

Supporting Information for

Ferroelectricity in Hydrogen-Bonded Alternating Donor-Acceptor Supramolecular Copolymer

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EXPERIMENTAL PROCEDURES

Materials and methods: HPLC-grade solvents were used for all the spectroscopic studies and other physical experiments. UV-Vis spectra were recorded in a JASCO V-750 spectrometer. AFM images were captured in Bruker Innova instrument in tapping mode where samples were spin-coated upon freshly cleaned mica surface. Multicell micro-DSC from TA instrument was used for DSC measurement at a heating rate of 1 °C/min under N₂ atmosphere.

Synthesis: Synthesis of NDI and Py was reported in our previous paper.¹

Sample preparation of NDI/ Py for UV-Vis study: A stock solution of NDI/ Py in THF (1.0 mM) was prepared by dissolving desired amount of NDI in that solvent. Then aliquot was transferred to a glass vial and THF was evaporated by gentle heating to make a thin film and MCH was added to get 0.5 mM NDI in MCH. Obtained solution was sonicated and heated in a water bath (75 °C) until a homogeneous solution was formed. Then the solution was allowed to cool at room temperature for 20 minutes before recording UV-Vis spectra.

Studies with NDI + Py (1:1) mixed sample: 5.0 mM stock solution of NDI and Py were prepared in THF. Equal volume of both stock solutions were taken in a screw capped glass vial and the solvent was evaporated by air blowing to get a red film. Then measured amount of MCH was added into it to get 5.0 mM solution. Then, the vial was capped tightly and obtained solution was sonicated and heated in a water bath (75 °C) until a homogeneous solution was produced. Then, the solution was allowed to equilibrate at room temperature for ~ 10 minutes to get red colour gel and UV-Vis spectra was recorded of that gel in 0.1cm path-length cuvette at 25 °C. For Job's plot experiment, solutions of different NDI/ Py ratio in MCH were prepared following above-mentioned procedure while keeping the total concentration fixed at 5.0 mM and

UV/ Vis were recorded at 25 °C. For solid state studies, 5.0 mM NDI + Py (1:1) solution in MCH was drop-casted on a cleaned quartz plate and dried at rt for 12 h and then UV-Vis spectra was recorded.

Microscopy experiments: For AFM studies, a solution of NDI, Py and NDI + Py (1:1) with appropriate concentration in MCH (mentioned in the respective figure captions), was drop-casted on freshly cleaned mica surface and dried in the air for 24 h before the images were taken.

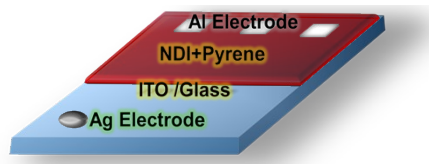
Calculation for α_{agg} : In a typical cooling experiment, a given sample solution in MCH containing 1:1 (D: A) CT mixture (5.0 mM) was placed in the UV/Vis spectrophotometer and the temperature was reduced from 90 °C to 15 °C at a rate 1K/min using the in-built temperature-controlled program in the equipment. Spectra were recorded in 5 °C interval. Then mole fraction of aggregate at each temperature was estimated from the absorbance at 510 nm using the following equation (1)

$$\alpha_{agg} = \frac{A(T) - A(min)}{A(max) - A(min)} \quad \text{--- (1)}$$

where A (max), A (min) and A (T) stand for maximum and minimum absorbance of the band at 510 nm and absorbance at the particular temperature (T) respectively. Similarly data were acquired for the heating experiment from 15 °C to 90 °C at a heating rate of 1K/ min.

Preparation of film: The film for the ferroelectric measurements was prepared from a 5.0 mM NDI + Py (1:1), NDI, Py or NDI + Py (2:1) solution in MCH upon a conducting ITO/Glass substrate. (5× 5) mm ITO coated glass substrates (purchased from Techinstro, India) with surface resistivity ~4 ohm-m were cleaned first with D.I water, absolute ethanol, acetone and then air dried at room temperature. Films were prepared by drop-casting of the respective samples and dried under vacuum for 12 h at room temperature. The thicknesses of the films were about 0.1mm, measured by a Mitutoyo Micrometer (Model No- 293-240-30).

Device Fabrication: The ferroelectric and dielectric capacitor devices were prepared by depositing Aluminium foil (Alfa Aesar) on the top of the film (top electrode) and on the conducting ITO surface (bottom electrode). 0.1mm Cu wires were attached on the both top and bottom electrode of the films. After that, it was dried at rt under vacuum for 12h and utilized in ferroelectric and dielectric measurements. To obtain precise data, we repeated the measurements for different sets of top-bottom electrodes geometry for all the films. A schematic device structure was shown below.



Dielectric, Ferroelectric and Piezoelectric properties measurements: Temperature dependent dielectric measurements was done by an impedance analyzer (4100, Wayne Kerr LCR Meter). An inert sealed bespoke chamber with a heating rate of 1°C min⁻¹ (using resistor heater) was used for the measurement and

the measuring frequencies ranging from 10 kHz to 1 MHz. The ferroelectric measurements were done by a Precision LCII Ferroelectric Tester (Radiant Technologies, Inc.) equipped with a micro-probe station. Bruker di INNOVA atomic force microscopy (spring constant 2 N/m) was used for PFM domain imaging and piezoelectricity measurements. The film was cast on an ITO coated glass using the similar process used for the dielectric and ferroelectric measurements. For PFM the sample was mounted on a standard conductive AFM holder disk, held and contacted by Ag-paint. The voltages were applied to the sample, while the tip was grounded. The AC Bias frequency used was 24 kHz.

Computational studies:³⁻⁶ For an understanding of the intermolecular charge-transfer effects that drive the dielectric response under field, the structure of NDI + Py oligomers in different ratios (1:1, 2:1, 2:2 and 3:3) were optimized using Gaussian16 (Rev. B.01) suite of quantum chemical package. All the initial NDI+Py complexes are optimized in the gas phase with the popular hybrid Minnesota M06-2X functional with the 6-31G (d, p) basis set.

ADDITIONAL FIGURES

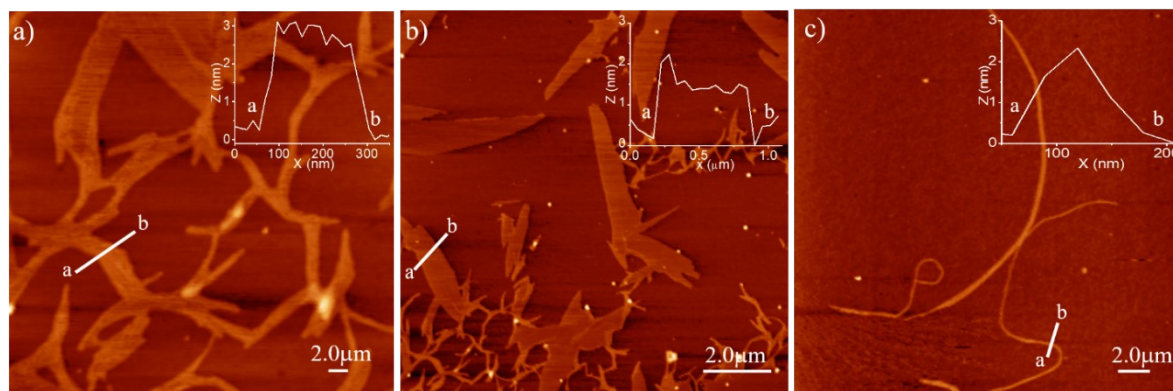


Figure S1: AFM images of 1:1 (NDI + Py) in MCH ($c = 0.5$ mM) at 25 °C.

