28A—C29A—H29A	119.7
C15A—O5A—C18A	118.8 (9)	C30A—C29A—H29A	119.7
C15B—O5B—C18B	118.6 (4)	C28B—C29B—C30B	120.5 (6)
C15C—O5C—C18C	106 (4)	C28B—C29B—H29B	119.7
C37A—O6A—C47A	117.2 (5)	C30B—C29B—H29B	119.7
C37B—O6B—C47B	116.5 (4)	C25A—C30A—C29A	121.3 (6)
C49A—O7A—C48A	113.7 (6)	C25A—C30A—H30A	119.4
C48B—O7B—C49B	112.5 (4)	C29A—C30A—H30A	119.4
C51A—O8A—C50A	117.0 (6)	C25B—C30B—C29B	120.0 (5)
C50B—O8B—C51B	112.1 (4)	C25B—C30B—H30B	120.0
C53A—O9A—C52A	115.3 (5)	C29B—C30B—H30B	120.0
C53B—O9B—C52B	115.0 (4)	C36A—C31A—C32A	118.5 (5)
C42A^{i}—O10A—C54A	117.5 (5)	C36A—C31A—Sn1A	121.7 (4)
C42B^{ii}—O10B—C54B	117.3 (4)	C32A—C31A—Sn1A	119.8 (4)
Sn1A—O11A—H11F	102.6	C36B—C31B—C32B	118.3 (5)
Sn1A—O11A—H11G	124.1	C36B—C31B—Sn1B	120.1 (4)
H11F—O11A—H11G	117.2	C32B—C31B—Sn1B	121.4 (4)
C6A—N1A—C3A	125.2 (4)	C31A—C32A—C33A	120.8 (6)
C6A—N1A—C8A	118.8 (4)	C31A—C32A—H32A	119.6
C3A—N1A—C8A	116.0 (4)	C33A—C32A—H32A	119.6
C6B—N1B—C3B	124.2 (4)	C33B—C32B—C31B	121.4 (5)
C6B—N1B—C8B	116.6 (4)	C33B—C32B—H32B	119.3
C3B—N1B—C8B	119.0 (4)	C31B—C32B—H32B	119.3
C2A—C1A—C7A^{i}	120.8 (5)	C34A—C33A—C32A	119.1 (6)
C2A—C1A—H1A	119.6	C34A—C33A—H33A	120.5
C7A^{i}—C1A—H1A	119.6	C32A—C33A—H33A	120.5
C2B—C1B—C7B^{ii}	121.1 (5)	C34B—C33B—C32B	119.5 (6)
C2B—C1B—H1B	119.5	C34B—C33B—H33B	120.3
C7B^{ii}—C1B—H1B	119.5	C32B—C33B—H33B	120.3
C1A—C2A—C4A	119.3 (4)	C35A—C34A—C33A	120.5 (6)
C1A—C2A—C3A	120.5 (5)	C35A—C34A—H34A	119.7
C4A—C2A—C3A	120.2 (4)	C33A—C34A—H34A	119.7
C1B—C2B—C4B	119.2 (5)	C33B—C34B—C35B	120.5 (5)
C1B—C2B—C3B	120.8 (5)	C33B—C34B—H34B	119.7
C4B—C2B—C3B	120.0 (4)	C35B—C34B—H34B	119.7
O1A—C3A—N1A	121.8 (5)	C34A—C35A—C36A	120.7 (6)
O1A—C3A—C2A	121.8 (5)	C34A—C35A—H35A	119.7

N1A—C3A—C2A	116.3 (4)	C36A—C35A—H35A	119.7
O1B—C3B—N1B	119.5 (5)	C34B—C35B—C36B	120.0 (6)
O1B—C3B—C2B	123.0 (5)	C34B—C35B—H35B	120.0
N1B—C3B—C2B	117.5 (4)	C36B—C35B—H35B	120.0
C4A^{i}—C4A—C5A	119.7 (5)	C31A—C36A—C35A	120.3 (6)
C4A^{i}—C4A—C2A	119.6 (5)	C31A—C36A—H36A	119.9
C5A—C4A—C2A	120.7 (4)	C35A—C36A—H36A	119.9
C4B^{ii}—C4B—C5B	119.4 (5)	C31B—C36B—C35B	120.3 (6)
C4B^{ii}—C4B—C2B	119.7 (6)	C31B—C36B—H36B	119.9
C5B—C4B—C2B	120.9 (5)	C35B—C36B—H36B	119.9
C7A—C5A—C4A	120.5 (4)	C38A—C37A—O6A	124.3 (5)
C7A—C5A—C6A	119.9 (4)	C38A—C37A—C46A	120.2 (5)
C4A—C5A—C6A	119.5 (4)	O6A—C37A—C46A	115.5 (5)
C7B—C5B—C4B	120.6 (5)	O6B—C37B—C38B	124.5 (5)
C7B—C5B—C6B	119.9 (5)	O6B—C37B—C46B	114.1 (4)
C4B—C5B—C6B	119.5 (4)	C38B—C37B—C46B	121.4 (5)
O2A—C6A—N1A	120.5 (5)	C37A—C38A—C39A	120.4 (5)
O2A—C6A—C5A	122.1 (5)	C37A—C38A—H38A	119.8
N1A—C6A—C5A	117.5 (4)	C39A—C38A—H38A	119.8
O2B—C6B—N1B	120.0 (5)	C37B—C38B—C39B	119.6 (5)
O2B—C6B—C5B	122.6 (5)	C37B—C38B—H38B	120.2
N1B—C6B—C5B	117.3 (4)	C39B—C38B—H38B	120.2
C5A—C7A—C1A^{i}	120.1 (5)	C40A—C39A—C38A	121.4 (5)
C5A—C7A—H7A	120.0	C40A—C39A—H39A	119.3
C1A^{i}—C7A—H7A	120.0	C38A—C39A—H39A	119.3
C5B—C7B—C1B^{ii}	120.1 (5)	C40B—C39B—C38B	122.0 (5)
C5B—C7B—H7B	119.9	C40B—C39B—H39B	119.0
C1B^{ii}—C7B—H7B	119.9	C38B—C39B—H39B	119.0
N1A—C8A—C9A	112.3 (4)	C39A—C40A—C41A	119.7 (5)
N1A—C8A—H8A1	109.1	C39A—C40A—H40A	120.2
C9A—C8A—H8A1	109.1	C41A—C40A—H40A	120.2
N1A—C8A—H8A2	109.1	C39B—C40B—C41B	119.0 (5)
C9A—C8A—H8A2	109.1	C39B—C40B—H40B	120.5
H8A1—C8A—H8A2	107.9	C41B—C40B—H40B	120.5
N1B—C8B—C9B	112.8 (4)	C46A—C41A—C40A	119.4 (5)
N1B—C8B—H8B1	109.0	C46A—C41A—C42A	118.5 (5)
C9B—C8B—H8B1	109.0	C40A—C41A—C42A	122.1 (5)
N1B—C8B—H8B2	109.0	C40B—C41B—C46B	120.7 (5)
C9B—C8B—H8B2	109.0	C40B—C41B—C42B	121.2 (5)
H8B1—C8B—H8B2	107.8	C46B—C41B—C42B	118.0 (5)
O3A—C9A—C8A	114.3 (4)	C43A—C42A—O10A^{i}	125.5 (5)
O3A—C9A—H9A1	108.7	C43A—C42A—C41A	120.7 (6)
C8A—C9A—H9A1	108.7	O10A^{i}—C42A—C41A	113.8 (5)

O3A—C9A—H9A2	108.7	C43B—C42B—O10B^{ii}	125.0 (5)
C8A—C9A—H9A2	108.7	C43B—C42B—C41B	121.3 (5)
H9A1—C9A—H9A2	107.6	O10B^{ii}—C42B—C41B	113.7 (4)
O3B—C9B—C8B	109.6 (4)	C42A—C43A—C44A	119.4 (6)
O3B—C9B—H9B1	109.8	C42A—C43A—H43A	120.3
C8B—C9B—H9B1	109.8	C44A—C43A—H43A	120.3
O3B—C9B—H9B2	109.8	C42B—C43B—C44B	119.6 (5)
C8B—C9B—H9B2	109.8	C42B—C43B—H43B	120.2
H9B1—C9B—H9B2	108.2	C44B—C43B—H43B	120.2
O3A—C10A—C11A	107.9 (4)	C45A—C44A—C43A	122.3 (6)
O3A—C10A—H10A	110.1	C45A—C44A—H44A	118.9
C11A—C10A—H10A	110.1	C43A—C44A—H44A	118.9
O3A—C10A—H10B	110.1	C45B—C44B—C43B	121.5 (5)
C11A—C10A—H10B	110.1	C45B—C44B—H44B	119.2
H10A—C10A—H10B	108.4	C43B—C44B—H44B	119.2
O3B—C10B—C11B	109.2 (4)	C44A—C45A—C46A	119.9 (6)
O3B—C10B—H10C	109.8	C44A—C45A—H45A	120.1
C11B—C10B—H10C	109.8	C46A—C45A—H45A	120.1
O3B—C10B—H10D	109.8	C44B—C45B—C46B	120.2 (5)
C11B—C10B—H10D	109.8	C44B—C45B—H45B	119.9
H10C—C10B—H10D	108.3	C46B—C45B—H45B	119.9
O4A—C11A—C10A	109.0 (4)	C41A—C46A—C37A	119.0 (5)
O4A—C11A—H11A	109.9	C41A—C46A—C45A	119.2 (5)
C10A—C11A—H11A	109.9	C37A—C46A—C45A	121.8 (5)
O4A—C11A—H11B	109.9	C45B—C46B—C37B	123.6 (5)
C10A—C11A—H11B	109.9	C45B—C46B—C41B	119.3 (5)
H11A—C11A—H11B	108.3	C37B—C46B—C41B	117.1 (5)
O4B—C11B—C10B	108.8 (4)	O6A—C47A—C48A	111.0 (6)
O4B—C11B—H11C	109.9	O6A—C47A—H47A	109.4
C10B—C11B—H11C	109.9	C48A—C47A—H47A	109.4
O4B—C11B—H11D	109.9	O6A—C47A—H47B	109.4
C10B—C11B—H11D	109.9	C48A—C47A—H47B	109.4
H11C—C11B—H11D	108.3	H47A—C47A—H47B	108.0
C13A—C12A—C17A	121.0 (8)	O6B—C47B—C48B	108.8 (4)
C13A—C12A—P1A	119.9 (8)	O6B—C47B—H47C	109.9
C17A—C12A—P1A	119.1 (8)	C48B—C47B—H47C	109.9
C13B—C12B—C17B	118.5 (5)	O6B—C47B—H47D	109.9
C13B—C12B—P1B	120.2 (4)	C48B—C47B—H47D	109.9
C17B—C12B—P1B	121.1 (4)	H47C—C47B—H47D	108.3
C13C—C12C—C17C	111.2 (18)	O7A—C48A—C47A	114.6 (5)
C13C—C12C—P1A	129.5 (19)	O7A—C48A—H48A	108.6
C17C—C12C—P1A	119.2 (19)	C47A—C48A—H48A	108.6
C12A—C13A—C14A	121.4 (8)	O7A—C48A—H48B	108.6

C12A—C13A—H13A	119.3	C47A—C48A—H48B	108.6
C14A—C13A—H13A	119.3	H48A—C48A—H48B	107.6
C14B—C13B—C12B	121.6 (5)	O7B—C48B—C47B	110.4 (4)
C14B—C13B—H13B	119.2	O7B—C48B—H48C	109.6
C12B—C13B—H13B	119.2	C47B—C48B—H48C	109.6
C12C—C13C—C14C	128 (2)	O7B—C48B—H48D	109.6
C12C—C13C—H13C	116.2	C47B—C48B—H48D	109.6
C14C—C13C—H13C	116.2	H48C—C48B—H48D	108.1
C15A—C14A—C13A	115.9 (10)	O7A—C49A—C50A	112.6 (6)
C15A—C14A—H14A	122.1	O7A—C49A—H49A	109.1
C13A—C14A—H14A	122.1	C50A—C49A—H49A	109.1
C13B—C14B—C15B	119.3 (5)	O7A—C49A—H49B	109.1
C13B—C14B—H14B	120.3	C50A—C49A—H49B	109.1
C15B—C14B—H14B	120.3	H49A—C49A—H49B	107.8
C13C—C14C—C15C	117 (2)	O7B—C49B—C50B	109.8 (5)
C13C—C14C—H14C	121.3	O7B—C49B—H49C	109.7
C15C—C14C—H14C	121.3	C50B—C49B—H49C	109.7
O5A—C15A—C16A	115.4 (9)	O7B—C49B—H49D	109.7
O5A—C15A—C14A	121.6 (11)	C50B—C49B—H49D	109.7
C16A—C15A—C14A	122.9 (10)	H49C—C49B—H49D	108.2
O5B—C15B—C14B	124.3 (5)	O8A—C50A—C49A	105.3 (5)
O5B—C15B—C16B	115.7 (5)	O8A—C50A—H50A	110.7
C14B—C15B—C16B	120.0 (5)	C49A—C50A—H50A	110.7
C16C—C15C—O5C	131 (3)	O8A—C50A—H50B	110.7
C16C—C15C—C14C	117 (2)	C49A—C50A—H50B	110.7
O5C—C15C—C14C	112 (2)	H50A—C50A—H50B	108.8
C15A—C16A—C17A	120.4 (8)	O8B—C50B—C49B	109.7 (5)
C15A—C16A—H16A	119.8	O8B—C50B—H50C	109.7
C17A—C16A—H16A	119.8	C49B—C50B—H50C	109.7
C17B—C16B—C15B	120.4 (5)	O8B—C50B—H50D	109.7
C17B—C16B—H16B	119.8	C49B—C50B—H50D	109.7
C15B—C16B—H16B	119.8	H50C—C50B—H50D	108.2
C15C—C16C—C17C	126 (3)	O8A—C51A—C52A	109.7 (6)
C15C—C16C—H16C	116.8	O8A—C51A—H51A	109.7
C17C—C16C—H16C	116.8	C52A—C51A—H51A	109.7
C16A—C17A—C12A	118.2 (9)	O8A—C51A—H51B	109.7
C16A—C17A—H17A	120.9	C52A—C51A—H51B	109.7
C12A—C17A—H17A	120.9	H51A—C51A—H51B	108.2
C16B—C17B—C12B	120.2 (5)	O8B—C51B—C52B	108.2 (4)
C16B—C17B—H17B	119.9	O8B—C51B—H51C	110.1
C12B—C17B—H17B	119.9	C52B—C51B—H51C	110.1
C16C—C17C—C12C	120 (2)	O8B—C51B—H51D	110.1
C16C—C17C—H17C	120.1	C52B—C51B—H51D	110.1

