

Electronic Supplementary Information

How do paramagnetic and diamagnetic LMOCs can detect
picric acid from surface water and intracellular
environment: a combined experimental and DFT-D3 study

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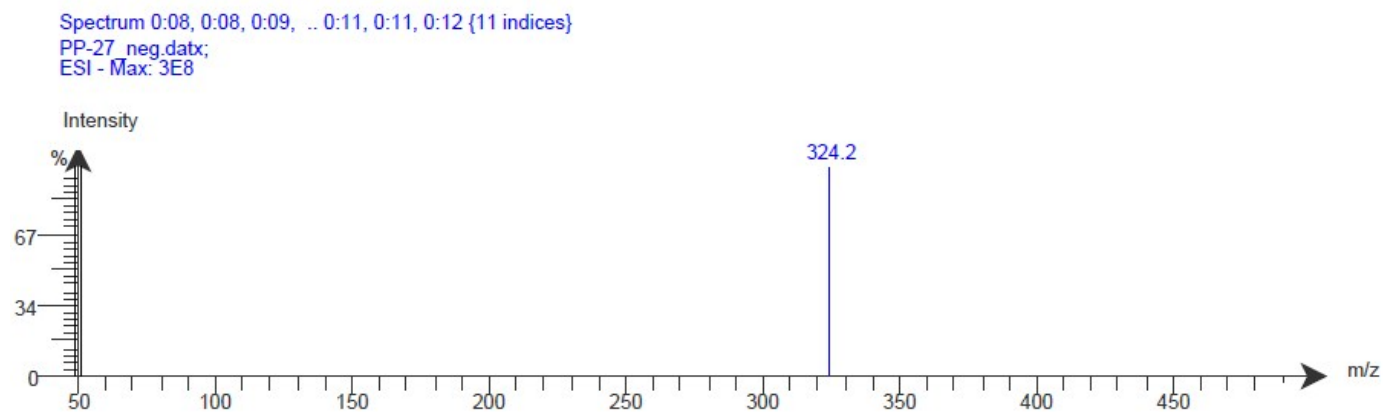


Figure S1. ESI-MS of **dtHBAP** in MeOH.

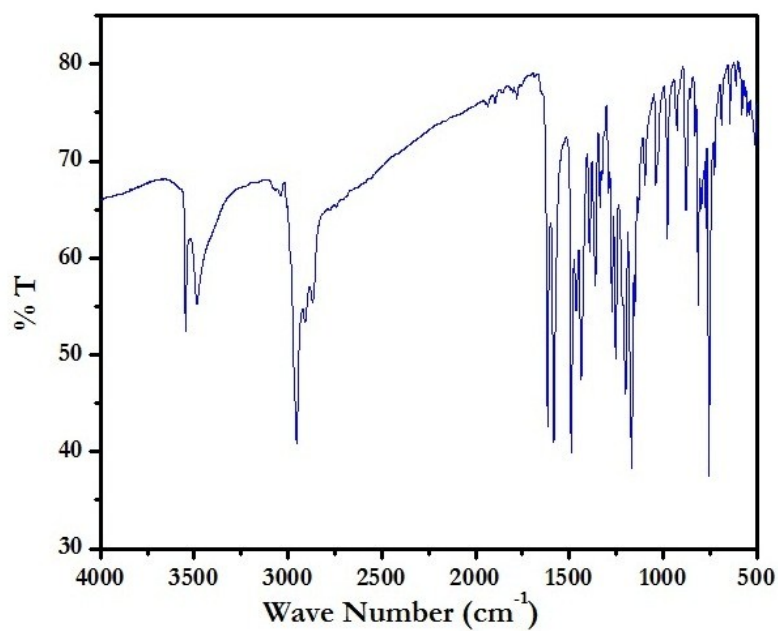


Figure S2. FT-IR of **dtHBAP** (KBr disk).

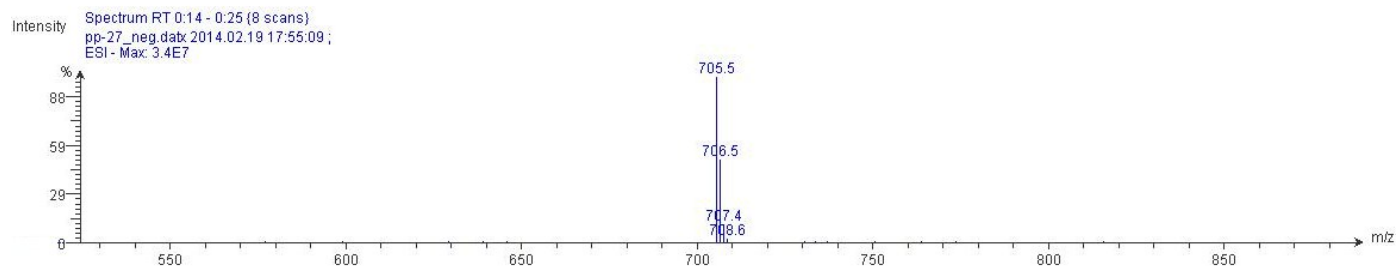


Figure S3. ESI-MS of **PP** in MeOH.

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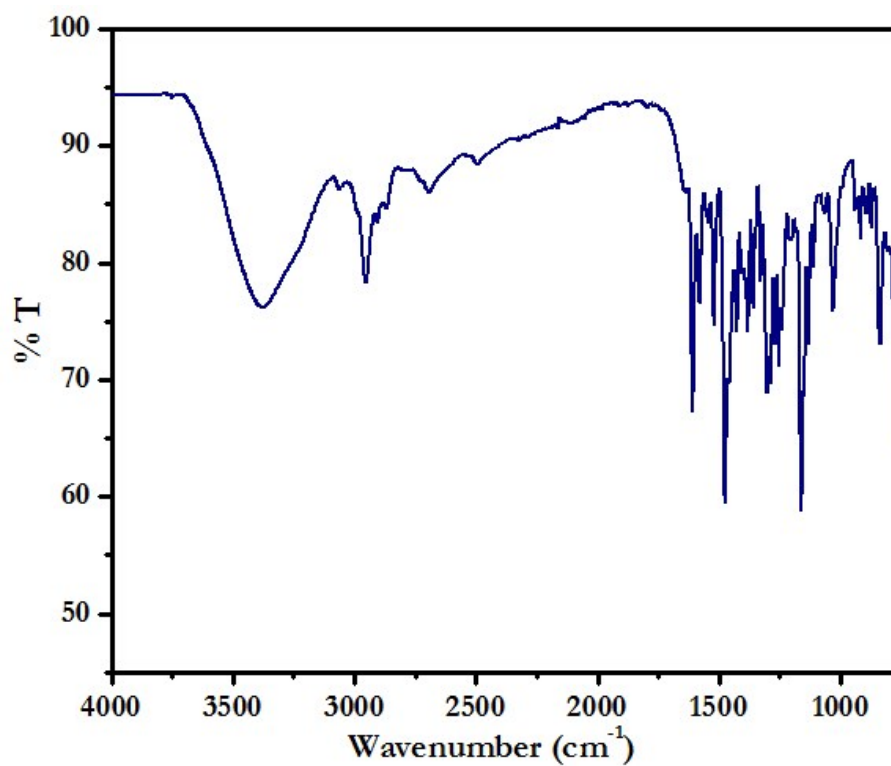


Figure S4. FT-IR of **PP** (KBr disk).

Table S1 Crystal data and details of the structure determination for **PP**.

<u>Crystal Data</u>				
Formula	$\text{C}_{42}\text{H}_{50}\text{CoN}_2\text{O}_4 \cdot \text{C}_6\text{H}_{15}\text{N}$			
Formula Weight	806.96			
Crystal System	monoclinic			
Space group	P21/c (No. 14)			
a, b, c [Angstrom]	17.028(4)	16.746(4)	17.575(4)	
alpha, beta, gamma [deg]	90	113.781(3)	90	

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V [Å ³]	4586.0(19)
Z	4
D(calc) [g/cm ³]	1.169
Mu(MoKa) [/mm]	0.418
F(000)	1732
Crystal Size [mm]	0.13 x 0.16 x 0.23

Data Collection

Temperature (K)	293
Radiation [Å]	MoKa 0.71073
Theta Min-Max [Deg]	1.3, 20.4
Dataset	-16: 16 ; -16: 16 ; -17: 17
Tot, Uniq. Data, R(int)	25730, 4519, 0.095
Observed Data [I > 2.0 sigma(I)]	3195

Refinement

Nref, Npar	4519, 520
R, wR2, S	0.0412, 0.0969, 1.01
$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 3.1419P]$ where $P = (F_o^2 + 2F_c^2)/3$	
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Å ³]	-0.26, 0.35

Table S2 Bond distances of **PP**.