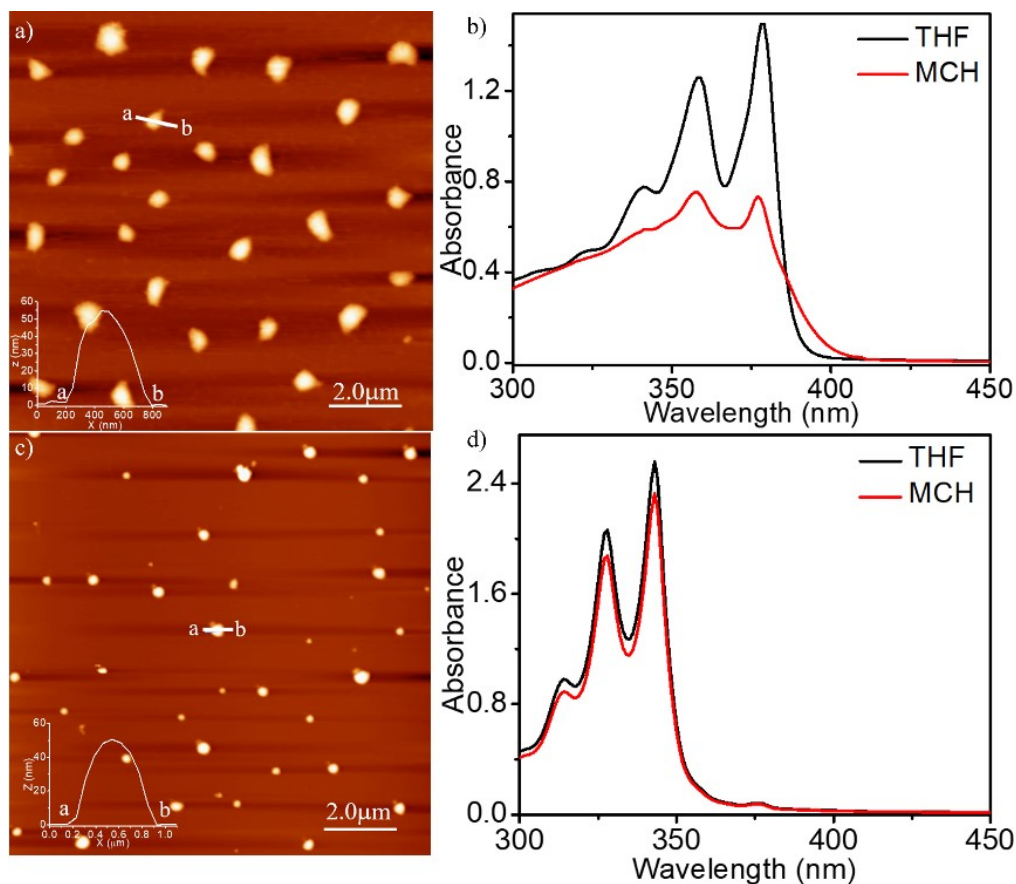


Figure S2: a) AFM image of NDI ($c = 0.1 \text{ mM}$) in MCH showing particles with average height 50-55 nm; b) UV-vis spectra of NDI in THF and MCH ($c = 0.5 \text{ mM}$, $l = 0.1 \text{ cm}$, $25 \text{ }^\circ\text{C}$) indicating aggregation in MCH; c) AFM image of Py ($c = 0.1 \text{ mM}$) in MCH showing particles with average height 40-45 nm; d) UV-vis spectra of Py in THF and MCH ($c = 0.5 \text{ mM}$, $l = 0.1 \text{ cm}$, $25 \text{ }^\circ\text{C}$) indicating no aggregation in MCH.

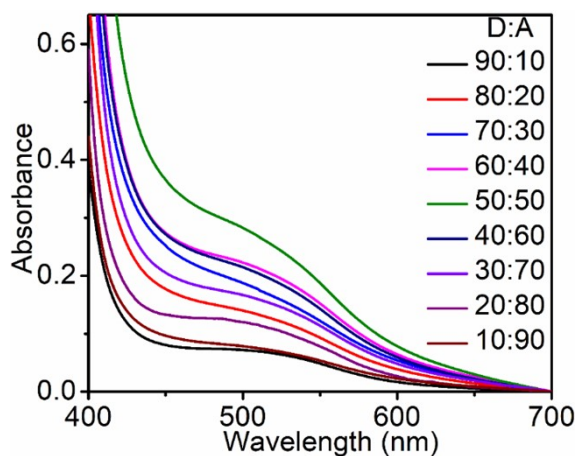


Figure S3: UV/Vis spectra (selected region shown) of Py (D) + NDI (A) with different ratio in MCH at $25 \text{ }^\circ\text{C}$. Total concentration of NDI + Py = 5.0 mM in all samples.

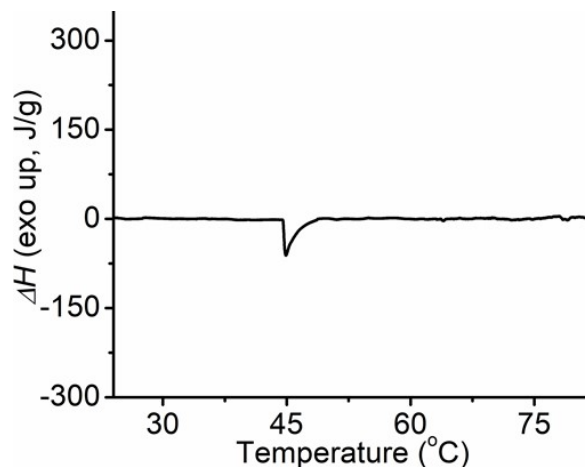


Figure S4: Micro-DSC trace of NDI + Py (1:1) gel in MCH ($c = 5.0$ mM in MCH, scan rate = 1K/min) showing single endothermic peaks near the Curie temperature (T_c). Minor discrepancy between the T_c and the phase transition temperature observed in DSC may be attributed to the fact that the DSC was done in MCH while electrical measurements were done in solid state.

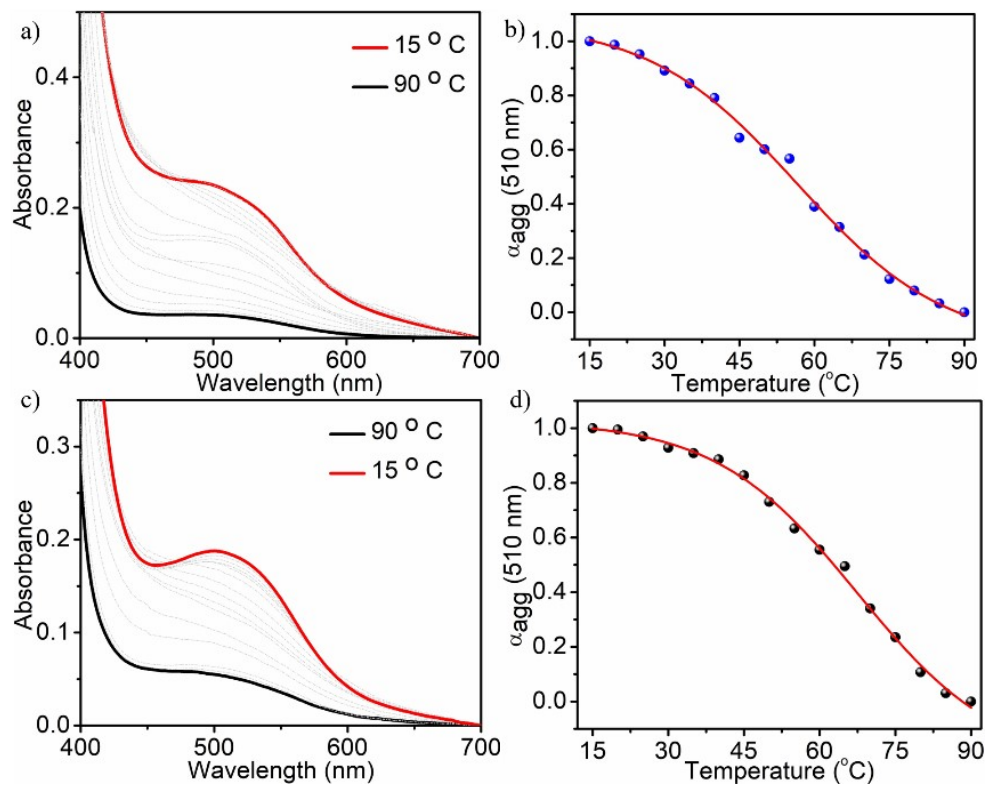


Figure S5: a, c) Variable temperature UV/Vis spectra (selected region is shown) of NDI + Py (1:1) in MCH ($c = 5.0$ mM; $l = 0.1$ cm; a- heating from 15 °C to 90 °C; c- cooling from 90 °C to 15 °C); Variation of the fraction of aggregate (α_{agg}) (Calculated from the intensity of the CT-band at $\lambda=510$ nm at different temperatures) is shown in b) and d) from corresponding heating and cooling spectra, respectively. The data were fitted using the isodesmic model.²

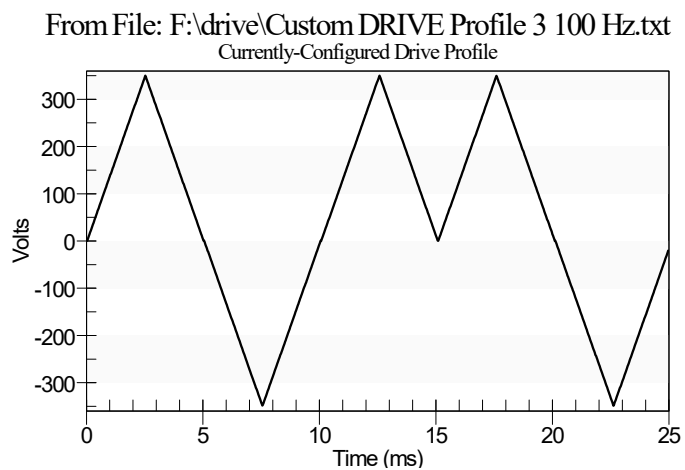


Figure S6: Representative Voltage Vs Time graph of the applied voltage in double-wave method at 100Hz frequency.

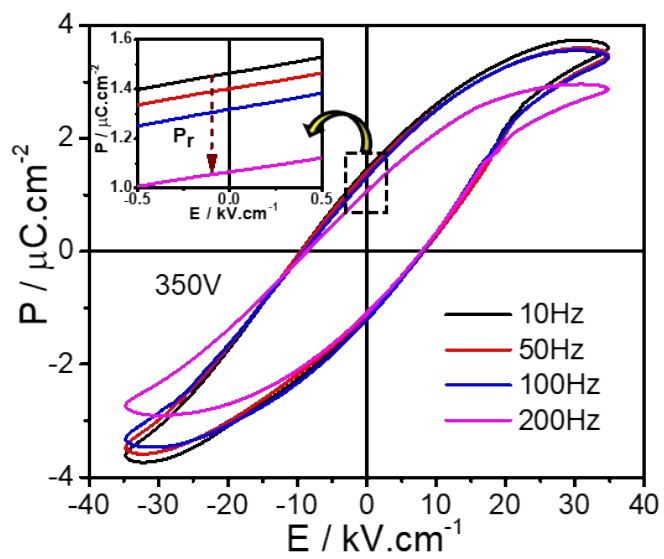


Figure S7: Room temperature frequency dependent ferroelectric hysteresis loops of NDI + Py (1:1) film measured by the double-wave method.