C12C—C17C—H17C	120.1	H51C—C51B—H51D	108.4
O5C—C18C—H18A	109.5	O9A—C52A—C51A	108.3 (6)
O5C—C18C—H18B	109.5	O9A—C52A—H52A	110.0
H18A—C18C—H18B	109.5	C51A—C52A—H52A	110.0
O5C—C18C—H18C	109.5	O9A—C52A—H52B	110.0
H18A—C18C—H18C	109.5	C51A—C52A—H52B	110.0
H18B—C18C—H18C	109.5	H52A—C52A—H52B	108.4
O5B—C18B—H18D	109.5	O9B—C52B—C51B	109.1 (5)
O5B—C18B—H18E	109.5	O9B—C52B—H52C	109.9
H18D—C18B—H18E	109.5	C51B—C52B—H52C	109.9
O5B—C18B—H18F	109.5	O9B—C52B—H52D	109.9
H18D—C18B—H18F	109.5	C51B—C52B—H52D	109.9
H18E—C18B—H18F	109.5	H52C—C52B—H52D	108.3
C20A—C19A—C24A	118.6 (5)	O9A—C53A—C54A	114.9 (5)
C20A—C19A—Sn1A	121.8 (4)	O9A—C53A—H53A	108.5
C24A—C19A—Sn1A	119.6 (4)	C54A—C53A—H53A	108.5
C20B—C19B—C24B	118.5 (6)	O9A—C53A—H53B	108.5
C20B—C19B—Sn1B	124.4 (4)	C54A—C53A—H53B	108.5
C24B—C19B—Sn1B	117.1 (5)	H53A—C53A—H53B	107.5
C19A—C20A—C21A	121.2 (5)	O9B—C53B—C54B	114.7 (5)
C19A—C20A—H20A	119.4	O9B—C53B—H53C	108.6
C21A—C20A—H20A	119.4	C54B—C53B—H53C	108.6
C21B—C20B—C19B	121.8 (6)	O9B—C53B—H53D	108.6
C21B—C20B—H20B	119.1	C54B—C53B—H53D	108.6
C19B—C20B—H20B	119.1	H53C—C53B—H53D	107.6
C22A—C21A—C20A	119.3 (5)	O10A—C54A—C53A	108.2 (6)
C22A—C21A—H21A	120.4	O10A—C54A—H54A	110.1
C20A—C21A—H21A	120.4	C53A—C54A—H54A	110.1
C20B—C21B—C22B	119.5 (7)	O10A—C54A—H54B	110.1
C20B—C21B—H21B	120.2	C53A—C54A—H54B	110.1
C22B—C21B—H21B	120.2	H54A—C54A—H54B	108.4
C21A—C22A—C23A	120.1 (6)	O10B—C54B—C53B	107.7 (4)
C21A—C22A—H22A	120.0	O10B—C54B—H54C	110.2
C23A—C22A—H22A	120.0	C53B—C54B—H54C	110.2
C23B—C22B—C21B	119.6 (7)	O10B—C54B—H54D	110.2
C23B—C22B—H22B	120.2	C53B—C54B—H54D	110.2
C21B—C22B—H22B	120.2	H54C—C54B—H54D	108.5
C19A—Sn1A—S1A—P1A	51.95 (15)	C31B—Sn1B—C19B—C20B	127.8 (5)
C31A—Sn1A—S1A—P1A	-72.13 (18)	S1B—Sn1B—C19B—C20B	10.1 (5)
C25A—Sn1A—S1A—P1A	168.63 (15)	C25B—Sn1B—C19B—C24B	71.5 (5)
O11A—Sn1A—S1A—P1A	-161.7 (11)	C31B—Sn1B—C19B—C24B	-55.2 (5)
C25B—Sn1B—S1B—P1B	-75.45 (16)	S1B—Sn1B—C19B—C24B	-173.0 (4)
C31B—Sn1B—S1B—P1B	52.29 (17)	C24A—C19A—C20A—C21A	0.6 (8)

C19B—Sn1B—S1B—P1B	169.26 (16)	Sn1A—C19A—C20A—C21A	178.9 (4)
Sn1A—S1A—P1A—O4A	-82.81 (15)	C24B—C19B—C20B—C21B	-0.9 (9)
Sn1A—S1A—P1A—C12A	163.8 (4)	Sn1B—C19B—C20B—C21B	176.0 (5)
Sn1A—S1A—P1A—C12C	179.8 (9)	C19A—C20A—C21A—C22A	0.5 (8)
Sn1A—S1A—P1A—S2A	41.24 (11)	C19B—C20B—C21B—C22B	1.9 (10)
Sn1B—S1B—P1B—O4B	-103.99 (15)	C20A—C21A—C22A—C23A	-0.6 (9)
Sn1B—S1B—P1B—C12B	151.06 (17)	C20B—C21B—C22B—C23B	-1.3 (11)
Sn1B—S1B—P1B—S2B	24.69 (10)	C21A—C22A—C23A—C24A	-0.4 (10)
C12A—P1A—O4A—C11A	-89.8 (6)	C21B—C22B—C23B—C24B	-0.2 (12)
C12C—P1A—O4A—C11A	-99.9 (12)	C20A—C19A—C24A—C23A	-1.6 (9)
S2A—P1A—O4A—C11A	31.0 (4)	Sn1A—C19A—C24A—C23A	-180.0 (5)
S1A—P1A—O4A—C11A	157.5 (3)	C22A—C23A—C24A—C19A	1.5 (10)
C12B—P1B—O4B—C11B	159.3 (4)	C20B—C19B—C24B—C23B	-0.6 (9)
S2B—P1B—O4B—C11B	-76.2 (4)	Sn1B—C19B—C24B—C23B	-177.8 (5)
S1B—P1B—O4B—C11B	52.5 (4)	C22B—C23B—C24B—C19B	1.2 (11)
C7A^{i}—C1A—C2A—C4A	0.7 (7)	C19A—Sn1A—C25A—C30A	-2.7 (6)
C7A^{i}—C1A—C2A—C3A	-178.7 (4)	C31A—Sn1A—C25A—C30A	153.7 (5)
C7B^{ii}—C1B—C2B—C4B	0.0 (8)	O11A—Sn1A—C25A—C30A	76.6 (5)
C7B^{ii}—C1B—C2B—C3B	-177.7 (5)	S1A—Sn1A—C25A—C30A	-105.6 (5)
C6A—N1A—C3A—O1A	175.6 (5)	C19A—Sn1A—C25A—C26A	177.8 (4)
C8A—N1A—C3A—O1A	-8.1 (7)	C31A—Sn1A—C25A—C26A	-25.8 (5)
C6A—N1A—C3A—C2A	-5.9 (7)	O11A—Sn1A—C25A—C26A	-102.9 (5)
C8A—N1A—C3A—C2A	170.5 (4)	S1A—Sn1A—C25A—C26A	74.9 (4)
C1A—C2A—C3A—O1A	5.1 (8)	C31B—Sn1B—C25B—C30B	34.2 (5)
C4A—C2A—C3A—O1A	-174.3 (5)	C19B—Sn1B—C25B—C30B	-90.1 (5)
C1A—C2A—C3A—N1A	-173.4 (4)	S1B—Sn1B—C25B—C30B	160.2 (4)
C4A—C2A—C3A—N1A	7.1 (7)	C31B—Sn1B—C25B—C26B	-150.4 (4)
C6B—N1B—C3B—O1B	170.8 (5)	C19B—Sn1B—C25B—C26B	85.3 (5)
C8B—N1B—C3B—O1B	-4.0 (7)	S1B—Sn1B—C25B—C26B	-24.4 (5)
C6B—N1B—C3B—C2B	-9.0 (7)	C30A—C25A—C26A—C27A	-3.3 (9)
C8B—N1B—C3B—C2B	176.2 (4)	Sn1A—C25A—C26A—C27A	176.3 (5)
C1B—C2B—C3B—O1B	6.5 (8)	C30B—C25B—C26B—C27B	-0.9 (8)
C4B—C2B—C3B—O1B	-171.2 (5)	Sn1B—C25B—C26B—C27B	-176.3 (4)
C1B—C2B—C3B—N1B	-173.7 (5)	C25A—C26A—C27A—C28A	2.4 (10)
C4B—C2B—C3B—N1B	8.6 (7)	C25B—C26B—C27B—C28B	-1.1 (9)
C1A—C2A—C4A—C4A^{i}	-1.2 (8)	C26A—C27A—C28A—C29A	0.3 (9)
C3A—C2A—C4A—C4A^{i}	178.2 (5)	C26B—C27B—C28B—C29B	1.9 (9)
C1A—C2A—C4A—C5A	178.8 (4)	C27A—C28A—C29A—C30A	-2.1 (10)
C3A—C2A—C4A—C5A	-1.8 (7)	C27B—C28B—C29B—C30B	-0.6 (9)
C1B—C2B—C4B—C4B^{ii}	-0.5 (9)	C26A—C25A—C30A—C29A	1.5 (9)
C3B—C2B—C4B—C4B^{ii}	177.2 (6)	Sn1A—C25A—C30A—C29A	-178.0 (5)
C1B—C2B—C4B—C5B	179.5 (5)	C28A—C29A—C30A—C25A	1.1 (10)
C3B—C2B—C4B—C5B	-2.8 (7)	C26B—C25B—C30B—C29B	2.2 (8)

C4A^{i}—C4A—C5A—C7A	-1.7 (8)	Sn1B—C25B—C30B—C29B	177.6 (4)
C2A—C4A—C5A—C7A	178.3 (4)	C28B—C29B—C30B—C25B	-1.4 (9)
C4A^{i}—C4A—C5A—C6A	174.9 (5)	C19A—Sn1A—C31A—C36A	37.4 (6)
C2A—C4A—C5A—C6A	-5.1 (7)	C25A—Sn1A—C31A—C36A	-117.8 (5)
C4B^{ii}—C4B—C5B—C7B	-1.0 (9)	O11A—Sn1A—C31A—C36A	-38.0 (5)
C2B—C4B—C5B—C7B	179.0 (5)	S1A—Sn1A—C31A—C36A	146.5 (5)
C4B^{ii}—C4B—C5B—C6B	176.9 (6)	C19A—Sn1A—C31A—C32A	-141.5 (5)
C2B—C4B—C5B—C6B	-3.1 (8)	C25A—Sn1A—C31A—C32A	63.3 (5)
C3A—N1A—C6A—O2A	178.5 (5)	O11A—Sn1A—C31A—C32A	143.1 (5)
C8A—N1A—C6A—O2A	2.2 (7)	S1A—Sn1A—C31A—C32A	-32.4 (5)
C3A—N1A—C6A—C5A	-0.7 (7)	C25B—Sn1B—C31B—C36B	-165.7 (4)
C8A—N1A—C6A—C5A	-177.0 (4)	C19B—Sn1B—C31B—C36B	-41.9 (5)
C7A—C5A—C6A—O2A	3.9 (7)	S1B—Sn1B—C31B—C36B	69.2 (4)
C4A—C5A—C6A—O2A	-172.8 (5)	C25B—Sn1B—C31B—C32B	19.7 (5)
C7A—C5A—C6A—N1A	-176.9 (4)	C19B—Sn1B—C31B—C32B	143.5 (4)
C4A—C5A—C6A—N1A	6.4 (6)	S1B—Sn1B—C31B—C32B	-105.4 (4)
C3B—N1B—C6B—O2B	-175.8 (5)	C36A—C31A—C32A—C33A	1.6 (9)
C8B—N1B—C6B—O2B	-0.9 (8)	Sn1A—C31A—C32A—C33A	-179.5 (5)
C3B—N1B—C6B—C5B	3.2 (8)	C36B—C31B—C32B—C33B	-0.2 (8)
C8B—N1B—C6B—C5B	178.2 (5)	Sn1B—C31B—C32B—C33B	174.5 (4)
C7B—C5B—C6B—O2B	-0.1 (8)	C31A—C32A—C33A—C34A	-3.3 (10)
C4B—C5B—C6B—O2B	-178.0 (5)	C31B—C32B—C33B—C34B	-1.5 (8)
C7B—C5B—C6B—N1B	-179.0 (5)	C32A—C33A—C34A—C35A	1.0 (11)
C4B—C5B—C6B—N1B	3.0 (7)	C32B—C33B—C34B—C35B	1.6 (9)
C4A—C5A—C7A—C1A^{i}	2.2 (7)	C33A—C34A—C35A—C36A	2.8 (11)
C6A—C5A—C7A—C1A^{i}	-174.4 (4)	C33B—C34B—C35B—C36B	0.0 (9)
C4B—C5B—C7B—C1B^{ii}	1.5 (8)	C32A—C31A—C36A—C35A	2.3 (9)
C6B—C5B—C7B—C1B^{ii}	-176.4 (5)	Sn1A—C31A—C36A—C35A	-176.6 (5)
C6A—N1A—C8A—C9A	-101.1 (5)	C34A—C35A—C36A—C31A	-4.5 (11)
C3A—N1A—C8A—C9A	82.3 (6)	C32B—C31B—C36B—C35B	1.7 (8)
C6B—N1B—C8B—C9B	82.4 (6)	Sn1B—C31B—C36B—C35B	-173.0 (4)
C3B—N1B—C8B—C9B	-102.4 (6)	C34B—C35B—C36B—C31B	-1.6 (8)
C10A—O3A—C9A—C8A	72.8 (5)	C47A—O6A—C37A—C38A	0.8 (7)
N1A—C8A—C9A—O3A	62.4 (6)	C47A—O6A—C37A—C46A	179.7 (4)
C10B—O3B—C9B—C8B	162.4 (4)	C47B—O6B—C37B—C38B	5.8 (8)
N1B—C8B—C9B—O3B	64.3 (6)	C47B—O6B—C37B—C46B	-174.5 (4)
C9A—O3A—C10A—C11A	164.9 (4)	O6A—C37A—C38A—C39A	-179.7 (5)
C9B—O3B—C10B—C11B	177.2 (4)	C46A—C37A—C38A—C39A	1.4 (8)
P1A—O4A—C11A—C10A	159.9 (3)	O6B—C37B—C38B—C39B	179.3 (5)
O3A—C10A—C11A—O4A	-71.0 (5)	C46B—C37B—C38B—C39B	-0.4 (9)
P1B—O4B—C11B—C10B	-177.3 (3)	C37A—C38A—C39A—C40A	-1.0 (8)
O3B—C10B—C11B—O4B	54.3 (6)	C37B—C38B—C39B—C40B	-2.8 (10)
O4A—P1A—C12A—C13A	-72.8 (10)	C38A—C39A—C40A—C41A	-0.1 (8)