Co1	-O1	1.936(3)	C10	-C16	1.417(7)	C1	-C2	1.406(7)	C29	-C30	1.414(7)
Co1	-O2	1.874(3)	C11	-C12	1.523(7)	C1	-C6	1.409(7)	C29	-C41	1.421(7)
Co1	-O3	1.899(3)	C11	-C13	1.539(8)	C2	-C3	1.367(7)	C30	-C31	1.371(8)
Co1	-O5	1.882(3)	C11	-C15	1.504(8)	C3	-C4	1.393(7)	C31	-C35	1.411(7)
Co1	-N1	1.882(3)	C16	-C17	1.380(7)	C4	-C5	1.384(7)	C31	-C32	1.515(7)
Co1	-N2	1.875(3)	C17	-C18	1.529(7)	C5	-C6	1.387(7)	C32	-C48	1.529(8)
O1	-C22	1.334(6)	C17	-C21	1.434(7)	C7	-C8	1.426(7)	C32	-C34	1.533(8)
O2	-C21	1.319(6)	C18	-C19	1.536(8)	C8	-C9	1.417(7)	C32	-C33	1.518(8)
O3	-C1	1.313(6)	C18	-C20	1.554(7)	C8	-C21	1.414(7)	C35	-C36	1.376(7)
O5	-C41	1.305(6)	C18	-C49	1.535(7)	C9	-C10	1.354(7)	C36	-C37	1.537(6)
N1	-C6	1.418(6)	C22	-C23	1.396(8)	C10	-C11	1.527(7)	C36	-C41	1.437(8)
N1	-C7	1.295(6)	C22	-C27	1.404(7)	N3	-C42	1.496(7)	C28	-C29	1.427(8)
N2	-C27	1.411(6)	C23	-C24	1.388(7)	N3	-C44	1.513(6)	C26	-C27	1.379(6)
N2	-C28	1.300(6)	C24	-C25	1.382(7)	N3	-C46	1.495(6)	C25	-C26	1.377(8)
C37	-C40	1.527(8)	C37	-C38	1.526(5)	C37	-C39	1.534(7)	C42	-C43	1.490(9)
C24	-H24	0.9300	C44	-C45	1.509(7)	C25	-H25	0.9300	C46	-C47	1.476(9)

Table S3 Bond angles of **PP**.

01	-Co1	-O2	90.70(12)	O3	-C1	-C2	122.6(4)
01	-Co1	-O3	86.77(12)	C2	-C1	-C6	117.4(5)
01	-Co1	-O5	179.33(12)	O3	-C1	-C6	120.1(4)
01	-Co1	-N1	92.24(14)	C1	-C2	-C3	121.4(5)
01	-Co1	-N2	85.78(13)	C2	-C3	-C4	120.4(5)
02	-Co1	-O3	176.61(13)	C3	-C4	-C5	119.5(5)
02	-Co1	-O5	88.91(13)	C4	-C5	-C6	120.2(5)
02	-Co1	-N1	95.65(13)	N1	-C6	-C1	111.5(4)
02	-Co1	-N2	89.18(13)	N1	-C6	-C5	127.7(5)
03	-Co1	-O5	93.64(13)	C1	-C6	-C5	120.8(5)
03	-Co1	-N1	86.70(13)	N1	-C7	-C8	125.9(4)
03	-Co1	-N2	88.39(13)	C7	-C8	-C21	123.1(5)
05	-Co1	-N1	87.26(14)	C7	-C8	-C9	117.0(4)
05	-Co1	-N2	94.76(14)	C9	-C8	-C21	119.9(5)
N1	-Co1	-N2	174.81(15)	C8	-C9	-C10	122.4(5)
Co1	-O1	-C22	108.9(3)	C9	-C10	-C11	124.4(4)
Co1	-O2	-C21	125.7(3)	C11	-C10	-C16	119.1(4)
Co1	-O3	-C1	109.5(3)	C9	-C10	-C16	116.5(5)
Co1	-O5	-C41	126.3(3)	C10	-C11	-C15	110.6(4)

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Co1	-N1	-C6	110.8(3)	C12	-C11	-C13	107.7(4)
Co1	-N1	-C7	124.2(3)	C13	-C11	-C15	109.2(5)
C6	-N1	-C7	124.9(4)	C10	-C11	-C12	111.4(4)
Co1	-N2	-C27	111.1(2)	C12	-C11	-C15	109.0(5)
Co1	-N2	-C28	125.0(3)	C10	-C11	-C13	108.9(4)
C27	-N2	-C28	123.9(3)	C10	-C16	-C17	125.2(5)
C44	-N3	-C46	113.2(4)	C18	-C17	-C21	121.4(4)
C42	-N3	-C44	112.0(4)	C16	-C17	-C18	121.8(4)
C42	-N3	-C46	109.0(4)	C16	-C17	-C21	116.9(4)
C17	-C18	-C19	111.2(4)	C31	-C32	-C34	109.2(4)
C17	-C18	-C20	112.0(4)	C31	-C32	-C48	110.0(4)
C17	-C18	-C49	109.6(4)	C34	-C32	-C48	109.0(4)
C19	-C18	-C20	106.6(4)	C33	-C32	-C34	108.9(4)
C20	-C18	-C49	107.2(4)	C33	-C32	-C48	107.8(4)
C19	-C18	-C49	110.0(4)	C31	-C35	-C36	125.8(5)
C8	-C21	-C17	119.1(5)	C35	-C36	-C37	121.0(5)
O2	-C21	-C17	117.3(4)	C35	-C36	-C41	117.8(4)
O2	-C21	-C8	123.6(4)	C37	-C36	-C41	121.2(4)
O1	-C22	-C23	123.8(5)	C38	-C37	-C39	111.0(4)
O1	-C22	-C27	118.9(5)	C38	-C37	-C40	107.2(4)
C23	-C22	-C27	117.3(4)	C39	-C37	-C40	107.0(4)
C22	-C23	-C24	120.6(5)	C36	-C37	-C39	109.6(4)

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C23	-C24	-C25	121.2(5)	C36	-C37	-C40	112.7(4)
C24	-C25	-C26	118.8(5)	C36	-C37	-C38	109.3(4)
C25	-C26	-C27	120.6(5)	O5	-C41	-C29	123.3(5)
N2	-C27	-C22	112.6(3)	O5	-C41	-C36	118.7(4)
N2	-C27	-C26	125.9(4)	C29	-C41	-C36	117.9(5)
C22	-C27	-C26	121.4(5)	C3	-C2	-H2	119.00
N2	-C28	-C29	125.6(4)	C1	-C2	-H2	119.00
C28	-C29	-C41	122.7(4)	C2	-C3	-H3	120.00
C28	-C29	-C30	117.1(4)	C4	-C3	-H3	120.00
C30	-C29	-C41	120.1(5)	C3	-C4	-H4	120.00
C29	-C30	-C31	123.0(5)	C5	-C4	-H4	120.00
C32	-C31	-C35	119.7(5)	C6	-C5	-H5	120.00
C30	-C31	-C35	115.3(5)	C4	-C5	-H5	120.00
C30	-C31	-C32	125.1(5)	N1	-C7	-H7	117.00
C31	-C32	-C33	111.9(4)	C8	-C7	-H7	117.00
C10	-C9	-H9	119.00	H20A	-C20	-H20B	109.00
C8	-C9	-H9	119.00	H20A	-C20	-H20C	109.00
C11	-C12	-H12A	109.00	H20B	-C20	-H20C	110.00
C11	-C12	-H12B	110.00	C18	-C20	-H20C	109.00
C11	-C12	-H12C	110.00	C18	-C20	-H20A	110.00
H12B	-C12	-H12C	109.00	C18	-C20	-H20B	109.00
H12A	-C12	-H12B	109.00	C22	-C23	-H23	120.00