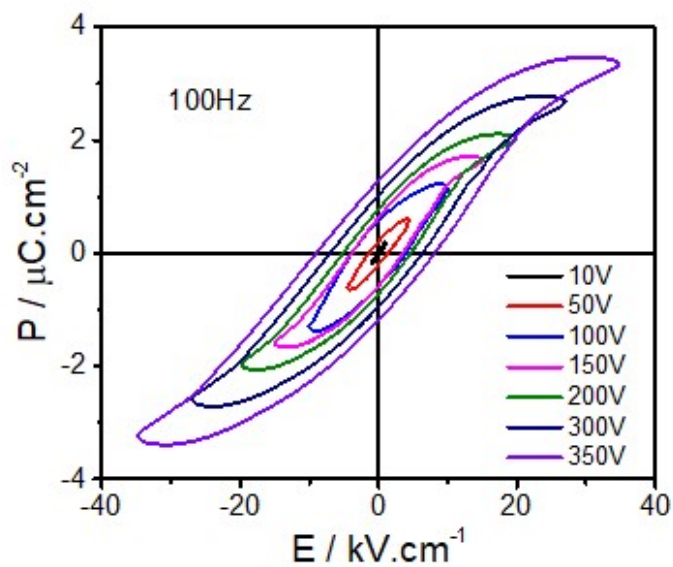


Figure S8: Room temperature voltage-dependent ferroelectric hysteresis loops of NDI + Py (1:1) film measured by double-wave method.

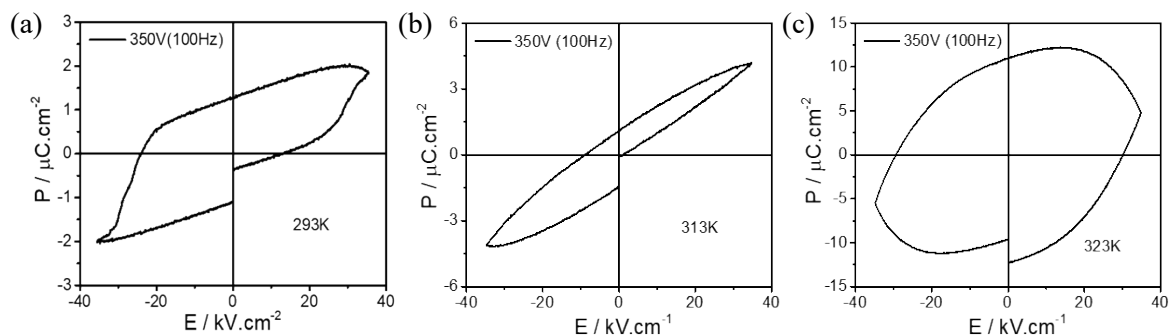


Figure S9: Ferroelectric hysteresis loop of NDI + Py (1:1) film at (a) 293K (b) 303K and (c) 313K.

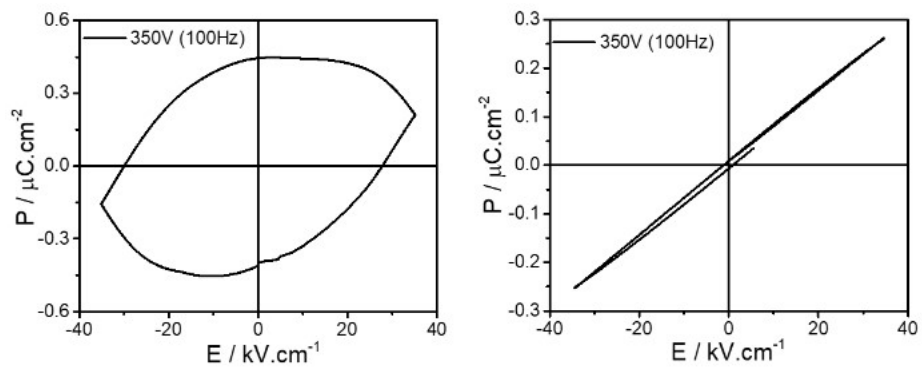


Figure S10: P - E loop of (left) NDI and (right) Py film.

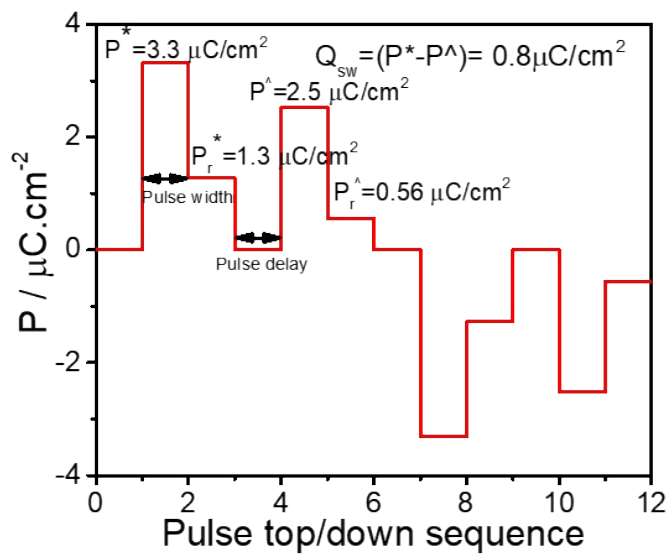


Figure S11: PUND sequence (Positive up and negative down) at 100Hz frequency of NDI + Py (1:1) film measured by square-wave method .

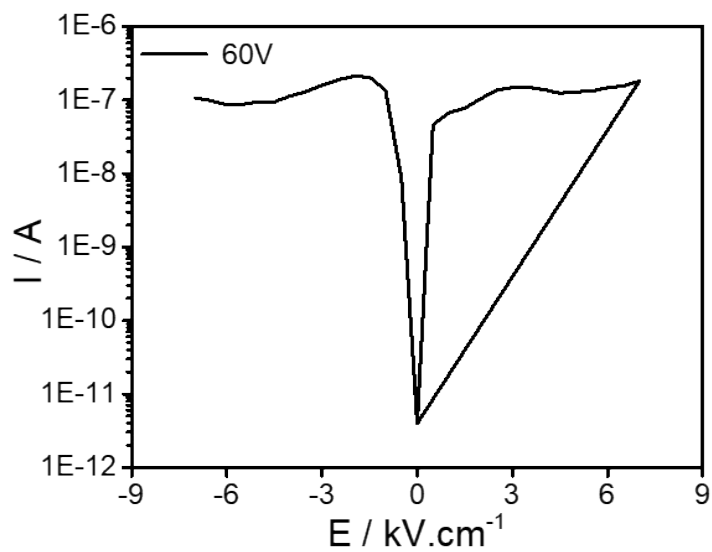


Figure S12: Leakage I - V of NDI + Py (1:1) film.

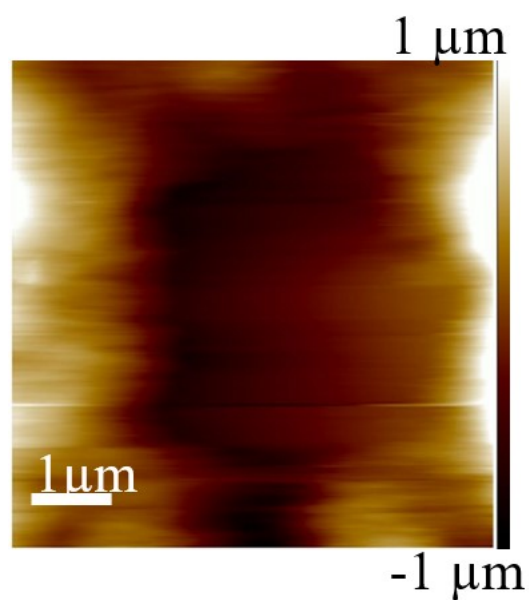


Figure S13: AFM image of the NDI + Py (1:1) sample studied by PFM after poling showing no change in topography.

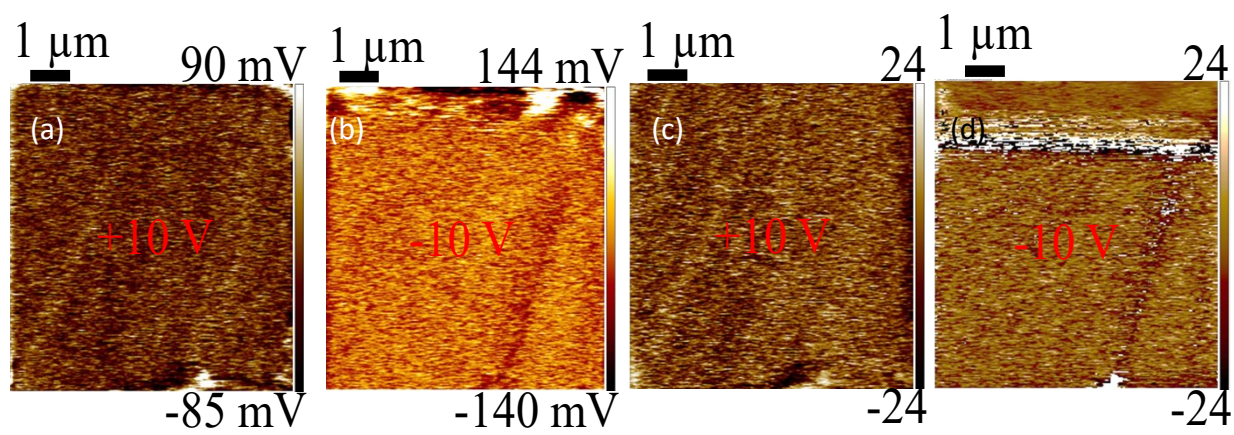


Figure S14. PFM imaging (a, b) Vertical PFM amplitude images at +10 V and -10V; (c, d) Vertical PFM phase images at applied tip Bias +10 V and -10V.