C12C—P1A—C12A—C13A	-35 (5)	C38B—C39B—C40B—C41B	3.6 (10)
S2A—P1A—C12A—C13A	163.5 (8)	C39A—C40A—C41A—C46A	0.6 (7)
S1A—P1A—C12A—C13A	35.8 (10)	C39A—C40A—C41A—C42A	-178.8 (5)
O4A—P1A—C12A—C17A	106.0 (9)	C39B—C40B—C41B—C46B	-1.2 (9)
C12C—P1A—C12A—C17A	144 (6)	C39B—C40B—C41B—C42B	177.7 (6)
S2A—P1A—C12A—C17A	-17.7 (10)	C46A—C41A—C42A—C43A	-0.6 (8)
S1A—P1A—C12A—C17A	-145.4 (8)	C40A—C41A—C42A—C43A	178.8 (5)
O4B—P1B—C12B—C13B	155.1 (4)	C46A—C41A—C42A—O10A^{i}	-179.5 (4)
S2B—P1B—C12B—C13B	30.9 (5)	C40A—C41A—C42A—O10A^{i}	-0.2 (7)
S1B—P1B—C12B—C13B	-95.2 (4)	C40B—C41B—C42B—C43B	-175.6 (5)
O4B—P1B—C12B—C17B	-29.7 (4)	C46B—C41B—C42B—C43B	3.4 (8)
S2B—P1B—C12B—C17B	-154.0 (4)	C40B—C41B—C42B—O10B^{ii}	5.1 (7)
S1B—P1B—C12B—C17B	79.9 (4)	C46B—C41B—C42B—O10B^{ii}	-175.9 (4)
O4A—P1A—C12C—C13C	-20 (4)	O10A^{i}—C42A—C43A—C44A	-179.0 (5)
C12A—P1A—C12C—C13C	-165 (9)	C41A—C42A—C43A—C44A	2.2 (8)
S2A—P1A—C12C—C13C	-143 (3)	O10B^{ii}—C42B—C43B—C44B	177.8 (5)
S1A—P1A—C12C—C13C	82 (4)	C41B—C42B—C43B—C44B	-1.4 (8)
O4A—P1A—C12C—C17C	158 (3)	C42A—C43A—C44A—C45A	-2.6 (9)
C12A—P1A—C12C—C17C	13 (3)	C42B—C43B—C44B—C45B	-1.3 (8)
S2A—P1A—C12C—C17C	35 (4)	C43A—C44A—C45A—C46A	1.3 (9)
S1A—P1A—C12C—C17C	-100 (3)	C43B—C44B—C45B—C46B	2.0 (8)
C17A—C12A—C13A—C14A	-3.1 (17)	C40A—C41A—C46A—C37A	-0.1 (7)
P1A—C12A—C13A—C14A	175.7 (8)	C42A—C41A—C46A—C37A	179.3 (5)
C17B—C12B—C13B—C14B	0.4 (8)	C40A—C41A—C46A—C45A	179.9 (5)
P1B—C12B—C13B—C14B	175.6 (4)	C42A—C41A—C46A—C45A	-0.7 (7)
C17C—C12C—C13C—C14C	4 (5)	C38A—C37A—C46A—C41A	-0.9 (8)
P1A—C12C—C13C—C14C	-178 (2)	O6A—C37A—C46A—C41A	-179.9 (4)
C12A—C13A—C14A—C15A	2.7 (16)	C38A—C37A—C46A—C45A	179.1 (5)
C12B—C13B—C14B—C15B	-1.1 (8)	O6A—C37A—C46A—C45A	0.1 (7)
C12C—C13C—C14C—C15C	-3 (4)	C44A—C45A—C46A—C41A	0.4 (8)
C18A—O5A—C15A—C16A	-179.3 (11)	C44A—C45A—C46A—C37A	-179.6 (5)
C18A—O5A—C15A—C14A	-1.7 (17)	C44B—C45B—C46B—C37B	177.9 (5)
C13A—C14A—C15A—O5A	179.4 (9)	C44B—C45B—C46B—C41B	0.0 (8)
C13A—C14A—C15A—C16A	-3.1 (18)	O6B—C37B—C46B—C45B	4.9 (7)
C18B—O5B—C15B—C14B	4.6 (7)	C38B—C37B—C46B—C45B	-175.4 (5)
C18B—O5B—C15B—C16B	-173.6 (5)	O6B—C37B—C46B—C41B	-177.2 (4)
C13B—C14B—C15B—O5B	-177.1 (5)	C38B—C37B—C46B—C41B	2.5 (8)
C13B—C14B—C15B—C16B	1.1 (8)	C40B—C41B—C46B—C45B	176.3 (5)
C18C—O5C—C15C—C16C	1 (5)	C42B—C41B—C46B—C45B	-2.6 (7)
C18C—O5C—C15C—C14C	-177 (4)	C40B—C41B—C46B—C37B	-1.7 (8)
C13C—C14C—C15C—C16C	3 (4)	C42B—C41B—C46B—C37B	179.3 (5)
C13C—C14C—C15C—O5C	-179 (2)	C37A—O6A—C47A—C48A	174.4 (5)
O5A—C15A—C16A—C17A	-178.5 (9)	C37B—O6B—C47B—C48B	176.6 (4)

C14A—C15A—C16A—C17A	3.9 (18)	C49A—O7A—C48A—C47A	-90.3 (8)
O5B—C15B—C16B—C17B	178.1 (4)	O6A—C47A—C48A—O7A	74.9 (8)
C14B—C15B—C16B—C17B	-0.2 (8)	C49B—O7B—C48B—C47B	-163.7 (4)
O5C—C15C—C16C—C17C	177 (2)	O6B—C47B—C48B—O7B	-62.1 (6)
C14C—C15C—C16C—C17C	-6 (5)	C48A—O7A—C49A—C50A	-162.9 (6)
C15A—C16A—C17A—C12A	-3.9 (15)	C48B—O7B—C49B—C50B	-177.1 (5)
C13A—C12A—C17A—C16A	3.6 (16)	C51A—O8A—C50A—C49A	179.4 (5)
P1A—C12A—C17A—C16A	-175.2 (8)	O7A—C49A—C50A—O8A	-65.0 (8)
C15B—C16B—C17B—C12B	-0.6 (8)	C51B—O8B—C50B—C49B	-168.9 (5)
C13B—C12B—C17B—C16B	0.5 (7)	O7B—C49B—C50B—O8B	-61.1 (6)
P1B—C12B—C17B—C16B	-174.7 (4)	C50A—O8A—C51A—C52A	178.8 (6)
C15C—C16C—C17C—C12C	8 (5)	C50B—O8B—C51B—C52B	-177.1 (5)
C13C—C12C—C17C—C16C	-6 (4)	C53A—O9A—C52A—C51A	176.0 (5)
P1A—C12C—C17C—C16C	175 (2)	O8A—C51A—C52A—O9A	69.2 (7)
C31A—Sn1A—C19A—C20A	170.2 (4)	C53B—O9B—C52B—C51B	-175.8 (5)
C25A—Sn1A—C19A—C20A	-33.9 (5)	O8B—C51B—C52B—O9B	-66.4 (6)
O11A—Sn1A—C19A—C20A	-115.1 (4)	C52A—O9A—C53A—C54A	89.5 (7)
S1A—Sn1A—C19A—C20A	62.4 (4)	C52B—O9B—C53B—C54B	-78.0 (6)
C31A—Sn1A—C19A—C24A	-11.5 (5)	C42A^{i}—O10A—C54A—C53A	-177.8 (5)
C25A—Sn1A—C19A—C24A	144.4 (4)	O9A—C53A—C54A—O10A	-69.8 (6)
O11A—Sn1A—C19A—C24A	63.2 (4)	C42B^{ii}—O10B—C54B—C53B	176.3 (4)
S1A—Sn1A—C19A—C24A	-119.3 (4)	O9B—C53B—C54B—O10B	73.8 (6)
C25B—Sn1B—C19B—C20B	-105.4 (5)		
Symmetry codes: (i) -*x*, -*y*+3, -*z*-1; (ii) -*x*, -*y*, -*z*.			

Table A13: Hydrogen-bond geometry (Å, °) for NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2(SnPh_3)_2]_2$ ⊂15DN38C10

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11*A*—H11*F*···O7*A*^{iii}	0.94	1.91	2.839 (6)	174
O11*A*—H11*G*···O9*A*^{iii}	1.01	1.73	2.736 (5)	170
Symmetry code: (iii) *x*+1, *y*-1, *z*.				

Table A14: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for NDI-$[CH_2CH_2O(An)PS_2]_2$-$[SnPh_2]_2$

	x	*y*	*z*	U_{iso}*/U_{eq}	
Sn1	0.913918 (14)	0.212481 (13)	0.238928 (8)	0.01781 (6)	
Cl1	1.19037 (7)	0.47718 (6)	0.02807 (4)	0.03414 (15)	
Cl2	1.11834 (7)	0.26962 (6)	0.04744 (4)	0.03635 (16)	
S1	0.75885 (6)	0.27596 (6)	0.05471 (4)	0.02583 (14)	
S2	0.67307 (6)	0.26165 (5)	0.23938 (3)	0.02182 (13)	

S3	0.89006 (6)	0.16983 (5)	0.37760 (3)	0.02190 (13)	
S4	1.17854 (6)	0.12296 (5)	0.30141 (3)	0.02311 (13)	
P1	0.62723 (6)	0.26158 (5)	0.12672 (3)	0.01816 (12)	
P2	1.08383 (6)	0.08986 (5)	0.39161 (3)	0.01879 (13)	
O1	0.81018 (18)	0.37978 (16)	0.60081 (10)	0.0268 (4)	
O2	0.58141 (18)	0.13184 (17)	0.60194 (10)	0.0279 (4)	
O3	0.30363 (17)	0.37702 (17)	0.25509 (10)	0.0260 (4)	
O4	0.53932 (19)	0.61955 (16)	0.24960 (11)	0.0290 (4)	
O5	0.48918 (16)	0.35967 (15)	0.11929 (9)	0.0200 (3)	
O6	0.47205 (19)	-0.15421 (16)	0.10953 (11)	0.0297 (4)	
O7	1.10923 (17)	-0.04258 (14)	0.41027 (9)	0.0210 (4)	
O8	1.2584 (2)	0.24244 (17)	0.67114 (11)	0.0309 (4)	
N1	0.6973 (2)	0.25523 (18)	0.60106 (11)	0.0214 (4)	
N2	0.4180 (2)	0.50167 (18)	0.25382 (11)	0.0201 (4)	
C1	0.8999 (2)	0.1193 (2)	0.64828 (14)	0.0224 (5)	
H1A	0.9532	0.1662	0.6292	0.027*	
H1B	0.9415	0.0742	0.6937	0.027*	
C2	0.7657 (3)	0.1964 (2)	0.66924 (14)	0.0236 (5)	
H2A	0.7167	0.1502	0.6948	0.028*	
H2B	0.7718	0.2538	0.7052	0.028*	
C3	0.7337 (2)	0.3461 (2)	0.56910 (14)	0.0214 (5)	
C4	0.6750 (2)	0.3966 (2)	0.49566 (13)	0.0191 (5)	
C5	0.5816 (2)	0.3568 (2)	0.46388 (13)	0.0185 (5)	
C6	0.5445 (2)	0.2671 (2)	0.49934 (14)	0.0201 (5)	
C7	0.6064 (2)	0.2115 (2)	0.57094 (14)	0.0216 (5)	
C8	0.4534 (2)	0.2296 (2)	0.46665 (14)	0.0227 (5)	
H8	0.4292	0.1691	0.4907	0.027*	
C9	0.3962 (2)	0.2802 (2)	0.39814 (14)	0.0232 (5)	
H9	0.3330	0.2543	0.3763	0.028*	
C10	0.4315 (2)	0.3672 (2)	0.36243 (14)	0.0204 (5)	
C11	0.5247 (2)	0.4070 (2)	0.39461 (13)	0.0182 (5)	
C12	0.5649 (2)	0.4939 (2)	0.35783 (13)	0.0192 (5)	
C13	0.6582 (2)	0.5300 (2)	0.38922 (14)	0.0211 (5)	
H13	0.6855	0.5877	0.3638	0.025*	
C14	0.7127 (2)	0.4812 (2)	0.45889 (14)	0.0217 (5)	
H14	0.7761	0.5069	0.4807	0.026*	
C15	0.3775 (2)	0.4138 (2)	0.28718 (14)	0.0210 (5)	
C16	0.5090 (2)	0.5450 (2)	0.28375 (14)	0.0204 (5)	
C17	0.3758 (2)	0.5415 (2)	0.17604 (14)	0.0229 (5)	
H17A	0.3601	0.6249	0.1705	0.027*	
H17B	0.2938	0.5273	0.1668	0.027*	
C18	0.4771 (2)	0.4799 (2)	0.11773 (14)	0.0215 (5)	
H18A	0.4519	0.5141	0.0664	0.026*	