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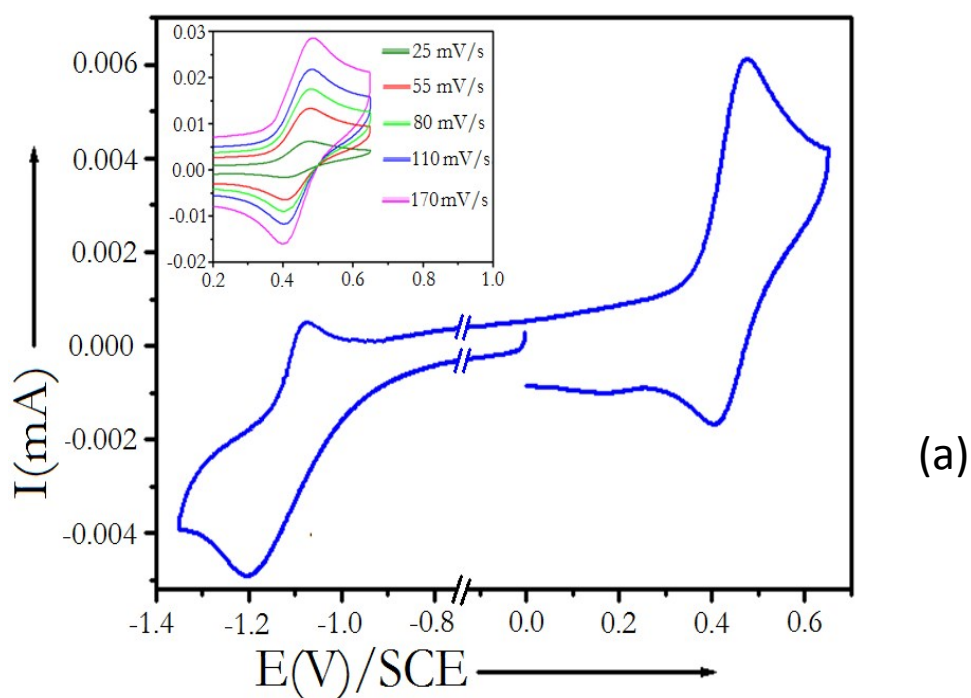
H12A	-C12	-H12C	109.00	C24	-C23	-H23	120.00
C11	-C13	-H13A	109.00	C23	-C24	-H24	119.00
C11	-C13	-H13B	109.00	C25	-C24	-H24	119.00
C11	-C13	-H13C	110.00	C26	-C25	-H25	121.00
H13A	-C13	-H13B	109.00	C24	-C25	-H25	121.00
H13B	-C13	-H13C	109.00	C25	-C26	-H26	120.00
H13A	-C13	-H13C	109.00	C27	-C26	-H26	120.00
C11	-C15	-H15C	109.00	N2	-C28	-H28	117.00
C11	-C15	-H15B	110.00	C29	-C28	-H28	117.00
H15B	-C15	-H15C	109.00	C31	-C30	-H30	118.00
H15A	-C15	-H15B	110.00	C29	-C30	-H30	118.00
H15A	-C15	-H15C	109.00	C32	-C33	-H33C	109.00
C11	-C15	-H15A	110.00	C32	-C33	-H33B	110.00
C10	-C16	-H16	117.00	H33B	-C33	-H33C	110.00
C17	-C16	-H16	117.00	H33A	-C33	-H33B	109.00
C18	-C19	-H19B	109.00	H33A	-C33	-H33C	109.00
H19A	-C19	-H19C	109.00	C32	-C33	-H33A	109.00
C18	-C19	-H19C	109.00	H34A	-C34	-H34B	109.00
H19A	-C19	-H19B	109.00	H34A	-C34	-H34C	109.00
C18	-C19	-H19A	110.00	H34B	-C34	-H34C	109.00
H19B	-C19	-H19C	109.00	C32	-C34	-H34C	110.00
C32	-C34	-H34A	109.00	C18	-C49	-H49C	109.00

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C32	-C34	-H34B	109.00	H49A	-C49	-H49C	109.00
C31	-C35	-H35	117.00	H49B	-C49	-H49C	110.00
C36	-C35	-H35	117.00	H49A	-C49	-H49B	109.00
H38A	-C38	-H38B	109.00	C18	-C49	-H49A	109.00
H38A	-C38	-H38C	109.00	C18	-C49	-H49B	109.00
C37	-C38	-H38C	110.00	N3	-C42	-C43	111.2(5)
C37	-C38	-H38A	110.00	N3	-C44	-C45	115.4(4)
C37	-C38	-H38B	109.00	N3	-C46	-C47	114.6(4)
H38B	-C38	-H38C	109.00	N3	-C42	-H42A	109.00
C37	-C39	-H39A	109.00	N3	-C42	-H42B	109.00
C37	-C39	-H39B	109.00	C43	-C42	-H42A	109.00
H39B	-C39	-H39C	109.00	C43	-C42	-H42B	109.00
C37	-C39	-H39C	109.00	H42A	-C42	-H42B	108.00
H39A	-C39	-H39B	110.00	C42	-C43	-H43A	110.00
H39A	-C39	-H39C	110.00	C42	-C43	-H43B	109.00
C37	-C40	-H40A	109.00	C42	-C43	-H43C	110.00
C37	-C40	-H40B	109.00	H43A	-C43	-H43B	109.00
C37	-C40	-H40C	109.00	H43A	-C43	-H43C	110.00
H40B	-C40	-H40C	110.00	H43B	-C43	-H43C	109.00
H40A	-C40	-H40B	110.00	N3	-C44	-H44A	108.00
H40A	-C40	-H40C	110.00	N3	-C44	-H44B	108.00
C32	-C48	-H48B	109.00	C45	-C44	-H44A	108.00

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H48A	-C48	-H48C	110.00	C45	-C44	-H44B	108.00
C32	-C48	-H48C	110.00	H44A	-C44	-H44B	107.00
H48A	-C48	-H48B	109.00	C44	-C45	-H45A	109.00
C32	-C48	-H48A	109.00	C44	-C45	-H45B	109.00
H48B	-C48	-H48C	109.00	C44	-C45	-H45C	110.00
H45A	-C45	-H45B	109.00	H46A	-C46	-H46B	108.00
H45A	-C45	-H45C	109.00	C46	-C47	-H47A	110.00
H45B	-C45	-H45C	110.00	C46	-C47	-H47B	109.00
N3	-C46	-H46A	109.00	C46	-C47	-H47C	109.00
N3	-C46	-H46B	109.00	H47A	-C47	-H47B	110.00
C47	-C46	-H46A	109.00	H47A	-C47	-H47C	109.00
C47	-C46	-H46B	109.00	H47B	-C47	-H47C	109.00



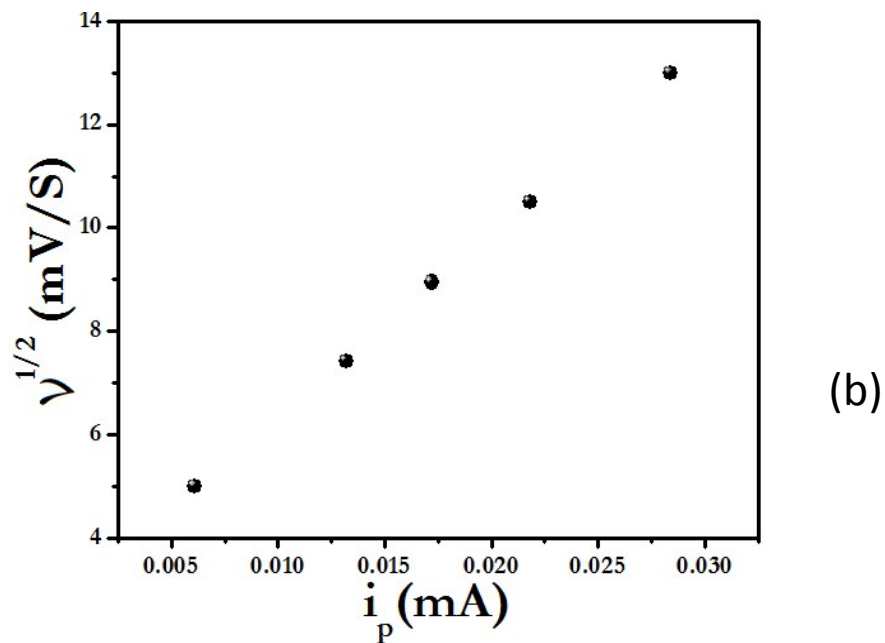


Figure S5. (a) Cyclic voltammetry of **PP** in dichloromethane, (b) Scan rate vs current graph of **PP**.

Randles–Sevcik (R-S) equation is as follows:

$$i_p = 0.4463nFAC\left(\frac{nFvD}{RT}\right)^{\frac{1}{2}}$$

where, i_p = current maximum in amps

n = number of electrons transferred in the redox event (usually 1)

A = electrode area in cm^2

F = Faraday Constant in C mol^{-1}

D = diffusion coefficient in cm^2/s

C = concentration in mol/cm³

v = scan rate in V/s

R = Gas constant in VC K⁻¹ mol⁻¹

T = temperature in K

now at 25 °C the equation will be

$$i_p = 268,000 n^{\frac{3}{2}} A D^{\frac{1}{2}} C v^{\frac{1}{2}}$$

Keeping every parameter constant when we just vary scan rates, the i_p vs scan rate curve it gives a straight line passing through the origin suggesting reversibility of the peak (Figure S5b).