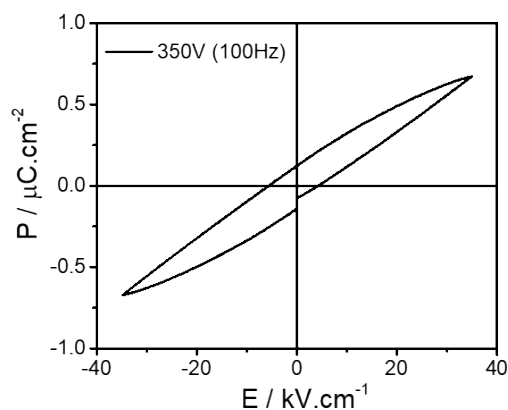


Figure S15: Room temperature P-E loop of NDI + Py (2:1) sample at applied voltage of 350V and frequency of 100Hz.

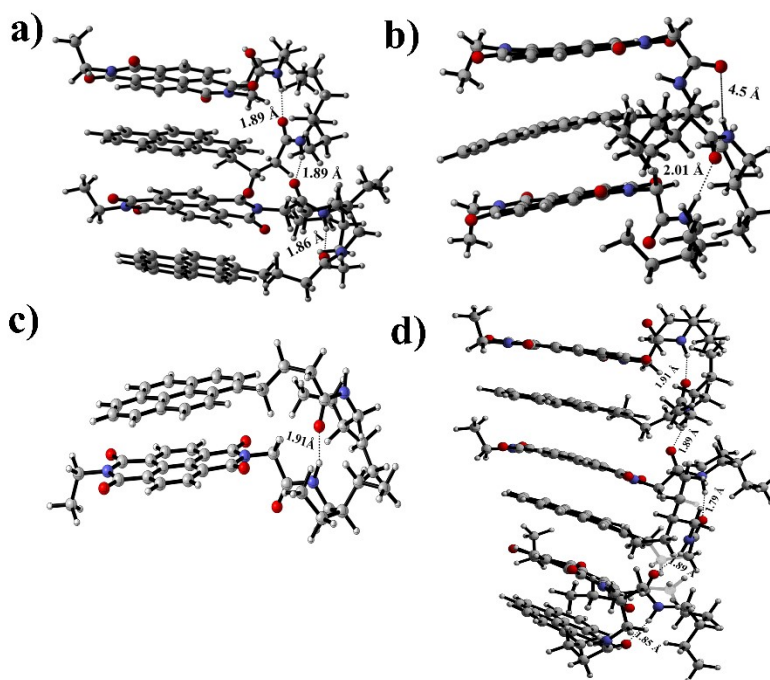


Figure S16: Optimized geometries for (a) 2:2 (b) 1:2 (c) 1:1 and (d) 3:3 Py: NDI complexes.

References

1. A. Sikder, B. Ghosh, S. Chakraborty, A. Paul, and S. Ghosh, *Chem. Eur. J.*, 2016, **22**, 1908.
2. M. M. J. Smulders, M. M. L. Nieuwenhuizen, T. F. A. de Greef, P. van der Schoot, A. P. H. J. Schenning and E. W. Meijer, *Chem. Eur. J.*, 2010, **16**, 362.
3. G. W. T. M. J. Frisch et. al. Gaussian 16, Revision B.01, Gaussian, Inc., Wallingford CT, 2016.
4. J. J. P. Stewart, *J. Mol. Model.* 2007, **13**, 1173.
5. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215.
6. W. J. Hehre, R. Ditchfield, and J. A. Pople, *J. Chem. Phys.* 1972, **56**, 2257.

Coordinate for 1:1 complex of NDI+ Py :

C	-3.82258300	-3.85971300	-2.42012500
C	-4.39626000	-3.57335000	-1.19939700
C	-3.58601200	-3.18420800	-0.08932000
C	-2.18808200	-3.04843900	-0.26849000
C	-1.61901900	-3.32845100	-1.54914700
C	-2.41603100	-3.74084000	-2.59574800
C	-4.15711400	-2.90374800	1.19078500
C	-3.35969800	-2.50806600	2.24263400
C	-1.95611300	-2.35483900	2.05909000
C	-1.38630500	-2.60906400	0.83070000
C	0.07529600	-2.38041800	0.64072600
N	0.60207500	-2.68594500	-0.65195600
C	-0.15428600	-3.14315100	-1.77142800
C	-5.88087700	-3.62977900	-1.05294400
N	-6.41165200	-3.33838100	0.23744200
C	-5.63333700	-3.00255100	1.38661200
O	-6.63459100	-3.88070900	-1.97259800
O	-6.18753600	-2.79263700	2.44674400
O	0.39649200	-3.30774200	-2.84223100
O	0.80766700	-1.91776100	1.49191700
C	2.06533100	-2.54689800	-0.82834700
C	2.82202700	-3.69963600	-0.15501600
O	2.33080400	-4.77991900	0.11676600
N	4.17229500	-3.40438300	0.01267900
C	5.05744200	-4.29192000	0.80170400
C	5.80243500	-3.55422700	1.93809700
C	6.57095800	-2.31896400	1.42287100
C	4.86775100	-3.19855800	3.11539300
C	7.86966000	-2.07723300	2.18423000
C	3.82646800	-2.12225300	2.82163300
C	-7.89979800	-3.44682600	0.41677500
C	-8.30024900	-4.85861400	0.82604500
H	-4.44777400	-4.16551500	-3.26675100
H	-1.97305100	-3.96504800	-3.57274800
H	-3.80223700	-2.28948500	3.22135700
H	-1.33638800	-2.01514400	2.89711500
H	2.31584400	-2.52750000	-1.92834500
H	2.39088200	-1.55211200	-0.40046200
H	4.47588600	-2.41574000	-0.01905700
H	4.46706100	-5.14366800	1.21494500

H	5.79837400	-4.73110900	0.08336400
H	6.55098400	-4.29121100	2.33225400
H	6.78768900	-2.41136200	0.33581400
H	5.91435800	-1.41848500	1.50354900
H	4.35395800	-4.11853000	3.45814400
H	5.49721900	-2.87004500	3.96673700
H	8.38078700	-1.18030800	1.81748800
H	2.93212100	-2.52845400	2.32867800
H	3.48444300	-1.63663600	3.74008600
H	-8.20892200	-2.70755300	1.19220400
H	-8.38644500	-3.16114600	-0.54497400
H	-8.00956000	-5.60016700	0.07053700
H	-7.83684800	-5.15380800	1.77676300
H	-9.38668100	-4.93370300	0.95579000
H	7.68459700	-1.92934700	3.25516100
H	8.56460100	-2.91797500	2.08404200
H	4.22300800	-1.33435800	2.16049400
C	-2.06532000	1.06543400	1.76061300
C	-3.35917400	0.72619800	1.19556500
C	-3.42554000	0.36638200	-0.17857600
C	-2.22058000	0.33021100	-0.97786600
C	-0.96287000	0.65415600	-0.39479000
C	-0.93973100	1.03052300	1.00891400
C	-4.67842600	0.01826100	-0.75687000
C	-4.72239800	-0.35485000	-2.16042000
C	-3.59579800	-0.38814100	-2.91100200
C	-2.30053700	-0.05718700	-2.34384700
C	-1.12197900	-0.12713100	-3.10127400
C	0.10682900	0.18461700	-2.52414700
C	0.20886600	0.58434100	-1.18341000
C	-4.53215900	0.72620200	1.96781400
C	-5.75428500	0.37541300	1.39126300
C	-5.83303300	0.02499500	0.04169100
C	1.55681200	0.87202600	-0.58238300
C	2.54749700	1.53493200	-1.54589300
C	3.93811200	1.68246200	-0.91558500
C	4.65091300	0.34283000	-0.90301000
N	5.56664900	0.13509500	-1.92595400
O	4.45720200	-0.49602900	-0.02815900
C	6.28485400	-1.14868300	-2.10334500
C	5.50567200	-2.21274400	-2.91311000
C	4.78838700	-1.64608100	-4.15701300

C	6.47482200	-3.34049400	-3.33405300
C	7.11731400	-4.06812000	-2.15737400
C	3.34000200	-1.24816000	-3.88300200
H	-2.03320200	1.34809200	2.81219400
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H	-5.69403400	-0.61017200	-2.58377800
H	-3.62594700	-0.66927800	-3.96349200
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H	-4.48906300	0.99754000	3.02095600
H	-6.65603600	0.36340500	2.00482600
H	-6.79373900	-0.24857900	-0.39154500
H	1.45335400	1.50071700	0.32953400
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H	2.16593100	2.53041600	-1.84760300
H	4.51917600	2.46505800	-1.43854700
H	3.85332500	2.04176600	0.13451100
H	5.59701700	0.76634500	-2.72165600
H	7.25840600	-0.92162700	-2.59096400
H	6.52426600	-1.57196100	-1.08913400
H	4.73232600	-2.66127200	-2.24095800
H	5.34928100	-0.79178500	-4.57715100
H	4.79054400	-2.41110700	-4.96256700
H	5.91210700	-4.07713300	-3.94544000
H	7.26173900	-2.93752700	-4.00024400
H	7.84299200	-3.44452200	-1.62554800
H	6.36526800	-4.39983100	-1.41901900
H	2.79549200	-1.07270500	-4.81803300
H	2.79042500	-2.04721400	-3.34790000
H	3.25780200	-0.33572400	-3.27442700
H	7.64826800	-4.96583500	-2.49484600