H18B	0.5610	0.4887	0.1293	0.026*	
C19	0.5780 (2)	0.1379 (2)	0.11745 (14)	0.0200 (5)	
C20	0.4761 (2)	0.1231 (2)	0.16294 (14)	0.0222 (5)	
H20	0.4298	0.1807	0.1968	0.027*	
C21	0.4439 (3)	0.0248 (2)	0.15823 (15)	0.0251 (5)	
H21	0.3745	0.0154	0.1885	0.030*	
C22	0.5126 (2)	-0.0612 (2)	0.10928 (15)	0.0237 (5)	
C23	0.6143 (3)	-0.0483 (2)	0.06506 (14)	0.0239 (5)	
H23	0.6617	-0.1068	0.0321	0.029*	
C24	0.6459 (2)	0.0513 (2)	0.06953 (14)	0.0233 (5)	
H24	0.7154	0.0605	0.0392	0.028*	
C25	0.5498 (3)	-0.2508 (2)	0.06882 (17)	0.0310 (6)	
H25A	0.5568	-0.2281	0.0153	0.046*	
H25B	0.5100	-0.3113	0.0727	0.046*	
H25C	0.6359	-0.2792	0.0906	0.046*	
C26	0.9737 (2)	0.0558 (2)	0.18008 (13)	0.0193 (5)	
C27	1.0949 (3)	0.0137 (2)	0.14495 (15)	0.0253 (5)	
H27	1.1513	0.0581	0.1431	0.030*	
C28	1.1333 (3)	-0.0929 (2)	0.11269 (16)	0.0296 (6)	
H28	1.2163	-0.1217	0.0894	0.035*	
C29	1.0501 (3)	-0.1580 (2)	0.11444 (16)	0.0303 (6)	
H29	1.0759	-0.2306	0.0919	0.036*	
C30	0.9301 (3)	-0.1160 (2)	0.14916 (16)	0.0277 (6)	
H30	0.8732	-0.1598	0.1502	0.033*	
C31	0.8920 (2)	-0.0098 (2)	0.18265 (15)	0.0229 (5)	
H31	0.8099	0.0178	0.2073	0.027*	
C32	0.9359 (2)	0.3780 (2)	0.23041 (14)	0.0214 (5)	
C33	1.0047 (3)	0.4086 (2)	0.28643 (15)	0.0262 (5)	
H33	1.0425	0.3555	0.3264	0.031*	
C34	1.0177 (3)	0.5167 (2)	0.28366 (16)	0.0297 (6)	
H34	1.0633	0.5379	0.3222	0.036*	
C35	0.9649 (3)	0.5929 (3)	0.22546 (18)	0.0344 (6)	
H35	0.9753	0.6663	0.2234	0.041*	
C36	0.8965 (3)	0.5636 (2)	0.16964 (18)	0.0340 (6)	
H36	0.8609	0.6164	0.1291	0.041*	
C37	0.8798 (3)	0.4564 (2)	0.17297 (16)	0.0292 (6)	
H37	0.8299	0.4373	0.1359	0.035*	
C38	1.1307 (2)	0.1313 (2)	0.47944 (14)	0.0203 (5)	
C39	1.2156 (3)	0.0513 (2)	0.52786 (15)	0.0243 (5)	
H39	1.2434	-0.0273	0.5159	0.029*	
C40	1.2601 (3)	0.0840 (2)	0.59284 (14)	0.0240 (5)	
H40	1.3173	0.0284	0.6253	0.029*	
C41	1.2198 (2)	0.1995 (2)	0.61011 (14)	0.0232 (5)	

C42	1.1330 (3)	0.2800 (2)	0.56298 (15)	0.0256 (5)	
H42	1.1039	0.3584	0.5755	0.031*	
C43	1.0892 (3)	0.2465 (2)	0.49826 (15)	0.0241 (5)	
H43	1.0307	0.3019	0.4664	0.029*	
C44	1.3444 (3)	0.1644 (3)	0.72298 (15)	0.0290 (6)	
H44A	1.3034	0.1104	0.7450	0.043*	
H44B	1.3649	0.2070	0.7636	0.043*	
H44C	1.4239	0.1222	0.6958	0.043*	
C45	1.1891 (3)	0.3615 (3)	0.09017 (16)	0.0319 (6)	
H45A	1.1401	0.3914	0.1372	0.038*	
H45B	1.2786	0.3175	0.1044	0.038*	

Table A15: Atomic displacement parameters ($Å^2$) for NDI-$[CH_2CH_2O(An)PS_2]_2$-$[SnPh_2]_2$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01943 (9)	0.01589 (9)	0.01950 (9)	-0.00736 (6)	-0.00010 (6)	-0.00298 (6)
Cl1	0.0438 (4)	0.0326 (4)	0.0304 (3)	-0.0182 (3)	-0.0075 (3)	0.0038 (3)
Cl2	0.0364 (4)	0.0318 (4)	0.0447 (4)	-0.0156 (3)	0.0006 (3)	-0.0069 (3)
S1	0.0283 (3)	0.0274 (3)	0.0259 (3)	-0.0146 (3)	0.0069 (2)	-0.0072 (2)
S2	0.0185 (3)	0.0262 (3)	0.0200 (3)	-0.0054 (2)	-0.0011 (2)	-0.0063 (2)
S3	0.0205 (3)	0.0233 (3)	0.0207 (3)	-0.0053 (2)	0.0004 (2)	-0.0015 (2)
S4	0.0231 (3)	0.0266 (3)	0.0210 (3)	-0.0099 (2)	0.0010 (2)	-0.0022 (2)
P1	0.0188 (3)	0.0186 (3)	0.0184 (3)	-0.0074 (2)	0.0001 (2)	-0.0042 (2)
P2	0.0208 (3)	0.0182 (3)	0.0178 (3)	-0.0066 (2)	0.0000 (2)	-0.0023 (2)
O1	0.0326 (10)	0.0219 (10)	0.0271 (9)	-0.0091 (8)	-0.0097 (8)	-0.0041 (7)
O2	0.0279 (10)	0.0311 (11)	0.0263 (9)	-0.0128 (8)	0.0009 (7)	0.0039 (8)
O3	0.0245 (9)	0.0330 (11)	0.0246 (9)	-0.0143 (8)	-0.0031 (7)	-0.0035 (7)
O4	0.0402 (11)	0.0251 (10)	0.0259 (9)	-0.0162 (8)	-0.0063 (8)	0.0010 (7)
O5	0.0204 (8)	0.0185 (9)	0.0224 (8)	-0.0076 (7)	-0.0021 (7)	-0.0023 (6)
O6	0.0344 (10)	0.0232 (10)	0.0358 (11)	-0.0151 (8)	0.0006 (8)	-0.0044 (8)
O7	0.0262 (9)	0.0171 (9)	0.0206 (8)	-0.0076 (7)	-0.0023 (7)	-0.0031 (6)
O8	0.0396 (11)	0.0336 (11)	0.0242 (9)	-0.0175 (9)	-0.0049 (8)	-0.0065 (8)
N1	0.0216 (10)	0.0232 (11)	0.0171 (10)	-0.0038 (8)	-0.0004 (8)	-0.0035 (8)
N2	0.0210 (10)	0.0199 (11)	0.0188 (10)	-0.0054 (8)	-0.0016 (8)	-0.0036 (8)
C1	0.0273 (13)	0.0153 (12)	0.0251 (12)	-0.0066 (10)	-0.0071 (10)	-0.0027 (9)
C2	0.0303 (14)	0.0207 (13)	0.0183 (12)	-0.0058 (10)	-0.0029 (10)	-0.0014 (9)
C3	0.0214 (12)	0.0181 (13)	0.0216 (12)	-0.0016 (9)	0.0001 (10)	-0.0065 (9)
C4	0.0185 (11)	0.0178 (12)	0.0188 (11)	-0.0023 (9)	0.0008 (9)	-0.0074 (9)
C5	0.0176 (11)	0.0183 (12)	0.0185 (11)	-0.0041 (9)	0.0038 (9)	-0.0066 (9)
C6	0.0179 (11)	0.0223 (13)	0.0196 (12)	-0.0056 (9)	0.0029 (9)	-0.0046 (9)
C7	0.0209 (12)	0.0214 (13)	0.0211 (12)	-0.0048 (10)	0.0049 (9)	-0.0040 (9)
C8	0.0232 (12)	0.0230 (13)	0.0243 (12)	-0.0109 (10)	0.0052 (10)	-0.0030 (10)
C9	0.0206 (12)	0.0277 (14)	0.0249 (13)	-0.0122 (10)	0.0011 (10)	-0.0059 (10)

C10	0.0174 (11)	0.0243 (13)	0.0194 (12)	-0.0063 (9)	0.0025 (9)	-0.0065 (9)
C11	0.0184 (11)	0.0166 (12)	0.0187 (11)	-0.0040 (9)	0.0029 (9)	-0.0065 (9)
C12	0.0197 (12)	0.0173 (12)	0.0188 (11)	-0.0029 (9)	0.0013 (9)	-0.0067 (9)
C13	0.0228 (12)	0.0195 (13)	0.0218 (12)	-0.0078 (10)	0.0021 (9)	-0.0052 (9)
C14	0.0208 (12)	0.0205 (13)	0.0241 (12)	-0.0063 (9)	0.0001 (10)	-0.0079 (9)
C15	0.0190 (12)	0.0210 (13)	0.0231 (12)	-0.0062 (9)	0.0027 (9)	-0.0054 (9)
C16	0.0246 (12)	0.0156 (12)	0.0211 (12)	-0.0061 (9)	0.0011 (10)	-0.0053 (9)
C17	0.0264 (13)	0.0206 (13)	0.0206 (12)	-0.0058 (10)	-0.0041 (10)	-0.0011 (9)
C18	0.0264 (13)	0.0180 (13)	0.0208 (12)	-0.0077 (10)	-0.0022 (10)	-0.0018 (9)
C19	0.0220 (12)	0.0199 (13)	0.0192 (11)	-0.0080 (9)	-0.0019 (9)	-0.0015 (9)
C20	0.0210 (12)	0.0225 (13)	0.0224 (12)	-0.0057 (10)	0.0004 (9)	-0.0036 (9)
C21	0.0229 (13)	0.0269 (14)	0.0261 (13)	-0.0090 (10)	0.0023 (10)	-0.0017 (10)
C22	0.0254 (13)	0.0208 (14)	0.0264 (13)	-0.0094 (10)	-0.0067 (10)	0.0009 (10)
C23	0.0268 (13)	0.0216 (14)	0.0228 (12)	-0.0067 (10)	-0.0008 (10)	-0.0048 (10)
C24	0.0247 (13)	0.0252 (14)	0.0205 (12)	-0.0087 (10)	0.0013 (10)	-0.0032 (10)
C25	0.0401 (16)	0.0204 (14)	0.0344 (15)	-0.0120 (12)	-0.0013 (12)	-0.0048 (11)
C26	0.0243 (12)	0.0153 (12)	0.0188 (11)	-0.0066 (9)	-0.0010 (9)	-0.0032 (9)
C27	0.0288 (14)	0.0256 (14)	0.0254 (13)	-0.0139 (11)	0.0027 (10)	-0.0041 (10)
C28	0.0306 (14)	0.0295 (15)	0.0276 (14)	-0.0082 (11)	0.0080 (11)	-0.0085 (11)
C29	0.0386 (16)	0.0195 (14)	0.0332 (14)	-0.0092 (11)	0.0039 (12)	-0.0095 (10)
C30	0.0303 (14)	0.0189 (14)	0.0381 (15)	-0.0129 (11)	-0.0025 (11)	-0.0053 (11)
C31	0.0218 (12)	0.0169 (13)	0.0305 (13)	-0.0069 (10)	0.0006 (10)	-0.0032 (10)
C32	0.0221 (12)	0.0190 (13)	0.0258 (12)	-0.0102 (9)	0.0035 (10)	-0.0048 (9)
C33	0.0287 (14)	0.0259 (15)	0.0254 (13)	-0.0103 (11)	-0.0015 (10)	-0.0033 (10)
C34	0.0284 (14)	0.0303 (16)	0.0340 (15)	-0.0133 (11)	-0.0009 (11)	-0.0108 (11)
C35	0.0378 (16)	0.0222 (15)	0.0476 (17)	-0.0151 (12)	0.0007 (13)	-0.0067 (12)
C36	0.0422 (17)	0.0199 (15)	0.0413 (16)	-0.0120 (12)	-0.0096 (13)	0.0050 (11)
C37	0.0330 (15)	0.0237 (15)	0.0336 (15)	-0.0122 (11)	-0.0072 (11)	-0.0019 (11)
C38	0.0216 (12)	0.0223 (13)	0.0189 (11)	-0.0097 (10)	0.0024 (9)	-0.0042 (9)
C39	0.0276 (13)	0.0219 (14)	0.0245 (13)	-0.0095 (10)	0.0026 (10)	-0.0028 (10)
C40	0.0260 (13)	0.0268 (14)	0.0205 (12)	-0.0103 (10)	-0.0012 (10)	0.0002 (10)
C41	0.0249 (13)	0.0284 (14)	0.0216 (12)	-0.0159 (10)	0.0024 (10)	-0.0039 (10)
C42	0.0326 (14)	0.0200 (14)	0.0275 (13)	-0.0127 (11)	0.0035 (11)	-0.0066 (10)
C43	0.0249 (13)	0.0240 (14)	0.0237 (13)	-0.0083 (10)	0.0013 (10)	-0.0006 (10)
C44	0.0374 (15)	0.0347 (16)	0.0207 (13)	-0.0196 (12)	-0.0016 (11)	-0.0013 (11)
C45	0.0351 (15)	0.0358 (17)	0.0298 (14)	-0.0186 (12)	-0.0041 (12)	0.0029 (11)

Table A16: Geometric parameters (Å, °) for NDI-$[CH_2CH_2O(An)PS_2]_2$-$[SnPh_2]_2$

Sn1—C26	2.135 (2)	C17—C18	1.521 (3)
Sn1—C32	2.136 (3)	C17—H17A	0.9900
Sn1—S3	2.4996 (6)	C17—H17B	0.9900
Sn1—S2	2.5111 (6)	C18—H18A	0.9900

Cl1—C45	1.766 (3)	C18—H18B	0.9900
Cl2—C45	1.773 (3)	C19—C24	1.390 (4)
S1—P1	1.9370 (9)	C19—C20	1.410 (4)
S2—P1	2.0629 (8)	C20—C21	1.377 (4)
S3—P2	2.0507 (9)	C20—H20	0.9500
S4—P2	1.9703 (9)	C21—C22	1.399 (4)
P1—O5	1.6089 (17)	C21—H21	0.9500
P1—C19	1.794 (3)	C22—C23	1.387 (4)
P2—O7	1.5909 (18)	C23—C24	1.389 (4)
P2—C38	1.792 (3)	C23—H23	0.9500
O1—C3	1.211 (3)	C24—H24	0.9500
O2—C7	1.210 (3)	C25—H25A	0.9800
O3—C15	1.214 (3)	C25—H25B	0.9800
O4—C16	1.209 (3)	C25—H25C	0.9800
O5—C18	1.448 (3)	C26—C31	1.390 (4)
O6—C22	1.361 (3)	C26—C27	1.395 (4)
O6—C25	1.428 (3)	C27—C28	1.387 (4)
O7—C1^{i}	1.458 (3)	C27—H27	0.9500
O8—C41	1.357 (3)	C28—C29	1.398 (4)
O8—C44	1.430 (3)	C28—H28	0.9500
N1—C3	1.401 (3)	C29—C30	1.381 (4)
N1—C7	1.405 (3)	C29—H29	0.9500
N1—C2	1.471 (3)	C30—C31	1.393 (4)
N2—C15	1.401 (3)	C30—H30	0.9500
N2—C16	1.402 (3)	C31—H31	0.9500
N2—C17	1.473 (3)	C32—C37	1.383 (4)
C1—O7^{i}	1.458 (3)	C32—C33	1.397 (4)
C1—C2	1.516 (4)	C33—C34	1.388 (4)
C1—H1A	0.9900	C33—H33	0.9500
C1—H1B	0.9900	C34—C35	1.369 (4)
C2—H2A	0.9900	C34—H34	0.9500
C2—H2B	0.9900	C35—C36	1.384 (4)
C3—C4	1.484 (3)	C35—H35	0.9500
C4—C14	1.375 (4)	C36—C37	1.393 (4)
C4—C5	1.412 (3)	C36—H36	0.9500
C5—C11	1.413 (3)	C37—H37	0.9500
C5—C6	1.415 (3)	C38—C39	1.398 (4)
C6—C8	1.381 (4)	C38—C43	1.398 (4)
C6—C7	1.484 (3)	C39—C40	1.384 (4)
C8—C9	1.404 (4)	C39—H39	0.9500
C8—H8	0.9500	C40—C41	1.396 (4)
C9—C10	1.378 (4)	C40—H40	0.9500
C9—H9	0.9500	C41—C42	1.397 (4)