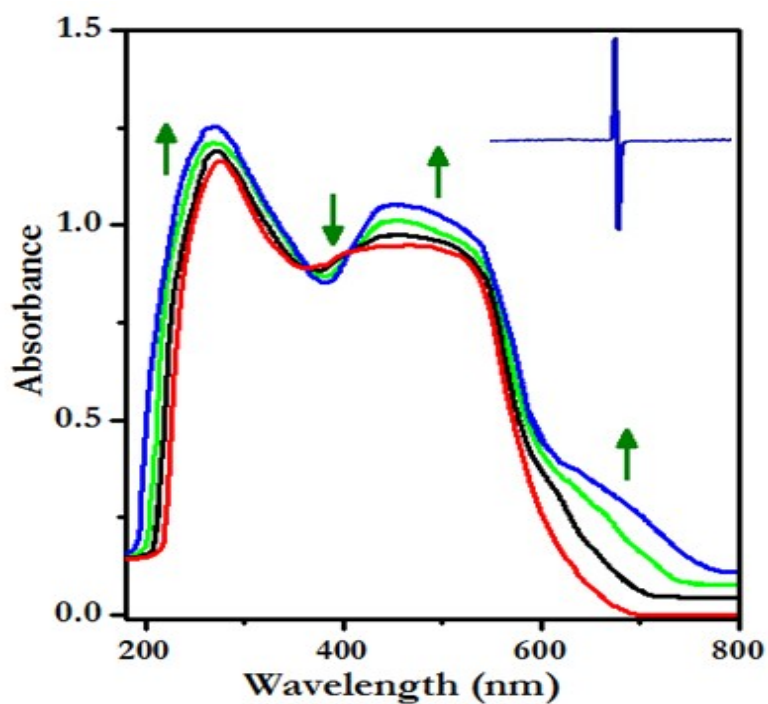


Figure S6. Spectroelectrochemistry of **PP** to **PP_{ox}**, inset shows EPR spectra of **PP_{ox}**.

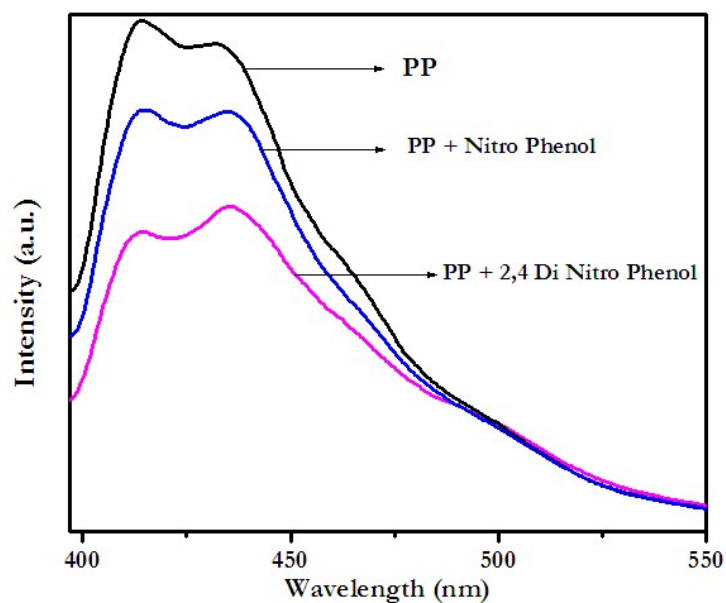


Figure S7. Fluorescence response of **PP** with nitro phenol and di nitro phenol.

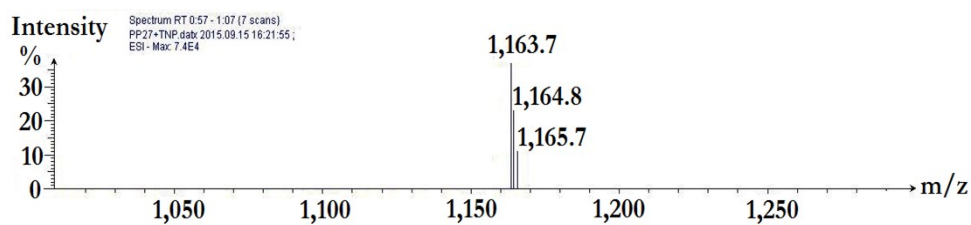


Figure S8. ESI-MS spectrum of **PP...PA** adduct (in methanol).

Table S4. Coordinates of geometry optimized file for **PP**.

Co	-3.469249000	1.943831000	12.464541001
O	-2.614158000	0.849272000	13.778424002
O	-4.327543001	3.064672000	11.167622001
C	-2.021823000	-2.518127000	12.404619001

O	-1.760504000	2.511926000	11.825692001
N	-3.617957000	3.334783000	13.787143002
N	-3.477509000	0.583444000	11.103410001
C	-4.502852001	2.422950000	10.030708001
C	-4.062155000	1.072010000	9.913769001
C	-5.121886001	3.025621000	8.908290001
C	-5.287290001	2.310815000	7.722894001
C	-4.233899001	0.365805000	8.713277001
C	-4.845056001	0.980227000	7.616930001
C	-2.432294000	-1.158750000	12.462543001
C	-1.668329000	-1.064607000	14.809221002
C	-2.262252000	-0.394221000	13.667982002
C	-1.452039000	-3.167387000	13.485307002
C	-1.296354000	-2.397509000	14.670428002
C	-3.020624000	-0.617842000	11.267371001
C	-0.997500000	-4.639807001	13.457660002
C	-1.462066000	-0.305587000	16.140496002
C	-1.776107000	-5.448333001	14.524226002
C	-2.825203000	0.187257000	16.689525002
C	0.518055000	-4.724429001	13.762491002
C	-1.244789000	-5.297628001	12.086440001
C	-0.827781000	-1.195544000	17.230213002

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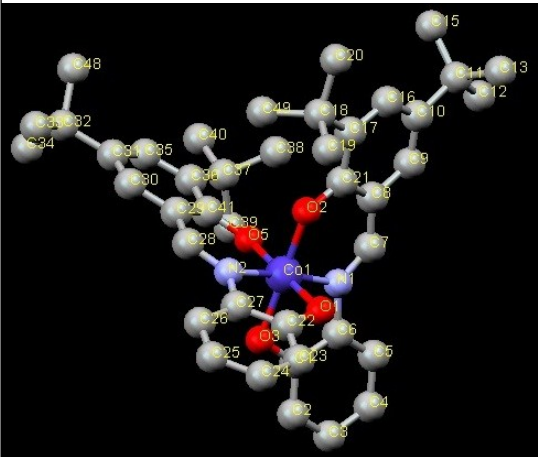
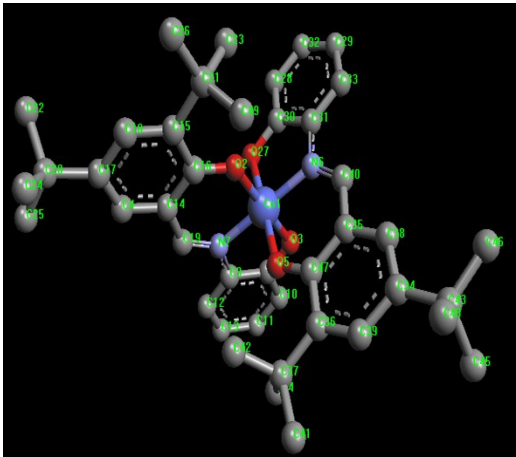
O	-5.180600001	1.349131000	13.085635002
C	-6.874239001	1.898962000	14.687885002
C	-6.521159001	3.826095000	16.133959002
C	-5.625870001	2.120060000	14.056755002
C	-4.833970001	3.221519000	14.495190002
C	-7.309544001	2.741746000	15.709872002
C	-5.285924001	4.061634000	15.524676002
C	0.573560000	5.745879001	13.113213002
C	-1.474131000	4.398868001	13.293862002
C	0.226153000	3.785464000	11.611535001
C	0.738865000	2.880210000	10.467711001
C	-0.651265000	5.483666001	13.700508002
C	0.970812000	4.867591001	12.068354001
C	-2.721837000	4.248164001	13.991091002
C	2.111970000	3.335528000	9.929843001
C	0.904063000	1.425778000	10.976727001
C	1.492822000	6.909530001	13.533866002
C	-0.251319000	2.912861000	9.275653001
C	1.721228000	7.858537001	12.332149001
C	0.891085000	7.735787001	14.686585002
C	-1.054007000	3.517879000	12.238564001
C	2.858004000	6.352615001	14.006798002