Coordinate for 2:1 complex of NDI+ Py :

C	3.26299400	-3.63109500	2.10226300
C	3.89428200	-3.49061400	0.88448300
C	3.16776200	-3.09387100	-0.25863700
C	1.79190800	-2.80540100	-0.13490900
C	1.16136200	-2.95574800	1.11912000
C	1.88462200	-3.37011700	2.21804900
C	3.79146200	-2.97515200	-1.52327500

C	3.07180400	-2.56203200	-2.62144400
C	1.70594400	-2.22846700	-2.48701400
C	1.07812100	-2.35257100	-1.26855000
C	-0.35253500	-1.98579400	-1.12585300
N	-0.95435200	-2.24426800	0.11012700
C	-0.28972300	-2.66851600	1.26050200
C	5.36208700	-3.71128900	0.78365100
N	5.93759500	-3.55001300	-0.47918800
C	5.23928200	-3.28518100	-1.66213800
O	6.04178400	-4.00726300	1.74655500
O	5.80763900	-3.28818300	-2.73552800
O	-0.87088200	-2.78476000	2.32512700
O	-0.99287500	-1.46489500	-2.01845800
C	-2.39118900	-2.05445900	0.16117800
C	-3.11591100	-3.08287200	-0.71146900
O	-2.54913600	-4.06398900	-1.16258600
N	-4.42164600	-2.78577400	-0.89840500
C	-5.33413600	-3.75422900	-1.48844100
C	-5.70913100	-3.49118600	-2.95241800
C	-6.39513900	-2.13037000	-3.10471000
C	-4.53186200	-3.70161400	-3.92687600
C	-6.97141900	-1.88584200	-4.49719900
C	-3.55927000	-2.53085500	-4.08167600
C	7.38257700	-3.78861100	-0.59096000
C	7.68761700	-5.26179900	-0.82702600
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H	-4.80070000	-2.00414800	-0.37089600
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H	-6.45709700	-4.26335200	-3.19036700
H	-7.20117400	-2.05716500	-2.36238500
H	-5.67571900	-1.34101900	-2.85332400
H	-3.97197900	-4.58477100	-3.59910400
H	-4.94220300	-3.94376400	-4.91508800
H	-7.50651700	-0.93270700	-4.54249700
H	-3.09567900	-2.24241000	-3.13693400
H	-2.75302600	-2.80503400	-4.76777300

H	7.73780500	-3.18022100	-1.42296400
H	7.83224100	-3.44140800	0.33966700
H	7.31418300	-5.86245300	0.00552900
H	7.22045000	-5.59908700	-1.75506500
H	8.76636900	-5.41579500	-0.90692100
H	-6.18737000	-1.86507700	-5.26006500
H	-7.67725000	-2.67713200	-4.77086700
H	-4.05595600	-1.64817400	-4.50099200
C	1.95323000	1.14705000	-2.14969600
C	3.31394100	0.71595800	-1.97656900
C	3.74470700	0.33652000	-0.67754000
C	2.82824500	0.36471400	0.41901800
C	1.46683500	0.71433400	0.20262500
C	1.07089700	1.13142900	-1.12007100
C	5.07288300	-0.13380700	-0.48313300
C	5.50048100	-0.48441600	0.84734500
C	4.64702200	-0.41229400	1.89653800
C	3.27320700	-0.01966400	1.71402800
C	2.34404300	-0.06031000	2.75533400
C	1.00338000	0.23194900	2.52636900
C	0.54181000	0.61987200	1.26633900
C	4.20520700	0.60555600	-3.05261800
C	5.48910100	0.10744700	-2.86122300
C	5.92137900	-0.25282300	-1.58821200
C	-0.91710500	0.91028300	1.00467900
C	-1.86693900	0.64528300	2.16779500
C	-3.32989900	0.97210000	1.78829700
C	-4.27913700	-0.17896300	2.06110100
N	-4.31346100	-0.59180800	3.34767200
O	-4.94549100	-0.72144400	1.17660700
C	-4.99637600	-1.80778700	3.75722600
C	-4.09354000	-3.05794600	3.77455400
C	-3.35789600	-3.22890800	5.10716300
C	-4.92087700	-4.30220400	3.42553800
C	-5.21089600	-4.39849900	1.92853700
C	-2.49954300	-2.03080000	5.51065900
H	1.63414400	1.46535800	-3.13878700
H	0.04653400	1.44517200	-1.29140600
H	6.52573200	-0.81780400	0.98978800
H	4.97493300	-0.68965600	2.89445200
H	2.67225400	-0.36274800	3.74622200
H	0.30218800	0.14072600	3.34939000

H	3.87285300	0.89554300	-4.04533500
H	6.15847900	-0.00443900	-3.70730600
H	6.92940400	-0.63332800	-1.44171400
H	-1.03216800	1.95007000	0.67163100
H	-1.24039400	0.32158300	0.13830200
H	-1.76915700	-0.40639700	2.46917500
H	-1.56956200	1.25290400	3.03137600
H	-3.68293700	1.85095800	2.33726000
H	-3.41722400	1.20426500	0.72232600
H	-3.71089600	-0.12257600	4.00719300
H	-5.43375100	-1.64778000	4.74996400
H	-5.82041700	-1.93992900	3.05306400
H	-3.32557100	-2.92850200	2.99920500
H	-4.09087900	-3.44509500	5.89724200
H	-2.71558600	-4.11310800	5.02774000
H	-4.38407600	-5.20020300	3.75187000
H	-5.85877600	-4.28127600	3.99785500
H	-5.61990400	-3.45830700	1.54218100
H	-4.28872400	-4.60213100	1.37246900
H	-1.89207600	-2.26126200	6.38959400
H	-1.82265800	-1.75441200	4.69409400
H	-3.11294800	-1.16094400	5.77277400
H	-5.92122200	-5.19821900	1.70247900
C	2.09064200	3.44897100	2.73091500
C	2.67094600	3.68697300	1.50696800
C	1.87521600	4.05797700	0.39689100
C	0.48006100	4.18949000	0.55659700
C	-0.09554700	3.96673800	1.82987400
C	0.69415000	3.59335000	2.89420600
C	2.45109900	4.28807800	-0.87043200
C	1.65824000	4.60202800	-1.95383500
C	0.26294900	4.71386900	-1.80073700
C	-0.31557900	4.52304300	-0.56174200
C	-1.77921500	4.70558200	-0.39574900
N	-2.30057900	4.53379100	0.88665800
C	-1.56500100	4.10741000	2.00823600
C	4.15117400	3.59062400	1.35421100
N	4.67740100	3.99802200	0.12596400
C	3.93181000	4.22202100	-1.03210900
O	4.87411500	3.23595700	2.26188300
O	4.47137500	4.40639900	-2.10364800
O	-2.12050300	3.88305500	3.06326000

O	-2.50654500	5.00847700	-1.32711400
C	-3.70816100	4.89669900	1.10613500
C	-4.71068600	3.76819700	0.83253200
O	-5.44295100	3.35530100	1.71723700
N	-4.71001200	3.28670700	-0.42989400
C	-5.64815200	2.24377700	-0.82438000
C	-5.27819600	1.58752800	-2.15585800
C	-5.29636000	2.58051600	-3.32559100
C	-3.98652700	0.75366500	-2.08343400
C	-5.07078200	1.90375300	-4.67692400
C	-2.66249100	1.52223300	-2.09641900
C	6.14017400	4.10589100	0.01544600
C	6.78210800	2.79520400	-0.40444900
H	2.72503000	3.15255600	3.55918500
H	0.22312500	3.41524300	3.85554700
H	2.13438900	4.76586500	-2.91459800
H	-0.37630000	4.96684500	-2.63987400
H	-3.82096600	5.16863900	2.15297700
H	-3.92383700	5.74814400	0.45693100
H	-4.17806700	3.78743600	-1.13123900
H	-5.66560100	1.49012000	-0.02941100
H	-6.66003900	2.66738600	-0.88793800
H	-6.09256500	0.87149600	-2.34282200
H	-6.26495600	3.09520200	-3.32833200
H	-4.53719200	3.36253100	-3.18643400
H	-4.05189700	0.12686600	-1.18431600
H	-3.97213800	0.05488400	-2.92690600
H	-5.21895500	2.60477300	-5.50193600
H	-2.52248400	2.12176000	-1.19029900
H	-1.83840200	0.80641700	-2.17291300
H	6.33484900	4.88844600	-0.71838300
H	6.50087000	4.42415500	0.99393100
H	6.59808800	2.02868800	0.35170700
H	6.36920800	2.46254100	-1.35971600
H	7.86166800	2.92611400	-0.51630100
H	-4.05674200	1.50118000	-4.75975600
H	-5.76761600	1.06890600	-4.81276000
H	-2.59542200	2.20299800	-2.95250000

Coordinate for 2:2 complex of NDI+ Py :