C10—C11	1.413 (3)	C42—C43	1.381 (4)
C10—C15	1.484 (3)	C42—H42	0.9500
C11—C12	1.414 (3)	C43—H43	0.9500
C12—C13	1.380 (4)	C44—H44A	0.9800
C12—C16	1.486 (3)	C44—H44B	0.9800
C13—C14	1.406 (4)	C44—H44C	0.9800
C13—H13	0.9500	C45—H45A	0.9900
C14—H14	0.9500	C45—H45B	0.9900
C26—Sn1—C32	139.28 (9)	O5—C18—H18B	109.7
C26—Sn1—S3	109.11 (7)	C17—C18—H18B	109.7
C32—Sn1—S3	106.16 (7)	H18A—C18—H18B	108.2
C26—Sn1—S2	101.49 (7)	C24—C19—C20	119.0 (2)
C32—Sn1—S2	101.74 (7)	C24—C19—P1	120.46 (19)
S3—Sn1—S2	84.113 (19)	C20—C19—P1	120.39 (19)
P1—S2—Sn1	104.91 (3)	C21—C20—C19	119.8 (2)
P2—S3—Sn1	93.87 (3)	C21—C20—H20	120.1
O5—P1—C19	99.32 (10)	C19—C20—H20	120.1
O5—P1—S1	115.35 (7)	C20—C21—C22	120.5 (2)
C19—P1—S1	115.47 (9)	C20—C21—H21	119.7
O5—P1—S2	104.29 (7)	C22—C21—H21	119.7
C19—P1—S2	105.90 (8)	O6—C22—C23	124.6 (2)
S1—P1—S2	114.75 (4)	O6—C22—C21	115.2 (2)
O7—P2—C38	100.01 (11)	C23—C22—C21	120.2 (2)
O7—P2—S4	114.57 (7)	C22—C23—C24	119.2 (2)
C38—P2—S4	114.34 (9)	C22—C23—H23	120.4
O7—P2—S3	109.11 (7)	C24—C23—H23	120.4
C38—P2—S3	109.18 (9)	C23—C24—C19	121.4 (2)
S4—P2—S3	109.22 (4)	C23—C24—H24	119.3
C18—O5—P1	121.51 (15)	C19—C24—H24	119.3
C22—O6—C25	117.3 (2)	O6—C25—H25A	109.5
C1^{i}—O7—P2	121.23 (15)	O6—C25—H25B	109.5
C41—O8—C44	118.3 (2)	H25A—C25—H25B	109.5
C3—N1—C7	125.4 (2)	O6—C25—H25C	109.5
C3—N1—C2	117.0 (2)	H25A—C25—H25C	109.5
C7—N1—C2	117.4 (2)	H25B—C25—H25C	109.5
C15—N2—C16	125.6 (2)	C31—C26—C27	119.5 (2)
C15—N2—C17	117.5 (2)	C31—C26—Sn1	117.97 (18)
C16—N2—C17	116.3 (2)	C27—C26—Sn1	122.34 (19)
O7^{i}—C1—C2	109.1 (2)	C28—C27—C26	120.2 (2)
O7^{i}—C1—H1A	109.9	C28—C27—H27	119.9
C2—C1—H1A	109.9	C26—C27—H27	119.9
O7^{i}—C1—H1B	109.9	C27—C28—C29	120.1 (3)
C2—C1—H1B	109.9	C27—C28—H28	119.9

H1A—C1—H1B	108.3	C29—C28—H28	119.9
N1—C2—C1	110.7 (2)	C30—C29—C28	119.5 (2)
N1—C2—H2A	109.5	C30—C29—H29	120.2
C1—C2—H2A	109.5	C28—C29—H29	120.2
N1—C2—H2B	109.5	C29—C30—C31	120.5 (3)
C1—C2—H2B	109.5	C29—C30—H30	119.7
H2A—C2—H2B	108.1	C31—C30—H30	119.7
O1—C3—N1	120.4 (2)	C26—C31—C30	120.1 (2)
O1—C3—C4	122.9 (2)	C26—C31—H31	119.9
N1—C3—C4	116.8 (2)	C30—C31—H31	119.9
C14—C4—C5	120.6 (2)	C37—C32—C33	119.6 (2)
C14—C4—C3	119.7 (2)	C37—C32—Sn1	121.76 (19)
C5—C4—C3	119.7 (2)	C33—C32—Sn1	118.58 (19)
C4—C5—C11	119.2 (2)	C34—C33—C32	120.0 (3)
C4—C5—C6	121.6 (2)	C34—C33—H33	120.0
C11—C5—C6	119.2 (2)	C32—C33—H33	120.0
C8—C6—C5	120.2 (2)	C35—C34—C33	120.1 (3)
C8—C6—C7	120.1 (2)	C35—C34—H34	119.9
C5—C6—C7	119.7 (2)	C33—C34—H34	119.9
O2—C7—N1	121.1 (2)	C34—C35—C36	120.4 (3)
O2—C7—C6	122.1 (2)	C34—C35—H35	119.8
N1—C7—C6	116.7 (2)	C36—C35—H35	119.8
C6—C8—C9	120.5 (2)	C35—C36—C37	120.0 (3)
C6—C8—H8	119.8	C35—C36—H36	120.0
C9—C8—H8	119.8	C37—C36—H36	120.0
C10—C9—C8	120.2 (2)	C32—C37—C36	119.8 (3)
C10—C9—H9	119.9	C32—C37—H37	120.1
C8—C9—H9	119.9	C36—C37—H37	120.1
C9—C10—C11	120.4 (2)	C39—C38—C43	118.7 (2)
C9—C10—C15	119.6 (2)	C39—C38—P2	121.1 (2)
C11—C10—C15	119.9 (2)	C43—C38—P2	120.05 (19)
C10—C11—C5	119.5 (2)	C40—C39—C38	121.5 (3)
C10—C11—C12	121.3 (2)	C40—C39—H39	119.3
C5—C11—C12	119.2 (2)	C38—C39—H39	119.3
C13—C12—C11	120.6 (2)	C39—C40—C41	119.2 (2)
C13—C12—C16	119.5 (2)	C39—C40—H40	120.4
C11—C12—C16	119.9 (2)	C41—C40—H40	120.4
C12—C13—C14	120.0 (2)	O8—C41—C40	124.8 (2)
C12—C13—H13	120.0	O8—C41—C42	115.4 (2)
C14—C13—H13	120.0	C40—C41—C42	119.9 (2)
C4—C14—C13	120.4 (2)	C43—C42—C41	120.4 (3)
C4—C14—H14	119.8	C43—C42—H42	119.8
C13—C14—H14	119.8	C41—C42—H42	119.8

O3—C15—N2	121.2 (2)	C42—C43—C38	120.3 (2)
O3—C15—C10	122.2 (2)	C42—C43—H43	119.8
N2—C15—C10	116.6 (2)	C38—C43—H43	119.8
O4—C16—N2	120.4 (2)	O8—C44—H44A	109.5
O4—C16—C12	123.0 (2)	O8—C44—H44B	109.5
N2—C16—C12	116.6 (2)	H44A—C44—H44B	109.5
N2—C17—C18	110.9 (2)	O8—C44—H44C	109.5
N2—C17—H17A	109.5	H44A—C44—H44C	109.5
C18—C17—H17A	109.5	H44B—C44—H44C	109.5
N2—C17—H17B	109.5	Cl1—C45—Cl2	111.43 (16)
C18—C17—H17B	109.5	Cl1—C45—H45A	109.3
H17A—C17—H17B	108.1	Cl2—C45—H45A	109.3
O5—C18—C17	109.8 (2)	Cl1—C45—H45B	109.3
O5—C18—H18A	109.7	Cl2—C45—H45B	109.3
C17—C18—H18A	109.7	H45A—C45—H45B	108.0
C26—Sn1—S2—P1	-54.72 (7)	C17—N2—C16—O4	7.3 (3)
C32—Sn1—S2—P1	91.60 (8)	C15—N2—C16—C12	-1.0 (3)
S3—Sn1—S2—P1	-163.07 (3)	C17—N2—C16—C12	-172.2 (2)
C26—Sn1—S3—P2	67.78 (8)	C13—C12—C16—O4	-1.6 (4)
C32—Sn1—S3—P2	-91.53 (7)	C11—C12—C16—O4	179.9 (2)
S2—Sn1—S3—P2	167.92 (3)	C13—C12—C16—N2	177.9 (2)
Sn1—S2—P1—O5	-146.36 (7)	C11—C12—C16—N2	-0.6 (3)
Sn1—S2—P1—C19	109.39 (9)	C15—N2—C17—C18	-94.4 (3)
Sn1—S2—P1—S1	-19.20 (5)	C16—N2—C17—C18	77.5 (3)
Sn1—S3—P2—O7	-112.54 (7)	P1—O5—C18—C17	-128.85 (18)
Sn1—S3—P2—C38	139.08 (9)	N2—C17—C18—O5	66.0 (3)
Sn1—S3—P2—S4	13.39 (4)	O5—P1—C19—C24	133.6 (2)
C19—P1—O5—C18	-175.52 (17)	S1—P1—C19—C24	9.7 (2)
S1—P1—O5—C18	-51.46 (18)	S2—P1—C19—C24	-118.51 (19)
S2—P1—O5—C18	75.32 (17)	O5—P1—C19—C20	-51.2 (2)
C38—P2—O7—C1^{i}	-172.32 (18)	S1—P1—C19—C20	-175.16 (17)
S4—P2—O7—C1^{i}	-49.58 (19)	S2—P1—C19—C20	56.7 (2)
S3—P2—O7—C1^{i}	73.21 (18)	C24—C19—C20—C21	-1.2 (4)
C3—N1—C2—C1	-75.2 (3)	P1—C19—C20—C21	-176.48 (19)
C7—N1—C2—C1	101.2 (3)	C19—C20—C21—C22	0.8 (4)
O7^{i}—C1—C2—N1	-53.6 (3)	C25—O6—C22—C23	8.3 (4)
C7—N1—C3—O1	177.7 (2)	C25—O6—C22—C21	-171.5 (2)
C2—N1—C3—O1	-6.2 (3)	C20—C21—C22—O6	180.0 (2)
C7—N1—C3—C4	-2.7 (3)	C20—C21—C22—C23	0.2 (4)
C2—N1—C3—C4	173.4 (2)	O6—C22—C23—C24	179.6 (2)
O1—C3—C4—C14	3.6 (4)	C21—C22—C23—C24	-0.6 (4)
N1—C3—C4—C14	-175.9 (2)	C22—C23—C24—C19	0.2 (4)
O1—C3—C4—C5	-176.8 (2)	C20—C19—C24—C23	0.8 (4)

N1—C3—C4—C5	3.6 (3)	P1—C19—C24—C23	176.0 (2)
C14—C4—C5—C11	-1.6 (3)	C32—Sn1—C26—C31	-149.57 (18)
C3—C4—C5—C11	178.9 (2)	S3—Sn1—C26—C31	61.8 (2)
C14—C4—C5—C6	177.7 (2)	S2—Sn1—C26—C31	-25.9 (2)
C3—C4—C5—C6	-1.8 (3)	C32—Sn1—C26—C27	35.7 (3)
C4—C5—C6—C8	-179.7 (2)	S3—Sn1—C26—C27	-113.0 (2)
C11—C5—C6—C8	-0.3 (3)	S2—Sn1—C26—C27	159.34 (19)
C4—C5—C6—C7	-1.1 (3)	C31—C26—C27—C28	0.1 (4)
C11—C5—C6—C7	178.2 (2)	Sn1—C26—C27—C28	174.8 (2)
C3—N1—C7—O2	179.3 (2)	C26—C27—C28—C29	0.8 (4)
C2—N1—C7—O2	3.2 (3)	C27—C28—C29—C30	-0.7 (4)
C3—N1—C7—C6	0.0 (3)	C28—C29—C30—C31	-0.3 (4)
C2—N1—C7—C6	-176.1 (2)	C27—C26—C31—C30	-1.1 (4)
C8—C6—C7—O2	1.3 (4)	Sn1—C26—C31—C30	-176.0 (2)
C5—C6—C7—O2	-177.3 (2)	C29—C30—C31—C26	1.2 (4)
C8—C6—C7—N1	-179.4 (2)	C26—Sn1—C32—C37	69.3 (3)
C5—C6—C7—N1	2.0 (3)	S3—Sn1—C32—C37	-141.4 (2)
C5—C6—C8—C9	-0.2 (4)	S2—Sn1—C32—C37	-54.2 (2)
C7—C6—C8—C9	-178.8 (2)	C26—Sn1—C32—C33	-113.3 (2)
C6—C8—C9—C10	0.6 (4)	S3—Sn1—C32—C33	35.9 (2)
C8—C9—C10—C11	-0.5 (4)	S2—Sn1—C32—C33	123.10 (19)
C8—C9—C10—C15	175.4 (2)	C37—C32—C33—C34	-0.8 (4)
C9—C10—C11—C5	-0.1 (3)	Sn1—C32—C33—C34	-178.2 (2)
C15—C10—C11—C5	-175.9 (2)	C32—C33—C34—C35	-1.0 (4)
C9—C10—C11—C12	178.2 (2)	C33—C34—C35—C36	1.1 (5)
C15—C10—C11—C12	2.3 (3)	C34—C35—C36—C37	0.7 (5)
C4—C5—C11—C10	179.8 (2)	C33—C32—C37—C36	2.6 (4)
C6—C5—C11—C10	0.4 (3)	Sn1—C32—C37—C36	179.9 (2)
C4—C5—C11—C12	1.5 (3)	C35—C36—C37—C32	-2.5 (5)
C6—C5—C11—C12	-177.8 (2)	O7—P2—C38—C39	23.5 (2)
C10—C11—C12—C13	-178.6 (2)	S4—P2—C38—C39	-99.4 (2)
C5—C11—C12—C13	-0.3 (3)	S3—P2—C38—C39	137.90 (19)
C10—C11—C12—C16	-0.1 (3)	O7—P2—C38—C43	-160.8 (2)
C5—C11—C12—C16	178.1 (2)	S4—P2—C38—C43	76.3 (2)
C11—C12—C13—C14	-0.8 (4)	S3—P2—C38—C43	-46.4 (2)
C16—C12—C13—C14	-179.3 (2)	C43—C38—C39—C40	-0.8 (4)
C5—C4—C14—C13	0.4 (4)	P2—C38—C39—C40	174.9 (2)
C3—C4—C14—C13	180.0 (2)	C38—C39—C40—C41	-0.4 (4)
C12—C13—C14—C4	0.8 (4)	C44—O8—C41—C40	-1.4 (4)
C16—N2—C15—O3	-175.7 (2)	C44—O8—C41—C42	178.3 (2)
C17—N2—C15—O3	-4.6 (3)	C39—C40—C41—O8	-178.7 (2)
C16—N2—C15—C10	3.1 (3)	C39—C40—C41—C42	1.6 (4)
C17—N2—C15—C10	174.2 (2)	O8—C41—C42—C43	178.6 (2)