C	-0.513212000	0.900437000	15.923262002
H	-2.178257000	-3.041132000	11.457841001
H	-5.465389001	4.060934000	8.997376001
H	-5.768413001	2.793957000	6.865063001
H	-3.892353000	-0.669688000	8.624202001
H	-4.977493001	0.424748000	6.683387001
H	-0.853002000	-2.895838000	15.533384002
H	-3.085574000	-1.315577000	10.421371001
H	-1.446907000	-6.504742001	14.528805002
H	-2.861466000	-5.428065001	14.316536002
H	-1.618977000	-5.046188001	15.540631002
H	-2.675984000	0.728334000	17.643469002
H	-3.494345000	-0.670698000	16.889225002
H	-3.326574000	0.862400000	15.979923002
H	0.763727000	-4.301887001	14.752894002
H	1.103099000	-4.171300000	13.004965002
H	0.856873000	-5.777411001	13.756091002
H	-0.905160000	-6.349189001	12.107026001
H	-0.692754000	-4.783828001	11.279495001
H	-2.316451000	-5.299148001	11.819444001
H	0.172432000	-1.564184000	16.940294002
H	-1.458344000	-2.069187000	17.476866002

H	-0.706220000	-0.605322000	18.156660002
H	-7.483829001	1.053901000	14.353051002
H	-6.869384001	4.484235001	16.935862002
H	-8.278927001	2.554134000	16.185061002
H	-4.678381001	4.907741001	15.858894002
H	-1.029344000	6.113011001	14.509790002
H	1.932995000	5.063521001	11.593438001
H	-2.914728000	4.996805001	14.771641002
H	2.897279000	3.305081000	10.706255001
H	2.078573000	4.358242001	9.513302001
H	2.427011000	2.658170000	9.115064001
H	1.261163000	0.775304000	10.155008001
H	-0.046391000	1.022709000	11.358149001
H	1.652203000	1.384356000	11.790236001
H	0.119700000	2.265241000	8.457994001
H	-0.341843000	3.940077000	8.874908001
H	-1.251967000	2.564335000	9.572258001
H	2.183933000	7.335671001	11.476444001
H	2.391737000	8.692186001	12.615605002
H	0.764806000	8.290816001	11.985874001
H	-0.074593000	8.191567001	14.404755002
H	1.579626000	8.556131001	14.960754002

H	0.729138000	7.121214001	15.589879002
H	2.731156000	5.685870001	14.879363002
H	3.533165000	7.178260001	14.301245002
H	3.363866000	5.775481001	13.212750002
H	0.480696000	0.555388000	15.581663002
H	-0.373080000	1.448792000	16.874669002
H	-0.915373000	1.596990000	15.172226002

Table S5. Correlation between experimental and theoretically calculated bond distances of **PP**.

PP	Exp.	Cald. (UKS)
		
Co1-O1	1.93	1.91
Co1-O2	1.87	1.91
Co1-O3	1.89	1.91
Co1-O5	1.88	1.91
Co1-N1	1.88	1.92
Co1-N2	1.88	1.92
C1-O3	1.31	1.31
C1-C6	1.41	1.42
C6-N1	1.41	1.41
N1-C7	1.29	1.29
C7-C8	1.43	1.43

C8-C21	1.41	1.43
C21-O2	1.31	1.29
O5-C41	1.30	1.29
C41-C29	1.42	1.43
C29-C28	1.43	1.43
C28-N2	1.30	1.29
N2-C27	1.41	1.41
C27-C22	1.40	1.42
C22-O1	1.33	1.31

Table S6. Coordinates of geometry optimized file for **PP_{ox}**.

Co -3.464100000 1.933679000 12.472132001

O -2.616026000 0.851589000 13.786238002

O -4.312311001 3.062367000 11.193450001

C -1.997947000 -2.513109000 12.403633001

O -1.753610000 2.520997000 11.844660001

N -3.627606000 3.336337000 13.791846002

N -3.473839000 0.585077000 11.115789001

C -4.500276001 2.423367000 10.047150001

C -4.067813000 1.074813000 9.928457001

C -5.118818001 3.037706000 8.935190001

C	-5.295886001	2.324229000	7.750295001
C	-4.250010001	0.367932000	8.729838001
C	-4.863740001	0.990569000	7.640877001
C	-2.417335000	-1.156078000	12.468826001
C	-1.669964000	-1.064761000	14.818715002
C	-2.256558000	-0.399141000	13.676581002
C	-1.428724000	-3.160700000	13.484504002
C	-1.286846000	-2.395002000	14.672933002
C	-3.009642000	-0.615292000	11.277786001
C	-0.961435000	-4.628712001	13.453317002
C	-1.479745000	-0.317330000	16.159686002
C	-1.736737000	-5.446020001	14.515383002
C	-2.851261000	0.156831000	16.704078002
C	0.553976000	-4.698168001	13.762809002
C	-1.198984000	-5.282891001	12.078757001
C	-0.847653000	-1.214679000	17.244744002
O	-5.183684001	1.352502000	13.110922002
C	-6.895819001	1.903731000	14.667848002
C	-6.531393001	3.875261000	16.061087002
C	-5.630219001	2.124557000	14.042095002
C	-4.822317001	3.250640000	14.468476002
C	-7.327629001	2.764784000	15.652240002

C	-5.299184001	4.116693000	15.480871002
C	0.564563000	5.728576001	13.129302002
C	-1.487682000	4.401513001	13.320823002
C	0.225879000	3.778972000	11.600837001
C	0.724432000	2.883351000	10.446237001
C	-0.652178000	5.483102001	13.725336002
C	0.961722000	4.848752001	12.065546001
C	-2.718449000	4.263722001	14.005280002
C	2.090126000	3.354808000	9.903937001
C	0.903187000	1.424952000	10.941476001
C	1.496758000	6.878066001	13.543654002
C	-0.278157000	2.926705000	9.263955001
C	1.725717000	7.818087001	12.333767001
C	0.912041000	7.711648001	14.699157002
C	-1.058166000	3.512469000	12.244215001
C	2.855684000	6.294629001	14.005548002
C	-0.537517000	0.897538000	15.965858002
H	-2.147283000	-3.032473000	11.454338001
H	-5.453597001	4.074947000	9.028511001
H	-5.778124001	2.810944000	6.895814001
H	-3.916376000	-0.669363000	8.636980001
H	-5.006488001	0.438237000	6.707459001

H	-0.845018000	-2.894043000	15.535685002
H	-3.075147000	-1.307554000	10.428690001
H	-1.398738000	-6.499202001	14.515596002
H	-2.821715000	-5.434095001	14.305343002
H	-1.584457000	-5.047749001	15.534002002
H	-2.714227000	0.686362000	17.665709002
H	-3.516331000	-0.707785000	16.885444002
H	-3.352205000	0.838548000	16.000515002
H	0.792773000	-4.278042001	14.755931002
H	1.136321000	-4.137079000	13.009153002
H	0.901847000	-5.747763001	13.753144002
H	-0.851092000	-6.331424001	12.097619001
H	-0.647380000	-4.762589001	11.275705001
H	-2.269644000	-5.292722001	11.807903001
H	0.157974000	-1.571344000	16.959496002
H	-1.473327000	-2.095456000	17.476516002
H	-0.739002000	-0.633272000	18.177940002
H	-7.494089001	1.049662000	14.341355002
H	-6.902602001	4.542710001	16.843584002
H	-8.297793001	2.599629000	16.130743002
H	-4.707514001	4.973677001	15.809490002
H	-1.018840000	6.115116001	14.535582002

H	1.922516000	5.052776001	11.593960001
H	-2.916684000	5.011837001	14.781330002
H	2.881871000	3.317339000	10.673011001
H	2.045919000	4.381623001	9.499335001
H	2.400379000	2.689182000	9.078975001
H	1.275987000	0.794685000	10.112721001
H	-0.041909000	0.994112000	11.305547001
H	1.645362000	1.380820000	11.759571001
H	0.101911000	2.303869000	8.433014001
H	-0.390552000	3.959539000	8.885600001
H	-1.271829000	2.550794000	9.550391001
H	2.183005000	7.292314001	11.477322001
H	2.404896000	8.643125001	12.617481002
H	0.772754000	8.260429001	11.992038001
H	-0.048225000	8.181616001	14.422882002
H	1.614361000	8.521660001	14.965384002
H	0.750539000	7.101083001	15.605040002
H	2.725260000	5.629935001	14.878631002
H	3.539143000	7.113273001	14.296274002
H	3.352217000	5.714782001	13.208014002
H	0.459632000	0.564933000	15.622504002
H	-0.404917000	1.430903000	16.926249002

H -0.940389000 1.605825000 15.226342002

Table S7. Bond distances of **PP** and **PP_{ox}** for visualizing quinoidal distortion

Bond distances to be investigated	Distance in PP	Distance in PP_{ox}	Remarks
C35-C38	1.420	1.425	long
C38-C34	1.383	1.376	short
C34-C39	1.421	1.436	long
C39-C36	1.390	1.379	short
C36-C47	1.450	1.461	long
C35-C47	1.437	1.460	long

Detection limit (DL) has been calculated through the following equation^{ref1}:

$$DL = CL \times ET$$

CL = Conc. of Complex **PP**; ET = Conc. of titrant at which change observed.