C	5.27246700	1.24713800	-3.90587600
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C	6.05677800	0.47492800	-3.07486000
C	5.92877500	0.57662600	-1.67236800
C	4.96230800	1.44648200	-1.12800300
C	4.13745600	2.19380800	-1.99616900
C	4.30376400	2.11260300	-3.36202600
C	6.73390100	-0.19297400	-0.80153700
C	6.60324700	-0.06835800	0.56306500
C	5.64408300	0.81114400	1.10899300
C	4.82730100	1.54095700	0.27663200
C	3.78786300	2.42849900	0.85803900
N	2.94202400	3.07366000	-0.04307900
C	3.05151500	3.03929200	-1.43095800
C	7.01786300	-0.49802800	-3.65755900
N	7.73458900	-1.29052100	-2.75669900
C	7.70023700	-1.17084100	-1.36369000
O	7.16720100	-0.62674400	-4.85732000
O	8.41781900	-1.85758700	-0.66308200
O	2.27143900	3.64078100	-2.14422000
O	3.65435700	2.57323200	2.05768600
C	2.01273300	4.02727200	0.52707600
C	2.71813900	5.38037300	0.69867900
O	3.78924700	5.60879500	0.16024700
N	2.02979900	6.24972300	1.47000800
C	2.58751800	7.53087500	1.86645800
C	2.49947900	7.77230000	3.37724600
C	1.03745000	7.87361500	3.83891200
C	3.33718800	6.78092400	4.20840500
C	0.89217300	8.20360600	5.32316700
C	2.79771600	5.35114600	4.33955000
C	8.66171100	-2.28030300	-3.32037000
C	10.04792200	-1.68646100	-3.53159700
H	5.40408900	1.15258100	-4.97852300
H	3.65769400	2.70718000	-3.99879000
H	7.23668800	-0.67518400	1.20137900
H	5.51544800	0.91119000	2.18117700
H	1.16527100	4.13357400	-0.15036000
H	1.66178200	3.65820900	1.49004900
H	1.20520100	5.89326700	1.94980500
H	3.62776600	7.53696500	1.53073400
H	2.06627800	8.34346600	1.34073100
H	2.94928000	8.76452100	3.53540800
H	0.54730600	8.65488400	3.24363900

H	0.49827200	6.94247700	3.62606900
H	4.34962600	6.74821300	3.78782400
H	3.44573500	7.20691600	5.21294200
H	-0.15268600	8.39060800	5.58416200
H	2.94982000	4.76264400	3.43249500
H	3.31751900	4.83169600	5.14987700
H	8.69688800	-3.11328200	-2.61797000
H	8.23126800	-2.61249700	-4.26474600
H	9.99581600	-0.84425900	-4.22556400
H	10.46108000	-1.34524000	-2.57965700
H	10.72104300	-2.43811700	-3.95104500
H	1.24746600	7.38105500	5.95073800
H	1.46987700	9.09662000	5.58589100
H	1.72658000	5.33353900	4.56504600
C	3.54643700	-1.61847900	2.10924200
C	4.00469100	-2.06163000	0.82018900
C	3.38032600	-1.52406600	-0.33583000
C	2.30918200	-0.58272900	-0.20424100
C	1.85117600	-0.17661000	1.08541600
C	2.53749700	-0.72021800	2.23459000
C	3.82310300	-1.93555200	-1.62329200
C	3.19440800	-1.36866300	-2.78792800
C	2.19128500	-0.46563700	-2.66773700
C	1.71202500	-0.04736500	-1.37690800
C	0.66011000	0.86151200	-1.24116800
C	0.19292100	1.22459700	0.01621600
C	0.76622800	0.72680700	1.19259300
C	5.05847900	-2.97143900	0.67452700
C	5.47273200	-3.38391300	-0.58683400
C	4.85920500	-2.87291900	-1.72627000
C	0.25852500	1.20055000	2.54367400
C	-1.25492900	1.50808000	2.61802700
C	-1.59296800	2.92478600	3.10410500
C	-1.06213600	4.05391400	2.23608400
N	-1.62928300	4.18472500	1.01808400
O	-0.17373200	4.80032400	2.65730000
C	-1.33179500	5.28824900	0.11440300
C	-1.17567400	4.84930000	-1.34403500
C	-2.48851900	4.28006900	-1.92523400
C	-0.68493200	6.01853800	-2.21237800
C	0.68989700	6.57932200	-1.85225400
C	-2.24734000	3.06329800	-2.81516200

H	4.03564200	-2.01519500	2.99565500
H	2.24640600	-0.39975500	3.22730900
H	3.55415300	-1.67356500	-3.76746600
H	1.72236500	-0.03308500	-3.54789900
H	0.20951900	1.28808100	-2.13380200
H	-0.63547500	1.92487700	0.07593000
H	5.55911400	-3.34272400	1.56311000
H	6.29145900	-4.08966300	-0.68192900
H	5.18766500	-3.18919000	-2.71345700
H	0.48917100	0.44667400	3.29896400
H	0.83934700	2.08934000	2.83413000
H	-1.74254600	1.32477200	1.65805900
H	-1.72838900	0.81351500	3.31982700
H	-2.68239800	3.02490000	3.17022900
H	-1.17363100	3.09493100	4.09865200
H	-2.33681700	3.50451600	0.74881000
H	-2.12977400	6.04373200	0.17656300
H	-0.41668800	5.75832100	0.47900700
H	-0.41395100	4.05503800	-1.38016700
H	-3.17849100	3.99108900	-1.12480500
H	-2.99706300	5.06977800	-2.49478600
H	-0.67213500	5.67572400	-3.25464700
H	-1.43915300	6.81737500	-2.16526400
H	0.70739700	7.02306900	-0.85201600
H	1.45530700	5.79944500	-1.89222200
H	-3.17068100	2.72211800	-3.29809200
H	-1.51947200	3.28499800	-3.60306200
H	-1.85802900	2.23384800	-2.21435600
H	0.97603400	7.36381900	-2.55809400
C	1.07271000	-3.72114700	-1.28344400
C	1.14161400	-3.87848900	0.08546000
C	0.25316200	-3.18103000	0.93001900
C	-0.74822500	-2.36867500	0.35794400
C	-0.78449500	-2.19201800	-1.04112900
C	0.12043300	-2.85211500	-1.84821700
C	0.33008700	-3.29669500	2.33824400
C	-0.58681500	-2.66424600	3.14637300
C	-1.65292300	-1.93961000	2.56739500
C	-1.72410600	-1.78773700	1.20091800
C	-2.87110300	-1.08619200	0.58184600
N	-2.74797600	-0.75062600	-0.76888100
C	-1.78986500	-1.28095600	-1.64356500

C	2.08837300	-4.86537300	0.67427000
N	2.10224900	-4.96954600	2.06829200
C	1.38495900	-4.15121100	2.94701000
O	2.78531300	-5.58848400	-0.00960100
O	1.58250300	-4.19285700	4.14461600
O	-1.80816400	-1.01077500	-2.82970700
O	-3.88286000	-0.79219300	1.19121200
C	-3.80301900	0.08114300	-1.32614400
C	-4.05649000	1.31730200	-0.46656100
O	-3.11780700	1.91907000	0.05632400
N	-5.33792100	1.70119600	-0.40224700
C	-5.81050800	2.87269600	0.32295600
C	-6.64819700	2.57535800	1.58992700
C	-7.49523200	1.30877800	1.40561200
C	-5.81987100	2.57586500	2.88456300
C	-8.44796800	1.04294500	2.56802200
C	-4.86200200	1.39951200	3.03798500
C	2.92988600	-6.03044500	2.65533600
C	4.39145900	-5.63592700	2.79435700
H	1.77176100	-4.27095800	-1.90506600
H	0.07707100	-2.69210100	-2.92015500
H	-0.50425900	-2.78270800	4.22144800
H	-2.43863900	-1.50980200	3.18066000
H	-3.45468600	0.40929800	-2.30767200
H	-4.72647400	-0.48947800	-1.45090700
H	-6.03508500	1.06850000	-0.79390400
H	-4.93436600	3.47945400	0.57165700
H	-6.42665500	3.45334700	-0.37188200
H	-7.34571000	3.42101700	1.67626200
H	-8.07073700	1.40009900	0.47423900
H	-6.83704300	0.44363900	1.26181600
H	-5.25560000	3.51731600	2.92670100
H	-6.50854100	2.60536100	3.73704200
H	-9.10975600	0.20230600	2.34567000
H	-4.12837900	1.37333700	2.22756600
H	-4.31819000	1.46769600	3.98619800
H	2.49593900	-6.25241600	3.63052700
H	2.83360800	-6.90041300	2.00212900
H	4.82738300	-5.46890000	1.80794200
H	4.48074600	-4.72522200	3.39317500
H	4.94785300	-6.43309500	3.29384800
H	-7.90159300	0.79955100	3.48391700

H	-9.07319400	1.91778700	2.77602400
H	-5.38645100	0.43998200	3.02421800
C	-4.21170300	-4.09919400	2.91187600
C	-3.05061900	-4.90882300	3.15950200
C	-2.32927000	-5.41735800	2.04833900
C	-2.73824400	-5.09108700	0.71882800
C	-3.88452400	-4.27708200	0.50011300
C	-4.61126400	-3.80222400	1.65101700
C	-1.17869600	-6.22623100	2.26428500
C	-0.45826600	-6.73357000	1.12441400
C	-0.83387200	-6.41387000	-0.13595300
C	-1.97683500	-5.57199500	-0.38196000
C	-2.35911600	-5.19930900	-1.66968800
C	-3.48030500	-4.40255600	-1.87879800
C	-4.27027800	-3.94888200	-0.82045300
C	-2.58921500	-5.17592200	4.45547900
C	-1.44877200	-5.94377800	4.65797500
C	-0.75814100	-6.47735000	3.57374700
C	-5.55122000	-3.16996900	-1.05712700
C	-5.92386400	-3.00895800	-2.53008900
C	-7.29851600	-2.35551100	-2.76526400
C	-7.22883900	-0.85368500	-2.59508700
N	-7.34347600	-0.12246400	-3.72488100
O	-7.03993000	-0.34777400	-1.48748100
C	-7.16235200	1.31966800	-3.77250200
C	-5.75372500	1.76814300	-4.19264500
C	-5.26519000	1.06436600	-5.47350000
C	-5.72982900	3.29279400	-4.36969800
C	-6.01618700	4.07727800	-3.09290200
C	-4.51145000	-0.24643300	-5.24118000
H	-4.76112500	-3.71188200	3.76559000
H	-5.47411800	-3.16301300	1.50287600
H	0.41203200	-7.36134100	1.30004200
H	-0.26418300	-6.77267100	-0.98915900
H	-1.77085800	-5.53968000	-2.51760400
H	-3.74035500	-4.14350800	-2.89900500
H	-3.13372500	-4.77015800	5.30367700
H	-1.09325900	-6.13005800	5.66577300
H	0.12752400	-7.08607900	3.73641100
H	-6.37125400	-3.70120600	-0.55507100
H	-5.50013300	-2.19073100	-0.56404200
H	-5.14849600	-2.43253200	-3.05285900