C9—C10—C15—O3	-0.8 (4)	C40—C41—C42—C43	-1.7 (4)
C11—C10—C15—O3	175.1 (2)	C41—C42—C43—C38	0.4 (4)
C9—C10—C15—N2	-179.6 (2)	C39—C38—C43—C42	0.8 (4)
C11—C10—C15—N2	-3.7 (3)	P2—C38—C43—C42	-175.0 (2)
C15—N2—C16—O4	178.5 (2)		
Symmetry code: (i) -*x*+2, -*y*, -*z*+1.			

Table A17: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$) for NDI-[$CH_2CH_2OCH_2CH_2O(An)PS_2]_2$-[$SnPh_2$]

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.61703 (2)	0.75565 (2)	0.148792 (15)	0.01718 (9)	
Cl1	0.2837 (3)	0.5750 (3)	0.26972 (15)	0.1375 (15)	
Cl2	0.10859 (16)	0.51821 (14)	0.12356 (10)	0.0581 (4)	
Cl3	0.40230 (15)	1.08169 (12)	0.38583 (12)	0.0634 (5)	
Cl4	0.430 (3)	0.9054 (9)	0.3048 (15)	0.072 (4)	0.41 (5)
Cl4A	0.4804 (16)	0.9124 (7)	0.3211 (5)	0.048 (2)	0.59 (5)
S1	0.71867 (10)	0.93521 (8)	0.21845 (6)	0.0219 (2)	
S2	0.63581 (10)	0.92705 (9)	0.02894 (6)	0.0248 (2)	
S3	0.66238 (10)	0.69511 (8)	0.27926 (6)	0.0221 (2)	
S4	0.50884 (10)	0.49599 (8)	0.14226 (6)	0.0235 (2)	
P1	0.72148 (10)	1.01913 (8)	0.12350 (6)	0.0186 (2)	
P2	0.61424 (9)	0.53345 (8)	0.24631 (6)	0.0175 (2)	
O1	0.6792 (3)	1.1200 (2)	0.13821 (18)	0.0237 (6)	
O2	0.7017 (3)	1.2413 (2)	0.27302 (17)	0.0242 (7)	
O3	1.2202 (3)	1.2406 (3)	0.15540 (19)	0.0284 (7)	
O4	0.9616 (3)	1.2265 (2)	0.35012 (17)	0.0228 (6)	
O5	0.6999 (3)	1.0570 (3)	0.47221 (19)	0.0283 (7)	
O6	1.1622 (3)	0.7700 (2)	0.3433 (2)	0.0298 (7)	
O7	0.9205 (3)	0.6097 (2)	0.48111 (17)	0.0218 (6)	
O8	0.9882 (3)	0.5299 (2)	0.28511 (17)	0.0242 (7)	
O9	0.7313 (3)	0.4976 (2)	0.26023 (17)	0.0228 (6)	
O10	0.4314 (3)	0.3145 (2)	0.48774 (18)	0.0269 (7)	
N1	0.8257 (3)	1.1395 (3)	0.4074 (2)	0.0194 (7)	
N2	1.0405 (3)	0.6892 (3)	0.4119 (2)	0.0184 (7)	
C1	0.5776 (4)	1.1176 (4)	0.1640 (3)	0.0250 (9)	
H1A	0.5649	1.0601	0.1978	0.030*	
H1B	0.5065	1.1048	0.1198	0.030*	
C2	0.6033 (4)	1.2247 (4)	0.2070 (3)	0.0272 (10)	
H2A	0.6192	1.2813	0.1732	0.033*	
H2B	0.5340	1.2292	0.2228	0.033*	
C3	0.6684 (4)	1.2195 (3)	0.3411 (2)	0.0221 (9)	
H3A	0.6168	1.1456	0.3351	0.027*	

H3B	0.6250	1.2694	0.3514	0.027*	
C4	0.7781 (4)	1.2327 (3)	0.4066 (2)	0.0220 (9)	
H4A	0.8384	1.2977	0.4024	0.026*	
H4B	0.7604	1.2428	0.4555	0.026*	
C5	0.9168 (4)	1.1455 (3)	0.3744 (2)	0.0191 (9)	
C6	0.9571 (4)	1.0480 (3)	0.3719 (2)	0.0188 (8)	
C7	0.9098 (4)	0.9586 (3)	0.4076 (2)	0.0173 (8)	
C8	0.8226 (4)	0.9591 (3)	0.4436 (2)	0.0189 (8)	
C9	0.7768 (4)	1.0534 (3)	0.4429 (2)	0.0206 (9)	
C10	0.7790 (4)	0.8725 (3)	0.4795 (2)	0.0200 (9)	
H10	0.7193	0.8730	0.5030	0.024*	
C11	0.8236 (4)	0.7831 (3)	0.4812 (2)	0.0191 (8)	
H11	0.7947	0.7241	0.5068	0.023*	
C12	0.9087 (4)	0.7808 (3)	0.4460 (2)	0.0169 (8)	
C13	0.9523 (4)	0.8684 (3)	0.4078 (2)	0.0166 (8)	
C14	1.0385 (4)	0.8672 (3)	0.3708 (2)	0.0190 (8)	
C15	1.0804 (4)	0.9535 (3)	0.3341 (2)	0.0204 (9)	
H15	1.1365	0.9512	0.3078	0.024*	
C16	1.0406 (4)	1.0448 (3)	0.3355 (2)	0.0214 (9)	
H16	1.0713	1.1046	0.3112	0.026*	
C17	1.0863 (4)	0.7728 (3)	0.3724 (2)	0.0191 (9)	
C18	0.9543 (4)	0.6869 (3)	0.4482 (2)	0.0185 (8)	
C19	1.0865 (4)	0.5948 (3)	0.4150 (3)	0.0228 (9)	
H19A	1.1026	0.5740	0.4678	0.027*	
H19B	1.1615	0.6140	0.4018	0.027*	
C20	1.0016 (4)	0.5008 (3)	0.3606 (2)	0.0220 (9)	
H20A	1.0322	0.4376	0.3666	0.026*	
H20B	0.9250	0.4826	0.3716	0.026*	
C21	0.8930 (4)	0.4566 (4)	0.2294 (3)	0.0245 (9)	
H21A	0.8669	0.3899	0.2523	0.029*	
H21B	0.9196	0.4387	0.1855	0.029*	
C22	0.7925 (4)	0.5032 (4)	0.2018 (3)	0.0251 (9)	
H22A	0.8216	0.5785	0.1923	0.030*	
H22B	0.7383	0.4627	0.1532	0.030*	
C23	0.8717 (4)	1.0854 (3)	0.1309 (2)	0.0196 (9)	
C24	0.9338 (4)	1.0379 (3)	0.0944 (3)	0.0230 (9)	
H24	0.8956	0.9711	0.0643	0.028*	
C25	1.0509 (4)	1.0867 (4)	0.1014 (3)	0.0266 (10)	
H25	1.0929	1.0531	0.0767	0.032*	
C26	1.1066 (4)	1.1857 (3)	0.1448 (2)	0.0217 (9)	
C27	1.0440 (4)	1.2337 (3)	0.1817 (2)	0.0225 (9)	
H27	1.0818	1.3008	0.2114	0.027*	
C28	0.9279 (4)	1.1842 (3)	0.1749 (2)	0.0208 (9)	

H28	0.8860	1.2171	0.2002	0.025*	
C29	1.2841 (4)	1.1965 (4)	0.1148 (3)	0.0328 (11)	
H29A	1.2923	1.1286	0.1338	0.049*	
H29B	1.3620	1.2464	0.1226	0.049*	
H29C	1.2419	1.1844	0.0600	0.049*	
C30	0.5594 (4)	0.4691 (3)	0.3200 (2)	0.0178 (8)	
C31	0.6330 (4)	0.4837 (3)	0.3950 (2)	0.0206 (9)	
H31	0.7110	0.5285	0.4067	0.025*	
C32	0.5935 (4)	0.4337 (3)	0.4525 (2)	0.0213 (9)	
H32	0.6440	0.4441	0.5034	0.026*	
C33	0.4791 (4)	0.3679 (3)	0.4355 (2)	0.0214 (9)	
C34	0.4050 (4)	0.3530 (3)	0.3603 (3)	0.0237 (9)	
H34	0.3270	0.3082	0.3487	0.028*	
C35	0.4449 (4)	0.4032 (3)	0.3036 (2)	0.0214 (9)	
H35	0.3942	0.3929	0.2528	0.026*	
C36	0.5063 (5)	0.3229 (4)	0.5638 (3)	0.0297 (10)	
H36A	0.5729	0.2959	0.5628	0.045*	
H36B	0.4625	0.2806	0.5955	0.045*	
H36C	0.5352	0.3978	0.5854	0.045*	
C37	0.4376 (4)	0.7462 (4)	0.0966 (3)	0.0270 (10)	
C38	0.3934 (5)	0.8268 (4)	0.1177 (3)	0.0386 (12)	
H38	0.4409	0.8793	0.1589	0.046*	
C39	0.2815 (5)	0.8318 (5)	0.0797 (4)	0.0438 (14)	
H39	0.2524	0.8864	0.0956	0.053*	
C40	0.2122 (5)	0.7568 (5)	0.0183 (3)	0.0403 (13)	
H40	0.1351	0.7590	-0.0079	0.048*	
C41	0.2559 (5)	0.6810 (5)	-0.0034 (3)	0.0434 (13)	
H41	0.2090	0.6300	-0.0457	0.052*	
C42	0.3680 (5)	0.6751 (5)	0.0343 (3)	0.0405 (13)	
H42	0.3966	0.6212	0.0169	0.049*	
C43	0.7361 (4)	0.7145 (3)	0.0975 (2)	0.0210 (9)	
C44	0.8562 (4)	0.7651 (4)	0.1281 (3)	0.0303 (11)	
H44	0.8828	0.8175	0.1710	0.036*	
C45	0.9363 (5)	0.7394 (4)	0.0963 (4)	0.0414 (13)	
H45	1.0176	0.7739	0.1173	0.050*	
C46	0.8978 (5)	0.6631 (5)	0.0337 (4)	0.0429 (13)	
H46	0.9530	0.6450	0.0121	0.052*	
C47	0.7795 (5)	0.6131 (4)	0.0026 (3)	0.0358 (12)	
H47	0.7534	0.5617	-0.0408	0.043*	
C48	0.6990 (4)	0.6380 (4)	0.0347 (3)	0.0264 (10)	
H48	0.6179	0.6026	0.0136	0.032*	
C49	0.1832 (6)	0.6189 (5)	0.2009 (4)	0.0476 (14)	
H49A	0.2244	0.6839	0.1820	0.057*	

H49B	0.1261	0.6374	0.2239	0.057*	
C50	0.4209 (5)	0.9547 (5)	0.3909 (4)	0.0433 (13)	
H50A	0.4932	0.9571	0.4320	0.052*	
H50B	0.3539	0.9064	0.4039	0.052*	

Table A18: Atomic displacement parameters (Å^2) for NDI-[$CH_2CH_2OCH_2CH_2O$(An)PS_2]$_2$-[$SnPh_2$]