Thus; detection limit for PA:

$$DL = 1 \times 10^{-5} \times 0.025 \text{ equiv} = 25 \times 10^{-8} \text{ M.}$$

Table S8. Coordinates of geometry optimized file for **PP** with 1,3-DNB.

C	-4.2416626	2.5069179	1.1454874
C	-3.9640056	1.7340880	0.0065021
C	-4.3622905	0.3924760	-0.0078283
C	-5.0567088	-0.1577075	1.0792280
C	-5.3207850	0.6535507	2.1947221
C	-4.8994981	1.9874864	2.2641222
N	-6.0648960	0.0920364	3.3315559
O	-6.2205154	0.8035702	4.3318625
N	-3.7941696	3.9092129	1.1766092
O	-3.5391808	4.4563626	0.1009109
O	-3.6830648	4.4552906	2.2827736
O	-6.5166149	-1.0534724	3.2188120
C	-3.1012223	-0.4966471	4.1971728
C	-2.3571039	0.4346246	3.4575816
C	-1.8328142	0.0701231	2.2037721
C	-1.9986515	-1.2599228	1.6911901
C	-2.7903774	-2.1734243	2.4386693
C	-3.3249565	-1.7891287	3.6755171
N	-1.1147254	0.8903527	1.3252831
C	-1.0164242	2.1925068	1.4399962

C -0.2839570 3.0539883 0.5642057
C 0.5761755 2.5506230 -0.4826344
C 1.3029216 3.5206299 -1.2797354
C 1.0808771 4.8786968 -1.0390097
C 0.1992313 5.3887423 -0.0421731
C -0.4443856 4.4554961 0.7590341
O 0.7483430 1.2833725 -0.7275091
Co -0.3472583 -0.1174230 -0.0869905
O 0.9881757 -0.6517035 1.1408108
C 1.7286950 -1.7178088 1.0349911
C 1.8664146 -2.4785937 -0.1860762
C 2.6742399 -3.6505668 -0.2229242
C 3.3460884 -4.1174232 0.8984236
C 3.2404782 -3.3309898 2.0820737
C 2.4834385 -2.1619396 2.1914328
C 1.2025078 -2.1148344 -1.3994615
N 0.3064509 -1.1665497 -1.5261418
C -0.3243824 -0.8297361 -2.7298634
C -1.4476468 0.0404367 -2.5291502
C -2.2397214 0.3846375 -3.6581078
C -1.8745802 -0.0642302 -4.9342246
C -0.7302770 -0.8686152 -5.1250577

C 0.0430168 -1.2541542 -4.0199991
O -1.6984359 0.4749908 -1.3158761
C 2.4125647 -1.3662904 3.5088917
C 3.3304149 -1.9635592 4.5933087
C 4.1336475 -5.4367914 0.9144397
C 5.5950272 -5.1739017 1.3465721
C 2.2693688 3.0426987 -2.3805443
C 3.3541440 2.1249811 -1.7621984
C -0.0367990 6.9022954 0.0789738
C -1.0087707 7.2334931 1.2272902
O -1.4185536 -1.5736992 0.5560081
C 4.1391666 -6.1098548 -0.4711846
C 3.4616842 -6.4008660 1.9225444
C 2.8603896 0.0966256 3.2622408
C 0.9605876 -1.3896570 4.0463662
C 1.4767308 2.2672725 -3.4614434
C 2.9853320 4.2206903 -3.0697856
C 1.3057081 7.6250595 0.3379694
C -0.6530767 7.4150428 -1.2454614
O 1.0807451 -5.4158401 -2.8751830
N 0.2239050 -5.1961230 -2.0081819
O 0.2826190 -5.6137551 -0.8490825

C -0.9327676 -4.3648817 -2.3814596
C -1.6730176 -3.7417709 -1.3640109
C -2.7556843 -2.9302907 -1.7221505
C -3.1147347 -2.7721574 -3.0684124
C -2.3493722 -3.4172991 -4.0533664
C -1.2334862 -4.2024640 -3.7368645
N -2.7264611 -3.2705342 -5.4669127
O -1.9885450 -3.7790074 -6.3201922
O -3.7735749 -2.6666759 -5.7271199
H -1.3708665 -3.8415563 -0.3163505
H -3.3010915 -2.4002595 -0.9322652
H -3.3942447 2.1578008 -0.8270398
H -4.0987704 -0.2266297 -0.8736690
H 2.7266820 -4.1956961 -1.1757532
H -3.1223717 1.0248958 -3.5100187
H -2.4899141 0.2199777 -5.8015809
H 0.9361295 -1.8793639 -4.1652283
H -0.4474049 -1.1997101 -6.1345156
H 3.7836457 -3.6766643 2.9722374
H 1.4616977 -2.7074409 -2.2972882
H 4.0077281 -7.3667571 1.9655206
H 2.4138354 -6.6071210 1.6233443

H	3.4462052	-5.9753766	2.9463995
H	0.8916598	-0.8154127	4.9943387
H	0.6369528	-2.4306057	4.2530814
H	0.2579819	-0.9474650	3.3194702
H	5.6498660	-4.7207837	2.3570316
H	6.0978913	-4.4845585	0.6374312
H	6.1712625	-6.1224722	1.3732199
H	4.6853369	-7.0738844	-0.4216562
H	4.6430939	-5.4763949	-1.2298886
H	3.1102280	-6.3144933	-0.8288698
H	4.3942758	-1.9764915	4.2785535
H	3.0389574	-2.9989678	4.8642488
H	3.2598807	-1.3480178	5.5131971
H	-2.9506994	-3.1858485	2.0383086
H	-3.5138402	-0.2149649	5.1764754
H	-3.9261433	-2.5105257	4.2498445
H	-2.1791160	1.4417243	3.8621834
H	-1.1253267	4.7780104	1.5590121
H	1.6129011	5.6057453	-1.6676400
H	-1.5582077	2.6827553	2.2708858
H	3.5817223	4.8227663	-2.3536892
H	2.2740401	4.9001848	-3.5824506

H	3.6810406	3.8278111	-3.8389754
H	4.0469543	1.7679010	-2.5533368
H	2.8923280	1.2513797	-1.2671937
H	3.9523253	2.6808892	-1.0103061
H	2.1620820	1.9115404	-4.2594987
H	0.7144138	2.9216143	-3.9326213
H	0.9617510	1.3923028	-3.0290849
H	0.0150302	7.2215083	-2.1089806
H	-0.8339228	8.5094493	-1.1960359
H	-1.6211579	6.9116599	-1.4445076
H	-1.9873921	6.7311595	1.0908083
H	-1.1854725	8.3275410	1.2696644
H	-0.6003940	6.9203645	2.2101334
H	1.7661823	7.2741863	1.2844049
H	1.1508546	8.7217123	0.4151279
H	2.0328876	7.4467097	-0.4798786
H	3.9125705	0.1278696	2.9098169
H	2.7990954	0.6777466	4.2066362
H	2.2207572	0.5792020	2.5009318
H	-0.6335246	-4.6777664	-4.5205494
H	-3.9692485	-2.1556179	-3.3711304
H	-5.0916035	2.5974270	3.1535152