H	-5.94162400	-3.99859300	-2.99853000
H	-7.66274000	-2.60981100	-3.76540200
H	-8.02259700	-2.73905700	-2.03992600
H	-7.45273300	-0.61569800	-4.59795200
H	-7.89589100	1.72809300	-4.47878100
H	-7.40969000	1.69918300	-2.77795500
H	-5.07117100	1.51066300	-3.36851100
H	-6.11847500	0.90130800	-6.14877600
H	-4.59783900	1.74838900	-6.00984200
H	-4.73952900	3.57809500	-4.74267400
H	-6.44295100	3.56940900	-5.15891100
H	-7.03731800	3.92163700	-2.73049200
H	-5.32351000	3.76871500	-2.30186700
H	-4.16583800	-0.67079900	-6.18757200
H	-3.63068300	-0.09096200	-4.60926200
H	-5.13579900	-0.99654100	-4.74889700
H	-5.88634300	5.15039400	-3.25365700

Coordinate for 3:3 complex of NDI+ Py :

C	6.35232100	14.35433500	1.25620000
C	5.04199000	14.65599900	1.56245300
C	4.65567200	14.89208700	2.89988400
C	5.63091800	14.85694800	3.91701800
C	6.97185600	14.57383300	3.57975700
C	7.32469900	14.30798700	2.27394700
C	3.31348300	15.17950600	3.23962700
C	2.95611200	15.39494100	4.55111700
C	3.93332600	15.36501500	5.56919200
C	5.24910700	15.11761600	5.25395600
C	6.27995400	15.15123900	6.32381100
N	7.59940100	14.93188900	5.92438100
C	8.00971500	14.57034900	4.64537900
C	4.03644000	14.77612300	0.47449400
N	2.73924900	15.13249700	0.85351100
C	2.28943700	15.28369400	2.16937900
O	4.31746900	14.59776300	-0.69507300
O	1.11850600	15.51165300	2.40287500
O	9.17109300	14.29115700	4.41136600
O	6.00277300	15.39084400	7.48222500
C	8.58315400	14.81683500	6.98154500
C	8.67060800	13.35724800	7.44523500

O	7.86806700	12.52194600	7.05932400
N	9.67219000	13.13536100	8.32186900
C	9.78292900	11.88837600	9.05565000
C	9.45961100	12.03131700	10.54859100
C	10.47244600	12.95524800	11.24182700
C	7.99312800	12.41345600	10.82479700
C	10.23463100	13.10802700	12.74271300
C	7.56447100	13.84500600	10.46512200
C	1.74290900	15.28353500	-0.21452200
C	1.03701800	13.96639400	-0.50735600
H	6.61387300	14.17249700	0.21922800
H	8.36224700	14.08153900	2.05278200
H	1.91731600	15.61234200	4.77564400
H	3.67609100	15.55936100	6.60464800
H	9.54773700	15.17848900	6.62893900
H	8.26348000	15.42902600	7.82516700
H	10.19850300	13.94789400	8.63458000
H	9.09572600	11.18610600	8.57796300
H	10.80157300	11.49490700	8.94088400
H	9.60068700	11.02611200	10.97554500
H	11.47637900	12.54373600	11.07353300
H	10.46792300	13.94805400	10.77667900
H	7.34634600	11.70237400	10.29754700
H	7.81212600	12.24711700	11.89288200
H	11.05096000	13.66038400	13.21535400
H	7.23015900	13.92260800	9.42830100
H	6.72098100	14.15415500	11.08906400
H	1.03365900	16.03987100	0.12256800
H	2.27642400	15.64433800	-1.09355800
H	1.76075700	13.21444600	-0.83055800
H	0.51956300	13.60950200	0.38601200
H	0.30042200	14.10106100	-1.30321900
H	9.30743300	13.65239100	12.94466800
H	10.16094500	12.13085100	13.23279600
H	8.37111900	14.57164800	10.61208500
C	4.08055700	18.64934700	6.11574400
C	3.89834400	18.52655400	4.69479700
C	5.03989200	18.28314600	3.88711100
C	6.33592900	18.17842800	4.48617100
C	6.49851500	18.33750700	5.89390800
C	5.30868600	18.55068300	6.68361700
C	4.88411800	18.15374000	2.47879600

C	6.04884900	17.88727200	1.67418400
C	7.27462400	17.77277700	2.23951300
C	7.46276100	17.92248600	3.65900800
C	8.72431300	17.83967400	4.25026300
C	8.87866900	18.02587200	5.61833100
C	7.79400200	18.28240800	6.46076000
C	2.63524800	18.60171100	4.09593700
C	2.49258300	18.48648000	2.71830600
C	3.60817800	18.27093000	1.91481100
C	8.00490100	18.47896300	7.95125000
C	9.37825400	19.05039500	8.37381300
C	10.20891600	18.12562700	9.27287800
C	10.76955700	16.85955300	8.64191200
N	11.56573800	17.02021300	7.55898700
O	10.53275300	15.75864800	9.14571200
C	12.33233100	15.92237700	6.98071900
C	12.03285200	15.61022600	5.50872400
C	12.45343400	16.75338500	4.57595100
C	12.68512300	14.27709200	5.11576300
C	12.10410600	13.05838300	5.83306600
C	12.08928000	16.49306900	3.11029500
H	3.20320600	18.81869600	6.73543500
H	5.39537700	18.61998400	7.76119400
H	5.91708000	17.76370500	0.60203500
H	8.14917400	17.55754100	1.63059700
H	9.59812400	17.65131700	3.63159600
H	9.87731000	17.96513000	6.03167700
H	1.76326100	18.74426800	4.72690900
H	1.50590600	18.54461500	2.27017800
H	3.49715800	18.18048700	0.83708000
H	7.23205700	19.15704900	8.32200200
H	7.81753700	17.52051700	8.45827100
H	9.96495800	19.35178300	7.50238700
H	9.21978500	19.97673500	8.93575300
H	11.06131400	18.69238100	9.66615400
H	9.61495500	17.78990900	10.12649200
H	11.71920900	17.96275600	7.20088400
H	13.40562300	16.14522900	7.08554800
H	12.12209600	15.05158900	7.60395700
H	10.94953800	15.48665300	5.38780600
H	11.97211200	17.68184700	4.90421900
H	13.53736200	16.92453000	4.66614700

H	12.54794900	14.13228500	4.03977400
H	13.77062900	14.34345100	5.28330100
H	12.30439400	13.06427800	6.90850800
H	11.01934400	13.02105500	5.69382100
H	12.79467800	15.81385700	2.62455700
H	11.09571400	16.03392700	3.04038500
H	12.07814900	17.42428900	2.53673400
H	12.52922800	12.13509000	5.43003600
C	6.44675300	21.16733900	2.80912800
C	5.66756500	21.46373400	3.90775000
C	6.26269400	21.65251900	5.17461300
C	7.66760500	21.61506100	5.29376200
C	8.45078300	21.35629300	4.14867200
C	7.84738300	21.10034000	2.93427400
C	5.48075000	21.92729000	6.32000000
C	6.07597400	22.12504500	7.54517900
C	7.48288800	22.10800300	7.66058500
C	8.26397300	21.87698500	6.55029800
C	9.74085400	21.96725900	6.65953000
N	10.46508000	21.80743300	5.47609100
C	9.93205300	21.42527600	4.24248700
C	4.20722900	21.70126500	3.73956900
N	3.50005700	22.09040400	4.88183900
C	4.00896300	22.09071000	6.18283400
O	3.65715000	21.64504800	2.65738700
O	3.28268400	22.29692500	7.13533000
O	10.65462600	21.21692600	3.28583800
O	10.31085900	22.19668100	7.70964000
C	11.90711400	21.87442200	5.59857100
C	12.47077600	20.52807700	6.05164600
O	11.72985000	19.54929000	6.16370800
N	13.78286400	20.52498000	6.30767300
C	14.50581600	19.34947600	6.76530600
C	15.01282700	19.45416700	8.20949100
C	15.94558200	20.66365400	8.37251200
C	13.89183300	19.39291400	9.26181300
C	16.54914700	20.78462700	9.77007100
C	12.94765000	20.59889700	9.33245100
C	2.13546000	22.60250300	4.69995200
C	1.06469400	21.52657300	4.77193600
H	5.95945100	21.01014100	1.85245200
H	8.47580300	20.88291000	2.07683500