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01803 (15)	0.01494 (14)	0.01646 (14)	0.00315 (10)	0.00281 (10)	0.00365 (10)
Cl1	0.132 (2)	0.216 (3)	0.0802 (15)	0.140 (3)	-0.0277 (15)	-0.0345 (18)
Cl2	0.0694 (11)	0.0604 (9)	0.0543 (9)	0.0171 (8)	0.0349 (8)	0.0038 (7)
Cl3	0.0568 (10)	0.0394 (8)	0.1114 (15)	0.0136 (7)	0.0516 (10)	0.0168 (8)
Cl4	0.092 (11)	0.058 (4)	0.062 (6)	-0.010 (4)	0.050 (7)	-0.016 (3)
Cl4A	0.081 (5)	0.030 (3)	0.040 (2)	0.017 (2)	0.029 (3)	0.0025 (14)
S1	0.0272 (5)	0.0156 (5)	0.0177 (5)	0.0004 (4)	0.0034 (4)	0.0041 (4)
S2	0.0278 (6)	0.0229 (5)	0.0195 (5)	0.0064 (4)	0.0005 (4)	0.0013 (4)
S3	0.0328 (6)	0.0139 (5)	0.0167 (5)	0.0024 (4)	0.0062 (4)	0.0036 (4)
S4	0.0276 (6)	0.0219 (5)	0.0171 (5)	0.0032 (4)	0.0035 (4)	0.0018 (4)
P1	0.0225 (5)	0.0145 (5)	0.0185 (5)	0.0056 (4)	0.0049 (4)	0.0035 (4)
P2	0.0218 (5)	0.0146 (5)	0.0162 (5)	0.0047 (4)	0.0058 (4)	0.0033 (4)
O1	0.0298 (17)	0.0180 (14)	0.0279 (16)	0.0095 (13)	0.0130 (13)	0.0057 (12)
O2	0.0228 (16)	0.0269 (16)	0.0212 (15)	0.0079 (13)	0.0024 (12)	0.0038 (12)
O3	0.0252 (17)	0.0275 (17)	0.0306 (17)	0.0023 (14)	0.0102 (14)	0.0014 (13)
O4	0.0270 (16)	0.0133 (14)	0.0250 (16)	0.0040 (12)	0.0039 (13)	0.0044 (12)
O5	0.0319 (18)	0.0271 (17)	0.0323 (18)	0.0148 (14)	0.0128 (15)	0.0116 (14)
O6	0.0336 (18)	0.0176 (15)	0.044 (2)	0.0081 (14)	0.0200 (16)	0.0068 (14)
O7	0.0297 (17)	0.0152 (14)	0.0217 (15)	0.0072 (12)	0.0078 (13)	0.0078 (12)
O8	0.0314 (17)	0.0179 (14)	0.0204 (15)	0.0033 (13)	0.0057 (13)	0.0051 (12)
O9	0.0263 (16)	0.0278 (16)	0.0186 (15)	0.0111 (13)	0.0096 (12)	0.0064 (12)
O10	0.0319 (18)	0.0231 (16)	0.0272 (16)	0.0028 (14)	0.0150 (14)	0.0090 (13)
N1	0.0222 (18)	0.0141 (16)	0.0201 (17)	0.0071 (14)	0.0015 (14)	0.0020 (13)
N2	0.0198 (18)	0.0136 (16)	0.0207 (17)	0.0055 (14)	0.0032 (14)	0.0030 (13)
C1	0.016 (2)	0.031 (2)	0.026 (2)	0.0084 (19)	0.0029 (18)	0.0008 (19)
C2	0.026 (2)	0.031 (2)	0.025 (2)	0.015 (2)	0.0007 (19)	0.0058 (19)
C3	0.023 (2)	0.019 (2)	0.025 (2)	0.0094 (18)	0.0063 (18)	0.0048 (17)
C4	0.027 (2)	0.015 (2)	0.023 (2)	0.0090 (18)	0.0039 (18)	0.0012 (16)
C5	0.021 (2)	0.017 (2)	0.0156 (19)	0.0051 (17)	-0.0014 (16)	-0.0008 (15)
C6	0.021 (2)	0.0131 (19)	0.017 (2)	0.0019 (16)	-0.0011 (16)	0.0031 (15)
C7	0.019 (2)	0.0139 (19)	0.0142 (19)	0.0030 (16)	-0.0008 (16)	0.0035 (15)
C8	0.017 (2)	0.019 (2)	0.016 (2)	0.0046 (17)	-0.0007 (16)	0.0028 (16)
C9	0.022 (2)	0.018 (2)	0.020 (2)	0.0054 (17)	0.0026 (17)	0.0026 (16)
C10	0.021 (2)	0.020 (2)	0.018 (2)	0.0054 (17)	0.0043 (16)	0.0032 (16)
C11	0.022 (2)	0.0161 (19)	0.016 (2)	0.0028 (17)	0.0024 (16)	0.0035 (15)

C12	0.019 (2)	0.0145 (19)	0.0139 (19)	0.0038 (16)	0.0006 (16)	0.0024 (15)
C13	0.016 (2)	0.0136 (18)	0.0148 (19)	0.0018 (16)	-0.0014 (15)	-0.0001 (15)
C14	0.020 (2)	0.0137 (19)	0.020 (2)	0.0038 (16)	0.0010 (16)	0.0025 (15)
C15	0.020 (2)	0.017 (2)	0.024 (2)	0.0044 (17)	0.0066 (17)	0.0032 (16)
C16	0.022 (2)	0.0153 (19)	0.022 (2)	0.0020 (17)	0.0020 (17)	0.0063 (16)
C17	0.019 (2)	0.0140 (19)	0.023 (2)	0.0032 (16)	0.0058 (17)	0.0006 (16)
C18	0.023 (2)	0.0133 (19)	0.0153 (19)	0.0033 (16)	0.0006 (16)	0.0005 (15)
C19	0.029 (2)	0.018 (2)	0.024 (2)	0.0117 (18)	0.0055 (18)	0.0051 (17)
C20	0.032 (2)	0.0128 (19)	0.023 (2)	0.0074 (18)	0.0092 (18)	0.0059 (16)
C21	0.029 (2)	0.023 (2)	0.023 (2)	0.0096 (19)	0.0083 (18)	-0.0008 (17)
C22	0.027 (2)	0.034 (2)	0.021 (2)	0.013 (2)	0.0120 (18)	0.0071 (18)
C23	0.024 (2)	0.0149 (19)	0.019 (2)	0.0042 (17)	0.0056 (17)	0.0060 (16)
C24	0.029 (2)	0.016 (2)	0.024 (2)	0.0047 (18)	0.0084 (18)	0.0015 (17)
C25	0.032 (3)	0.023 (2)	0.029 (2)	0.010 (2)	0.013 (2)	0.0027 (18)
C26	0.021 (2)	0.022 (2)	0.022 (2)	0.0053 (18)	0.0069 (17)	0.0088 (17)
C27	0.030 (2)	0.017 (2)	0.020 (2)	0.0051 (18)	0.0076 (18)	0.0028 (16)
C28	0.027 (2)	0.017 (2)	0.022 (2)	0.0080 (18)	0.0101 (18)	0.0043 (16)
C29	0.028 (3)	0.031 (3)	0.043 (3)	0.008 (2)	0.016 (2)	0.008 (2)
C30	0.023 (2)	0.0114 (18)	0.021 (2)	0.0062 (16)	0.0083 (17)	0.0044 (15)
C31	0.024 (2)	0.0146 (19)	0.024 (2)	0.0050 (17)	0.0089 (18)	0.0032 (16)
C32	0.027 (2)	0.017 (2)	0.021 (2)	0.0079 (18)	0.0068 (17)	0.0042 (16)
C33	0.029 (2)	0.0148 (19)	0.024 (2)	0.0069 (18)	0.0135 (18)	0.0067 (16)
C34	0.021 (2)	0.019 (2)	0.030 (2)	0.0025 (18)	0.0086 (18)	0.0041 (18)
C35	0.023 (2)	0.019 (2)	0.022 (2)	0.0060 (18)	0.0063 (17)	0.0015 (16)
C36	0.037 (3)	0.029 (2)	0.027 (2)	0.009 (2)	0.015 (2)	0.0127 (19)
C37	0.021 (2)	0.025 (2)	0.033 (3)	0.0057 (19)	0.0054 (19)	0.0013 (19)
C38	0.037 (3)	0.030 (3)	0.045 (3)	0.005 (2)	0.011 (2)	0.004 (2)
C39	0.042 (3)	0.034 (3)	0.061 (4)	0.015 (3)	0.019 (3)	0.011 (3)
C40	0.034 (3)	0.046 (3)	0.043 (3)	0.012 (3)	0.011 (2)	0.021 (3)
C41	0.036 (3)	0.049 (3)	0.038 (3)	0.012 (3)	-0.003 (2)	0.005 (2)
C42	0.035 (3)	0.052 (3)	0.032 (3)	0.017 (3)	0.002 (2)	0.002 (2)
C43	0.021 (2)	0.022 (2)	0.022 (2)	0.0078 (18)	0.0086 (17)	0.0110 (17)
C44	0.025 (2)	0.022 (2)	0.043 (3)	0.0072 (19)	0.008 (2)	0.007 (2)
C45	0.026 (3)	0.031 (3)	0.068 (4)	0.007 (2)	0.015 (3)	0.007 (3)
C46	0.036 (3)	0.044 (3)	0.063 (4)	0.017 (3)	0.029 (3)	0.015 (3)
C47	0.040 (3)	0.041 (3)	0.034 (3)	0.018 (2)	0.018 (2)	0.004 (2)
C48	0.024 (2)	0.031 (2)	0.026 (2)	0.008 (2)	0.0071 (18)	0.0094 (19)
C49	0.051 (4)	0.039 (3)	0.058 (4)	0.018 (3)	0.018 (3)	0.008 (3)
C50	0.043 (3)	0.037 (3)	0.051 (3)	0.003 (3)	0.024 (3)	-0.001 (2)

Table A19: Geometric parameters (Å, °) for NDI-$[CH_2CH_2OCH_2CH_2O(An)PS_2]_2$-$[SnPh_2]$

Sn1—C43	2.114 (4)	C15—H15	0.9500
Sn1—C37	2.129 (5)	C16—H16	0.9500
Sn1—S1	2.4730 (10)	C19—C20	1.512 (6)
Sn1—S3	2.4904 (10)	C19—H19A	0.9900
Cl1—C49	1.733 (7)	C19—H19B	0.9900
Cl2—C49	1.769 (6)	C20—H20A	0.9900
Cl3—C50	1.733 (6)	C20—H20B	0.9900
Cl4—C50	1.728 (13)	C21—C22	1.496 (6)
Cl4A—C50	1.777 (10)	C21—H21A	0.9900
S1—P1	2.0754 (14)	C21—H21B	0.9900
S2—P1	1.9424 (15)	C22—H22A	0.9900
S3—P2	2.0608 (14)	C22—H22B	0.9900
S4—P2	1.9517 (15)	C23—C24	1.386 (6)
P1—O1	1.580 (3)	C23—C28	1.401 (6)
P1—C23	1.796 (4)	C24—C25	1.388 (7)
P2—O9	1.594 (3)	C24—H24	0.9500
P2—C30	1.795 (4)	C25—C26	1.398 (6)
O1—C1	1.450 (5)	C25—H25	0.9500
O2—C2	1.423 (5)	C26—C27	1.400 (6)
O2—C3	1.423 (5)	C27—C28	1.380 (6)
O3—C26	1.356 (5)	C27—H27	0.9500
O3—C29	1.429 (6)	C28—H28	0.9500
O4—C5	1.212 (5)	C29—H29A	0.9800
O5—C9	1.221 (6)	C29—H29B	0.9800
O6—C17	1.204 (5)	C29—H29C	0.9800
O7—C18	1.222 (5)	C30—C35	1.396 (6)
O8—C20	1.415 (5)	C30—C31	1.398 (6)
O8—C21	1.428 (5)	C31—C32	1.381 (6)
O9—C22	1.458 (5)	C31—H31	0.9500
O10—C33	1.366 (5)	C32—C33	1.392 (6)
O10—C36	1.426 (6)	C32—H32	0.9500
N1—C9	1.392 (5)	C33—C34	1.401 (6)
N1—C5	1.401 (6)	C34—C35	1.373 (6)
N1—C4	1.483 (5)	C34—H34	0.9500
N2—C18	1.394 (6)	C35—H35	0.9500
N2—C17	1.401 (5)	C36—H36A	0.9800
N2—C19	1.484 (5)	C36—H36B	0.9800
C1—C2	1.499 (6)	C36—H36C	0.9800
C1—H1A	0.9900	C37—C42	1.373 (7)
C1—H1B	0.9900	C37—C38	1.397 (7)
C2—H2A	0.9900	C38—C39	1.387 (8)

C2—H2B	0.9900	C38—H38	0.9500
C3—C4	1.509 (6)	C39—C40	1.388 (9)
C3—H3A	0.9900	C39—H39	0.9500
C3—H3B	0.9900	C40—C41	1.344 (9)
C4—H4A	0.9900	C40—H40	0.9500
C4—H4B	0.9900	C41—C42	1.391 (8)
C5—C6	1.488 (6)	C41—H41	0.9500
C6—C16	1.379 (6)	C42—H42	0.9500
C6—C7	1.419 (6)	C43—C48	1.392 (7)
C7—C8	1.407 (6)	C43—C44	1.402 (7)
C7—C13	1.409 (6)	C44—C45	1.381 (8)
C8—C10	1.380 (6)	C44—H44	0.9500
C8—C9	1.483 (6)	C45—C46	1.386 (9)
C10—C11	1.412 (6)	C45—H45	0.9500
C10—H10	0.9500	C46—C47	1.383 (8)
C11—C12	1.379 (6)	C46—H46	0.9500
C11—H11	0.9500	C47—C48	1.384 (7)
C12—C13	1.416 (6)	C47—H47	0.9500
C12—C18	1.475 (6)	C48—H48	0.9500
C13—C14	1.411 (6)	C49—H49A	0.9900
C14—C15	1.379 (6)	C49—H49B	0.9900
C14—C17	1.498 (6)	C50—H50A	0.9900
C15—C16	1.406 (6)	C50—H50B	0.9900
C43—Sn1—C37	127.94 (18)	O8—C21—H21A	109.4
C43—Sn1—S1	106.07 (12)	C22—C21—H21A	109.4
C37—Sn1—S1	109.09 (13)	O8—C21—H21B	109.4
C43—Sn1—S3	105.34 (11)	C22—C21—H21B	109.4
C37—Sn1—S3	115.48 (13)	H21A—C21—H21B	108.0
S1—Sn1—S3	83.74 (3)	O9—C22—C21	108.5 (3)
P1—S1—Sn1	97.51 (5)	O9—C22—H22A	110.0
P2—S3—Sn1	97.60 (5)	C21—C22—H22A	110.0
O1—P1—C23	99.02 (18)	O9—C22—H22B	110.0
O1—P1—S2	117.02 (13)	C21—C22—H22B	110.0
C23—P1—S2	114.65 (15)	H22A—C22—H22B	108.4
O1—P1—S1	105.85 (13)	C24—C23—C28	119.5 (4)
C23—P1—S1	107.91 (14)	C24—C23—P1	120.2 (3)
S2—P1—S1	111.29 (6)	C28—C23—P1	120.3 (3)
O9—P2—C30	99.51 (18)	C23—C24—C25	120.9 (4)
O9—P2—S4	114.53 (13)	C23—C24—H24	119.6
C30—P2—S4	115.89 (15)	C25—C24—H24	119.6
O9—P2—S3	107.53 (13)	C24—C25—C26	119.6 (4)
C30—P2—S3	106.04 (14)	C24—C25—H25	120.2
S4—P2—S3	112.21 (6)	C26—C25—H25	120.2