H -5.3934676 -1.2010704 1.0831523

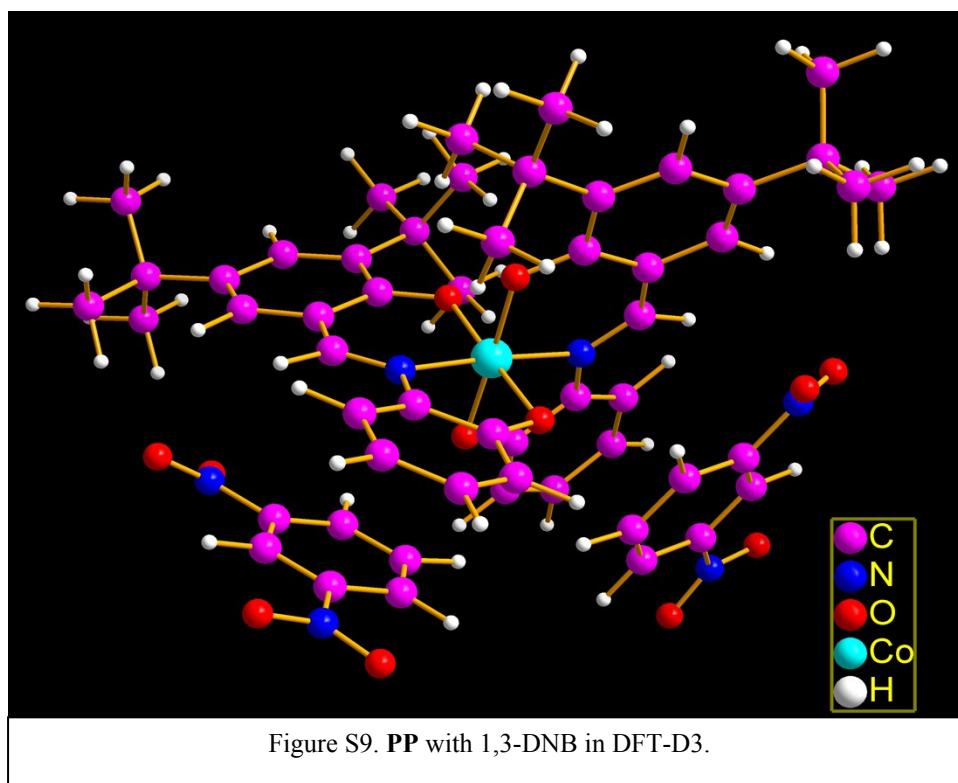


Table S9. Coordinates of geometry optimized file for **PP** with 2,4-DNT.

C -0.9657791 -4.2784233 -3.6512189

C -0.6207974 -4.3608952 -2.3028339

C -1.3564711 -3.6934953 -1.3136237

C -2.4708455 -2.9509972 -1.7044957

C -2.9245068 -2.8923006 -3.0419024

C -2.1253445 -3.5709238 -4.0019087

N 0.5644108 -5.1384929 -1.9148005

O 0.6512893 -5.5046723 -0.7399520
N -2.4463558 -3.5475330 -5.4379375
O -3.5823305 -3.2023998 -5.7845414
O 1.4144200 -5.3720548 -2.7855965
O -1.5632983 -3.8919870 -6.2343652
C 2.9468035 -3.4848545 -0.1897592
C 2.0857211 -2.3515334 -0.1415442
C 1.9136553 -1.6127728 1.0883632
C 2.6784941 -2.0414264 2.2440322
C 3.4866841 -3.1744573 2.1233748
C 3.6344843 -3.9365565 0.9283339
O 1.1318109 -0.5788664 1.2052450
Co -0.1865381 -0.0408680 -0.0359779
O -1.2770039 -1.4832466 0.6088584
C -1.8444070 -1.1607332 1.7505667
C -1.6759987 0.1731716 2.2508857
C -2.2099438 0.5543280 3.4973368
C -2.9552861 -0.3674323 4.2454319
C -3.1625138 -1.6714558 3.7447006
C -2.6150653 -2.0723997 2.5187020
N -0.9398497 0.9803043 1.3753897
C -0.7891621 2.2757850 1.5093094

C	-0.0328539	3.1231935	0.6398966
C	0.8007794	2.6058530	-0.4210406
C	1.5483124	3.5610394	-1.2163996
C	1.3753952	4.9226763	-0.9559340
C	0.5242393	5.4483306	0.0591933
C	-0.1420761	4.5265812	0.8553800
O	0.9328784	1.3371698	-0.6804977
C	2.4829144	3.0632489	-2.3356956
C	3.2223932	4.2251358	-3.0273488
C	0.3414524	6.9672134	0.2042757
C	-0.2701978	7.5205487	-1.1059011
C	1.4028371	-2.0082377	-1.3505602
N	0.4675794	-1.0971541	-1.4719275
C	-0.1777767	-0.7804236	-2.6735396
C	-1.2773570	0.1210336	-2.4807258
C	-2.0491770	0.4909715	-3.6134910
C	-1.7164989	-0.0024807	-4.8816417
C	-0.6124641	-0.8647521	-5.0631854
C	0.1590743	-1.2493732	-3.9580070
C	4.4782972	-5.2208150	0.9305807
C	3.8349876	-6.2309738	1.9119665
C	2.5626657	-1.2683893	3.5718133

C 1.1075420 -1.3570640 4.0944215
O -1.5225813 0.5681793 -1.2689219
C 3.4929603 -1.8447527 4.6569295
C 2.9545461 0.2146617 3.3506981
C 5.9215632 -4.9041523 1.3865293
C 4.5299111 -5.8675940 -0.4665142
C 3.5494891 2.1091886 -1.7409572
C 1.6516653 2.3194812 -3.4100868
C -0.6070002 7.3144843 1.3675203
C 1.7104311 7.6399142 0.4593113
C -4.9862139 0.0169140 1.0738163
C -4.1994216 0.5889107 0.0478625
C -3.7267768 1.8998457 0.0951743
C -4.0006916 2.6650746 1.2372616
C -4.7081583 2.1388025 2.3170932
C -5.2159539 0.8347544 2.2143700
N -3.4996067 4.0440543 1.3137311
O -3.3816393 4.5575441 2.4351388
N -5.9835613 0.3580230 3.3768649
O -6.6087437 -0.7046843 3.2792787
O -5.9814895 1.0558781 4.3995425
O -3.2121751 4.6093513 0.2550511

H	-1.0336505	-3.6947123	-0.2667898
H	-2.9943763	-2.3722385	-0.9329977
H	-3.1035565	2.2941349	-0.7145028
H	-3.9246581	-0.0248962	-0.8190676
H	3.0274005	-4.0153776	-1.1488050
H	-2.9027445	1.1708644	-3.4722563
H	-2.3219879	0.2955455	-5.7520287
H	1.0247491	-1.9126808	-4.0989019
H	-0.3577906	-1.2366841	-6.0658187
H	4.0385361	-3.5094005	3.0123081
H	1.6874274	-2.5837989	-2.2516187
H	4.4203399	-7.1740322	1.9448938
H	2.8006244	-6.4742408	1.5943909
H	3.7886494	-5.8254475	2.9429803
H	1.0076971	-0.8007618	5.0502878
H	0.8238843	-2.4131439	4.2825075
H	0.3943425	-0.9314490	3.3677956
H	5.9447037	-4.4674093	2.4053730
H	6.4035115	-4.1814283	0.6963220
H	6.5373126	-5.8277755	1.4042188
H	5.1200289	-6.8058849	-0.4275196
H	5.0115896	-5.1975413	-1.2081122

H	3.5155720	-6.1136013	-0.8392652
H	4.5596736	-1.8094437	4.3537231
H	3.2413328	-2.8953900	4.9085226
H	3.3879073	-1.2472999	5.5854215
H	-2.7628909	-3.0929901	2.1348826
H	-3.3801495	-0.0714450	5.2151040
H	-3.7554002	-2.3908567	4.3309119
H	-2.0387604	1.5676710	3.8887610
H	-0.8033020	4.8610768	1.6667875
H	1.9237721	5.6397750	-1.5820294
H	-1.3015246	2.7736318	2.3539628
H	3.8486642	4.8029683	-2.3167828
H	2.5230908	4.9301192	-3.5218092
H	3.8929447	3.8185004	-3.8116194
H	4.2195105	1.7383472	-2.5453190
H	3.0694734	1.2453680	-1.2460598
H	4.1750981	2.6410519	-0.9939660
H	2.3143848	1.9534161	-4.2225349
H	0.8993490	2.9985610	-3.8617451
H	1.1200056	1.4547719	-2.9772178
H	0.3823101	7.3175102	-1.9791080
H	-0.4130244	8.6196228	-1.0385416

H	-1.2568698	7.0535338	-1.3023693
H	-1.6031834	6.8468941	1.2344034
H	-0.7464557	8.4131225	1.4270706
H	-0.1993235	6.9738432	2.3414541
H	2.1678699	7.2599637	1.3959445
H	1.5944196	8.7400808	0.5532865
H	2.4227882	7.4479962	-0.3684354
H	4.0078862	0.2924303	3.0090453
H	2.8617242	0.7788937	4.3027706
H	2.3034044	0.6831566	2.5903343
H	-0.3619823	-4.7649380	-4.4246574
C	-4.1858141	-2.1372020	-3.3458871
H	-4.8865450	2.7278141	3.2228010
C	-5.5175750	-1.3741209	0.8813767
H	-5.2693921	-2.0270654	1.7369732
H	-6.6229062	-1.3660607	0.8008683
H	-5.0963182	-1.8118425	-0.0425686
H	-4.9999253	-2.8343284	-3.6295902
H	-4.5032427	-1.5634034	-2.4555060
H	-4.0544039	-1.4417954	-4.1934502