H	5.44390700	22.33785500	8.40076400
H	7.97277400	22.31664100	8.60629400
H	12.32900000	22.15045600	4.63125100
H	12.16859900	22.63593300	6.33391500
H	14.26122000	21.42833500	6.28635300
H	13.83910500	18.49096800	6.64957700
H	15.36058300	19.19245000	6.09474400
H	15.62533700	18.55248200	8.36297300
H	16.75336300	20.57203900	7.63438300
H	15.41778500	21.59190000	8.12565700
H	13.30888100	18.47904600	9.08511000
H	14.36661500	19.25481100	10.23969000
H	17.30632800	21.57195100	9.80181200
H	12.19278700	20.58890500	8.54212500
H	12.40990400	20.60422000	10.28566300
H	1.98470500	23.34662900	5.48422900
H	2.11717300	23.09122000	3.72417700
H	1.17351800	20.83448100	3.93560600
H	1.14337800	20.97771700	5.71409200
H	0.07416100	21.98605200	4.72131400
H	15.78605000	21.03133200	10.51396400
H	17.02473700	19.84727300	10.07828000
H	13.48774700	21.54863500	9.25914300
C	7.94570900	25.52584300	7.98590800
C	6.86632400	25.34831600	7.05244500
C	7.18652700	25.07004200	5.69844800
C	8.55429400	24.99865400	5.28273000
C	9.60912700	25.24516700	6.21134800
C	9.24189300	25.47604800	7.58916500
C	6.13824900	24.89329600	4.75375300
C	6.47701300	24.57840500	3.39016000
C	7.77052300	24.46927300	3.00207900
C	8.84993300	24.69209400	3.92758600
C	10.18680400	24.64805400	3.52611100
C	11.20803700	24.95217700	4.41988200
C	10.95083100	25.26268700	5.76030600
C	5.52317100	25.42082500	7.44115800
C	4.50415500	25.28643700	6.50537900
C	4.80893500	25.03351800	5.17124900
C	12.09403000	25.59340600	6.70620300
C	13.30528800	26.30574900	6.06117200
C	14.64220100	25.56674200	6.21686000

C	14.66741800	24.16492400	5.63832800
N	14.73227800	24.07448300	4.29521600
O	14.64199700	23.18408400	6.39036900
C	14.88539700	22.81530200	3.58058500
C	13.91885700	22.65694500	2.40455900
C	14.16280900	23.71813100	1.30771500
C	14.03060200	21.24639000	1.80326800
C	13.72688000	20.08739700	2.75316800
C	12.86396700	24.28077700	0.73583700
H	7.70146000	25.70807800	9.02955300
H	10.02111400	25.59919200	8.33144900
H	5.66786500	24.41147200	2.68274700
H	8.02426300	24.22274600	1.97429800
H	10.42186500	24.39369500	2.49575100
H	12.23128100	24.95009300	4.05393700
H	5.28709500	25.58788500	8.48727800
H	3.46844000	25.36427100	6.81968700
H	4.01241900	24.92787700	4.43824000
H	11.71227800	26.23097300	7.50671900
H	12.42586900	24.66832500	7.20105100
H	13.12617600	26.50795100	5.00317300
H	13.43698000	27.28714800	6.52758400
H	15.43042200	26.15873500	5.73980000
H	14.88972600	25.45351300	7.27508700
H	14.68064900	24.94137000	3.76384200
H	15.91753800	22.72676400	3.20965100
H	14.73628200	22.01767200	4.30941500
H	12.89432800	22.78591600	2.78643400
H	14.75497300	24.55361200	1.69817000
H	14.76402600	23.26885600	0.50601300
H	13.34855400	21.19573800	0.94563400
H	15.04421000	21.13079000	1.39365000
H	14.44177800	20.03006200	3.58012200
H	12.71997700	20.17631200	3.17203300
H	13.05002500	24.94880200	-0.11355200
H	12.20004200	23.47976300	0.39309500
H	12.33807200	24.85755600	1.50432300
H	13.78445900	19.13627300	2.21637000
C	6.89058500	27.92887100	3.98191200
C	7.26135900	28.30307500	5.25644200
C	8.62267900	28.48420400	5.57968700
C	9.59749800	28.33432900	4.57088300

C	9.20550600	27.90809800	3.28433900
C	7.87119700	27.70277700	2.99737100
C	9.02812200	28.84650700	6.88567300
C	10.35104000	29.10637800	7.16345300
C	11.30872800	29.06497200	6.12567300
C	10.94028500	28.67103800	4.85849400
C	11.92389500	28.67962200	3.75129700
N	11.54731000	28.03223300	2.57113800
C	10.23352900	27.66999200	2.24132600
C	6.21863600	28.62076900	6.27104900
N	6.66935100	29.00643100	7.53680700
C	8.00454800	29.00880400	7.95340600
O	5.03125100	28.59944200	6.01419300
O	8.29773800	29.19686800	9.11679800
O	9.96904400	27.20219400	1.14969300
O	13.01949900	29.20270300	3.83386200
C	12.56832900	27.90622200	1.54253000
C	13.87005100	27.32824600	2.09149400
O	13.85253200	26.42113500	2.92546300
N	14.98083500	27.83187500	1.53931900
C	16.33131300	27.38175900	1.84798500
C	17.21181000	28.39923200	2.60870700
C	16.92969400	29.83076000	2.13280800
C	17.15808600	28.23689700	4.13591200
C	17.87038800	30.86821200	2.73975100
C	15.83653200	28.63746200	4.78225400
C	5.65964300	29.46061500	8.50111600
C	4.98458100	28.31627700	9.23981900
H	5.83505700	27.80369800	3.76385900
H	7.59639700	27.37291300	2.00137000
H	10.62530700	29.39779200	8.17165000
H	12.33845900	29.35996300	6.30064000
H	12.17378900	27.20960900	0.79964100
H	12.75605900	28.86753600	1.05805500
H	14.87513500	28.64160700	0.92802900
H	16.24549900	26.44692100	2.41038200
H	16.81766700	27.14915200	0.89435300
H	18.24348300	28.15784300	2.31416900
H	17.00918300	29.86035300	1.03737300
H	15.89072200	30.09720200	2.35995400
H	17.38058800	27.18769300	4.37392700
H	17.97625200	28.81943600	4.57516500

H	17.71114900	31.85054200	2.28853000
H	15.00822400	28.02847400	4.41054900
H	15.88678400	28.51397600	5.86930800
H	6.17790600	30.11763600	9.19991700
H	4.92161600	30.03292400	7.93502800
H	4.42407500	27.69847500	8.53611200
H	5.73304300	27.70354600	9.74991700
H	4.29314300	28.71135700	9.98832200
H	17.71005700	30.97019400	3.81701800
H	18.91855400	30.59184900	2.58376600
H	15.58094000	29.68120600	4.57937900
C	11.77672000	32.31532200	5.43890000
C	10.58255500	32.29623100	6.23792000
C	9.34751400	32.00222200	5.60395200
C	9.31350500	31.69656100	4.20866400
C	10.51199800	31.70854800	3.44187200
C	11.74442000	32.04102000	4.11175600
C	8.14829400	31.98329400	6.36958500
C	6.90313800	31.68562000	5.70887200
C	6.86904800	31.38205800	4.39031700
C	8.07267500	31.36325500	3.59865300
C	8.06593200	31.01726000	2.24827400
C	9.24045000	31.02897800	1.50277900
C	10.46669600	31.39031300	2.06447100
C	10.60601200	32.51880800	7.62135500
C	9.43448600	32.47066200	8.36735400
C	8.21444700	32.22043100	7.74587300
C	11.72583700	31.50635800	1.22487400
C	11.50822800	31.26469000	-0.26809800
C	12.75176000	31.52734300	-1.13803700
C	13.72782500	30.37409600	-1.06079900
N	13.81867800	29.59912000	-2.16312200
O	14.36322600	30.14829500	-0.02924800
C	14.59647800	28.37207400	-2.22787800
C	13.77787000	27.08881000	-2.01315400
C	12.50632300	27.04345600	-2.88203900
C	14.66129500	25.86334600	-2.28496600
C	15.85426900	25.72873900	-1.34347000
C	11.26288500	27.66326600	-2.24163400
H	12.72018900	32.54189200	5.92801600
H	12.66985900	32.03510900	3.54727500
H	5.99040900	31.68826600	6.29981400

H	5.92964800	31.12672400	3.90702100
H	7.12786000	30.73751800	1.77640400
H	9.18337600	30.75765200	0.45464900
H	11.55575100	32.72690400	8.10643900
H	9.46841200	32.62972700	9.43986900
H	7.29889100	32.19410900	8.33104000
H	12.12778400	32.52092700	1.35065600
H	12.50689400	30.83958600	1.61215500
H	11.15340800	30.23836700	-0.43418600
H	10.71107400	31.92804900	-0.61955500
H	12.44740700	31.70139000	-2.17469600
H	13.26958200	32.42528800	-0.78753600
H	13.23499500	29.83124900	-2.95242200
H	15.07785400	28.33005800	-3.21300700
H	15.38464900	28.46108400	-1.47595700
H	13.48014900	27.06397100	-0.95388300
H	12.71232300	27.51411200	-3.85502500
H	12.28263100	25.99504100	-3.10942700
H	14.03819700	24.96623400	-2.19476500
H	14.99909200	25.89424600	-3.33028400
H	16.57911900	26.53831100	-1.47523400
H	15.51285900	25.74412400	-0.30211200
H	10.39224100	27.55004000	-2.89299800
H	11.02548800	27.18109400	-1.28750400
H	11.39144200	28.73022500	-2.04234700
H	16.38258800	24.78677100	-1.51028700