C1—O1—P1	125.0 (3)	O3—C26—C25	124.7 (4)
C2—O2—C3	112.4 (3)	O3—C26—C27	115.7 (4)
C26—O3—C29	116.8 (4)	C25—C26—C27	119.6 (4)
C20—O8—C21	113.2 (3)	C28—C27—C26	120.4 (4)
C22—O9—P2	121.3 (3)	C28—C27—H27	119.8
C33—O10—C36	117.2 (4)	C26—C27—H27	119.8
C9—N1—C5	125.4 (3)	C27—C28—C23	120.1 (4)
C9—N1—C4	116.5 (4)	C27—C28—H28	120.0
C5—N1—C4	118.1 (3)	C23—C28—H28	120.0
C18—N2—C17	125.5 (3)	O3—C29—H29A	109.5
C18—N2—C19	117.0 (3)	O3—C29—H29B	109.5
C17—N2—C19	117.5 (4)	H29A—C29—H29B	109.5
O1—C1—C2	106.1 (4)	O3—C29—H29C	109.5
O1—C1—H1A	110.5	H29A—C29—H29C	109.5
C2—C1—H1A	110.5	H29B—C29—H29C	109.5
O1—C1—H1B	110.5	C35—C30—C31	119.1 (4)
C2—C1—H1B	110.5	C35—C30—P2	121.3 (3)
H1A—C1—H1B	108.7	C31—C30—P2	119.7 (3)
O2—C2—C1	110.8 (4)	C32—C31—C30	120.8 (4)
O2—C2—H2A	109.5	C32—C31—H31	119.6
C1—C2—H2A	109.5	C30—C31—H31	119.6
O2—C2—H2B	109.5	C31—C32—C33	119.6 (4)
C1—C2—H2B	109.5	C31—C32—H32	120.2
H2A—C2—H2B	108.1	C33—C32—H32	120.2
O2—C3—C4	108.3 (4)	O10—C33—C32	124.4 (4)
O2—C3—H3A	110.0	O10—C33—C34	115.7 (4)
C4—C3—H3A	110.0	C32—C33—C34	119.8 (4)
O2—C3—H3B	110.0	C35—C34—C33	120.2 (4)
C4—C3—H3B	110.0	C35—C34—H34	119.9
H3A—C3—H3B	108.4	C33—C34—H34	119.9
N1—C4—C3	112.3 (3)	C34—C35—C30	120.5 (4)
N1—C4—H4A	109.1	C34—C35—H35	119.7
C3—C4—H4A	109.1	C30—C35—H35	119.7
N1—C4—H4B	109.1	O10—C36—H36A	109.5
C3—C4—H4B	109.1	O10—C36—H36B	109.5
H4A—C4—H4B	107.9	H36A—C36—H36B	109.5
O4—C5—N1	121.7 (4)	O10—C36—H36C	109.5
O4—C5—C6	121.7 (4)	H36A—C36—H36C	109.5
N1—C5—C6	116.6 (4)	H36B—C36—H36C	109.5
C16—C6—C7	120.2 (4)	C42—C37—C38	117.2 (5)
C16—C6—C5	120.2 (4)	C42—C37—Sn1	123.2 (4)
C7—C6—C5	119.6 (4)	C38—C37—Sn1	118.7 (4)
C8—C7—C13	119.6 (4)	C39—C38—C37	121.4 (5)

C8—C7—C6	121.2 (4)	C39—C38—H38	119.3
C13—C7—C6	119.2 (4)	C37—C38—H38	119.3
C10—C8—C7	120.7 (4)	C38—C39—C40	119.7 (5)
C10—C8—C9	119.5 (4)	C38—C39—H39	120.1
C7—C8—C9	119.8 (4)	C40—C39—H39	120.1
O5—C9—N1	120.5 (4)	C41—C40—C39	118.9 (5)
O5—C9—C8	122.4 (4)	C41—C40—H40	120.6
N1—C9—C8	117.1 (4)	C39—C40—H40	120.6
C8—C10—C11	119.7 (4)	C40—C41—C42	121.9 (6)
C8—C10—H10	120.2	C40—C41—H41	119.1
C11—C10—H10	120.2	C42—C41—H41	119.1
C12—C11—C10	120.6 (4)	C37—C42—C41	120.8 (5)
C12—C11—H11	119.7	C37—C42—H42	119.6
C10—C11—H11	119.7	C41—C42—H42	119.6
C11—C12—C13	120.1 (4)	C48—C43—C44	118.9 (4)
C11—C12—C18	120.0 (4)	C48—C43—Sn1	122.0 (3)
C13—C12—C18	119.9 (4)	C44—C43—Sn1	119.0 (3)
C7—C13—C14	119.6 (4)	C45—C44—C43	120.4 (5)
C7—C13—C12	119.3 (4)	C45—C44—H44	119.8
C14—C13—C12	121.0 (4)	C43—C44—H44	119.8
C15—C14—C13	120.3 (4)	C44—C45—C46	119.9 (5)
C15—C14—C17	119.7 (4)	C44—C45—H45	120.1
C13—C14—C17	120.0 (4)	C46—C45—H45	120.1
C14—C15—C16	120.3 (4)	C47—C46—C45	120.3 (5)
C14—C15—H15	119.9	C47—C46—H46	119.9
C16—C15—H15	119.9	C45—C46—H46	119.9
C6—C16—C15	120.3 (4)	C46—C47—C48	120.0 (5)
C6—C16—H16	119.8	C46—C47—H47	120.0
C15—C16—H16	119.8	C48—C47—H47	120.0
O6—C17—N2	121.9 (4)	C47—C48—C43	120.4 (5)
O6—C17—C14	121.9 (4)	C47—C48—H48	119.8
N2—C17—C14	116.2 (4)	C43—C48—H48	119.8
O7—C18—N2	120.1 (4)	Cl1—C49—Cl2	110.2 (3)
O7—C18—C12	122.5 (4)	Cl1—C49—H49A	109.6
N2—C18—C12	117.4 (4)	Cl2—C49—H49A	109.6
N2—C19—C20	112.1 (4)	Cl1—C49—H49B	109.6
N2—C19—H19A	109.2	Cl2—C49—H49B	109.6
C20—C19—H19A	109.2	H49A—C49—H49B	108.1
N2—C19—H19B	109.2	Cl4—C50—Cl3	111.0 (9)
C20—C19—H19B	109.2	Cl4—C50—Cl4A	19.3 (8)
H19A—C19—H19B	107.9	Cl3—C50—Cl4A	115.6 (4)
O8—C20—C19	107.8 (3)	Cl4—C50—H50A	109.4
O8—C20—H20A	110.1	Cl3—C50—H50A	109.4

C19—C20—H20A	110.1	Cl4A—C50—H50A	90.6
O8—C20—H20B	110.1	Cl4—C50—H50B	109.4
C19—C20—H20B	110.1	Cl3—C50—H50B	109.4
H20A—C20—H20B	108.5	Cl4A—C50—H50B	121.3
O8—C21—C22	111.0 (4)	H50A—C50—H50B	108.0
C43—Sn1—S1—P1	68.52 (13)	C17—N2—C18—O7	180.0 (4)
C37—Sn1—S1—P1	-72.44 (15)	C19—N2—C18—O7	0.4 (6)
S3—Sn1—S1—P1	172.73 (6)	C17—N2—C18—C12	-0.9 (6)
C43—Sn1—S3—P2	-65.34 (13)	C19—N2—C18—C12	179.5 (3)
C37—Sn1—S3—P2	81.48 (15)	C11—C12—C18—O7	-0.7 (6)
S1—Sn1—S3—P2	-170.33 (6)	C13—C12—C18—O7	179.2 (4)
Sn1—S1—P1—O1	133.15 (13)	C11—C12—C18—N2	-179.8 (4)
Sn1—S1—P1—C23	-121.60 (15)	C13—C12—C18—N2	0.2 (5)
Sn1—S1—P1—S2	5.01 (8)	C18—N2—C19—C20	75.9 (5)
Sn1—S3—P2—O9	106.27 (12)	C17—N2—C19—C20	-103.7 (4)
Sn1—S3—P2—C30	-148.01 (15)	C21—O8—C20—C19	-168.1 (3)
Sn1—S3—P2—S4	-20.55 (7)	N2—C19—C20—O8	63.8 (5)
C23—P1—O1—C1	-158.7 (3)	C20—O8—C21—C22	106.6 (4)
S2—P1—O1—C1	77.6 (3)	P2—O9—C22—C21	-175.8 (3)
S1—P1—O1—C1	-47.0 (3)	O8—C21—C22—O9	-76.9 (5)
C30—P2—O9—C22	162.2 (3)	O1—P1—C23—C24	-155.2 (3)
S4—P2—O9—C22	37.9 (3)	S2—P1—C23—C24	-29.8 (4)
S3—P2—O9—C22	-87.5 (3)	S1—P1—C23—C24	94.8 (3)
P1—O1—C1—C2	151.8 (3)	O1—P1—C23—C28	26.4 (4)
C3—O2—C2—C1	-98.6 (4)	S2—P1—C23—C28	151.8 (3)
O1—C1—C2—O2	-63.2 (5)	S1—P1—C23—C28	-83.6 (3)
C2—O2—C3—C4	176.5 (3)	C28—C23—C24—C25	0.3 (6)
C9—N1—C4—C3	-84.1 (5)	P1—C23—C24—C25	-178.1 (3)
C5—N1—C4—C3	97.3 (4)	C23—C24—C25—C26	-0.8 (7)
O2—C3—C4—N1	-78.3 (4)	C29—O3—C26—C25	4.3 (6)
C9—N1—C5—O4	-173.7 (4)	C29—O3—C26—C27	-176.4 (4)
C4—N1—C5—O4	4.8 (6)	C24—C25—C26—O3	-179.8 (4)
C9—N1—C5—C6	5.2 (6)	C24—C25—C26—C27	0.8 (7)
C4—N1—C5—C6	-176.3 (3)	O3—C26—C27—C28	-179.7 (4)
O4—C5—C6—C16	-5.7 (6)	C25—C26—C27—C28	-0.3 (6)
N1—C5—C6—C16	175.4 (4)	C26—C27—C28—C23	-0.2 (6)
O4—C5—C6—C7	173.9 (4)	C24—C23—C28—C27	0.3 (6)
N1—C5—C6—C7	-5.0 (5)	P1—C23—C28—C27	178.7 (3)
C16—C6—C7—C8	-178.5 (4)	O9—P2—C30—C35	-128.2 (4)
C5—C6—C7—C8	1.9 (6)	S4—P2—C30—C35	-4.9 (4)
C16—C6—C7—C13	2.4 (6)	S3—P2—C30—C35	120.4 (3)
C5—C6—C7—C13	-177.2 (4)	O9—P2—C30—C31	50.8 (4)
C13—C7—C8—C10	0.5 (6)	S4—P2—C30—C31	174.1 (3)

C6—C7—C8—C10	-178.7 (4)	S3—P2—C30—C31	-60.6 (3)
C13—C7—C8—C9	-179.4 (4)	C35—C30—C31—C32	0.1 (6)
C6—C7—C8—C9	1.4 (6)	P2—C30—C31—C32	-179.0 (3)
C5—N1—C9—O5	177.7 (4)	C30—C31—C32—C33	0.1 (6)
C4—N1—C9—O5	-0.8 (6)	C36—O10—C33—C32	-3.5 (6)
C5—N1—C9—C8	-2.1 (6)	C36—O10—C33—C34	176.5 (4)
C4—N1—C9—C8	179.4 (3)	C31—C32—C33—O10	179.8 (4)
C10—C8—C9—O5	-1.2 (6)	C31—C32—C33—C34	-0.2 (6)
C7—C8—C9—O5	178.8 (4)	O10—C33—C34—C35	-179.9 (4)
C10—C8—C9—N1	178.6 (4)	C32—C33—C34—C35	0.0 (7)
C7—C8—C9—N1	-1.5 (6)	C33—C34—C35—C30	0.1 (7)
C7—C8—C10—C11	1.0 (6)	C31—C30—C35—C34	-0.2 (6)
C9—C8—C10—C11	-179.1 (4)	P2—C30—C35—C34	178.8 (3)
C8—C10—C11—C12	-1.3 (6)	C43—Sn1—C37—C42	27.0 (5)
C10—C11—C12—C13	0.1 (6)	S1—Sn1—C37—C42	156.9 (4)
C10—C11—C12—C18	-180.0 (4)	S3—Sn1—C37—C42	-111.0 (4)
C8—C7—C13—C14	179.1 (4)	C43—Sn1—C37—C38	-141.9 (4)
C6—C7—C13—C14	-1.8 (6)	S1—Sn1—C37—C38	-12.0 (4)
C8—C7—C13—C12	-1.7 (6)	S3—Sn1—C37—C38	80.1 (4)
C6—C7—C13—C12	177.5 (4)	C42—C37—C38—C39	3.0 (8)
C11—C12—C13—C7	1.4 (6)	Sn1—C37—C38—C39	172.5 (4)
C18—C12—C13—C7	-178.6 (4)	C37—C38—C39—C40	-1.3 (9)
C11—C12—C13—C14	-179.4 (4)	C38—C39—C40—C41	-0.6 (8)
C18—C12—C13—C14	0.7 (6)	C39—C40—C41—C42	0.6 (9)
C7—C13—C14—C15	-0.5 (6)	C38—C37—C42—C41	-2.9 (8)
C12—C13—C14—C15	-179.7 (4)	Sn1—C37—C42—C41	-172.0 (4)
C7—C13—C14—C17	178.5 (4)	C40—C41—C42—C37	1.2 (9)
C12—C13—C14—C17	-0.8 (6)	C37—Sn1—C43—C48	-27.3 (4)
C13—C14—C15—C16	2.1 (6)	S1—Sn1—C43—C48	-158.3 (3)
C17—C14—C15—C16	-176.8 (4)	S3—Sn1—C43—C48	114.0 (3)
C7—C6—C16—C15	-0.7 (6)	C37—Sn1—C43—C44	153.3 (3)
C5—C6—C16—C15	178.9 (4)	S1—Sn1—C43—C44	22.3 (4)
C14—C15—C16—C6	-1.6 (6)	S3—Sn1—C43—C44	-65.5 (3)
C18—N2—C17—O6	178.8 (4)	C48—C43—C44—C45	0.0 (7)
C19—N2—C17—O6	-1.6 (6)	Sn1—C43—C44—C45	179.5 (4)
C18—N2—C17—C14	0.8 (6)	C43—C44—C45—C46	0.0 (8)
C19—N2—C17—C14	-179.6 (3)	C44—C45—C46—C47	0.5 (9)
C15—C14—C17—O6	1.0 (6)	C45—C46—C47—C48	-1.0 (8)
C13—C14—C17—O6	-177.9 (4)	C46—C47—C48—C43	1.1 (8)
C15—C14—C17—N2	179.0 (4)	C44—C43—C48—C47	-0.6 (7)
C13—C14—C17—N2	0.1 (6)	Sn1—C43—C48—C47	180.0 (4)