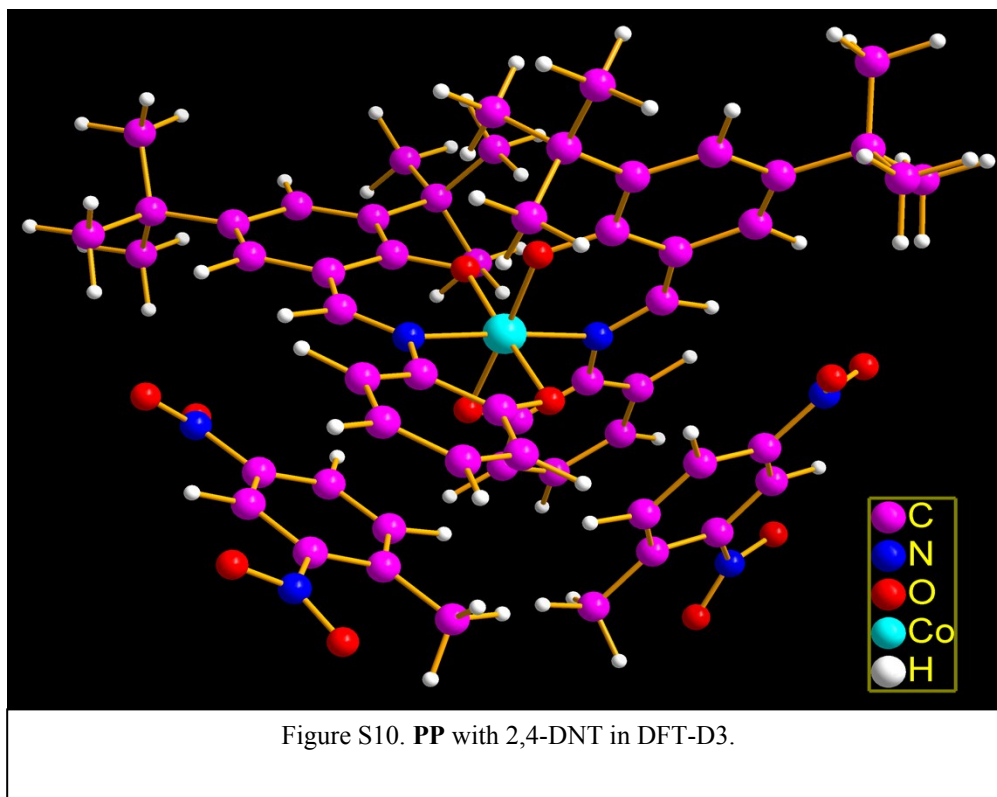


Table S10. Coordinates of geometry optimized file for PP with 3,4-DNT.

C	-2.4496397	5.4375100	0.5776578
C	-1.9649907	4.7303615	-0.5443886
C	-2.3314252	3.3950098	-0.7280537
C	-3.1690141	2.7722742	0.2081646
C	-3.6843279	3.4677465	1.3192848
C	-3.2961022	4.8115674	1.4984430
N	-0.9511712	5.2888345	-1.4487872

O -1.0831926 5.0687624 -2.6540639
H -3.6661013 5.3994343 2.3488848
O 0.0004831 5.8938560 -0.9387133
C 1.7195362 3.3794969 -2.5889976
C 1.2610206 2.3118735 -1.7642185
C 1.2498663 0.9555039 -2.2618146
C 1.7443292 0.7246469 -3.6049797
C 2.1629255 1.8242803 -4.3581788
C 2.1513824 3.1710840 -3.8924692
O 0.8383730 -0.0648521 -1.5668624
Co -0.1506806 0.0219575 0.0335786
O -1.6791895 0.4858815 -1.0263352
C -2.2598662 -0.5921978 -1.5065273
C -1.7294190 -1.8778700 -1.1538482
C -2.3247855 -3.0606733 -1.6317017
C -3.4601195 -2.9861557 -2.4504084
C -3.9889707 -1.7250978 -2.8083782
C -3.4011656 -0.5403201 -2.3507050
N -0.6391282 -1.7849337 -0.2785513
C -0.0650634 -2.8096817 0.3030231
C 0.9885844 -2.7392581 1.2703690
C 1.6626849 -1.5056266 1.6039103

C 2.7108845 -1.5580854 2.6039352
C 2.9841436 -2.7827686 3.2183386
C 2.3087326 -4.0016768 2.9206335
C 1.3364756 -3.9533613 1.9297717
O 1.3951338 -0.3626437 1.0408254
C 3.4705262 -0.2720797 2.9825533
C 4.5596092 -0.5369266 4.0400798
C 2.6317314 -5.2771579 3.7150833
C 2.2918826 -5.0335133 5.2057892
C 0.7906286 2.6629505 -0.4584521
N 0.1867279 1.8569686 0.3809302
C -0.3494014 2.2536974 1.6132653
C -1.0783290 1.1998223 2.2587761
C -1.7181297 1.4794366 3.4959676
C -1.6384669 2.7610272 4.0525785
C -0.9210713 3.7925697 3.4049839
C -0.2685082 3.5348130 2.1916054
C 2.5591524 4.3165036 -4.8326779
C 1.5841933 4.3430677 -6.0351175
C 1.7727892 -0.7076143 -4.1728828
C 0.3304007 -1.2707307 -4.2298349
O -1.1366001 0.0217989 1.6769050

C 2.3555833 -0.7499701 -5.5988507
C 2.6541797 -1.6090829 -3.2716406
C 4.0013315 4.0892209 -5.3428097
C 2.4935442 5.6824911 -4.1236215
C 4.1608734 0.3163509 1.7260410
C 2.4761900 0.7610643 3.5694968
C 1.8051655 -6.4784571 3.2183196
C 4.1343898 -5.6157819 3.5771491
C -4.8328080 -1.8639887 0.5708600
C -3.7074279 -1.4873588 1.3292760
C -2.8388629 -2.4389699 1.8826275
C -3.0688090 -3.7975581 1.6534045
C -4.1758649 -4.1947810 0.8720287
C -5.0438531 -3.2383921 0.3353586
N -2.0439847 -4.7471360 2.1080258
O -1.6469051 -5.5937868 1.2976882
H -5.9035753 -3.5869392 -0.2520889
O -1.6027482 -4.6005434 3.2492844
H -1.9035334 2.8037039 -1.5472427
H -3.3788703 1.7042454 0.0622281
H -1.9407756 -2.1047602 2.4169085
H -3.4565878 -0.4288370 1.4794019

H	1.6876435	4.3918312	-2.1627984
H	-2.2764728	0.6730956	3.9949568
H	-2.1458241	2.9678336	5.0078775
H	0.2763760	4.3434095	1.6831610
H	-0.8793357	4.8004925	3.8425099
H	2.5127467	1.6428366	-5.3836763
H	0.9239401	3.7199201	-0.1625149
H	1.8526609	5.1578098	-6.7401859
H	0.5439884	4.5119899	-5.6892645
H	1.6047918	3.3883312	-6.5987927
H	0.3380212	-2.3036804	-4.6374382
H	-0.3060177	-0.6473447	-4.8916124
H	-0.1296234	-1.2940480	-3.2265406
H	4.0957347	3.1317526	-5.8939913
H	4.7195095	4.0670027	-4.4974749
H	4.3051389	4.9045028	-6.0323929
H	2.7640936	6.4905927	-4.8333378
H	3.2004482	5.7331914	-3.2701444
H	1.4767144	5.8916042	-3.7351483
H	3.3980268	-0.3718236	-5.6347033
H	1.7502345	-0.1575693	-6.3152561
H	2.3666231	-1.7984451	-5.9602297

H	-3.8101382	0.4438275	-2.6245074
H	-3.9388798	-3.9107937	-2.8037829
H	-4.8798540	-1.6720520	-3.4536783
H	-1.9222693	-4.0429974	-1.3450647
H	0.7773706	-4.8562983	1.6475770
H	3.7621750	-2.8076330	3.9934870
H	-0.4406272	-3.8222439	0.0661186
H	5.3195930	-1.2622662	3.6834190
H	4.1349201	-0.9225461	4.9896161
H	5.0850352	0.4118311	4.2722439
H	4.7001165	1.2508274	1.9894956
H	3.4169700	0.5406402	0.9398579
H	4.9019459	-0.4016135	1.3167922
H	3.0110972	1.6948302	3.8437996
H	1.9940495	0.3621074	4.4859540
H	1.6843921	1.0109814	2.8420814
H	2.8756109	-4.1891630	5.6251830
H	2.5181188	-5.9355649	5.8124454
H	1.2151819	-4.7957572	5.3257880
H	0.7167570	-6.2837761	3.2953849
H	2.0386084	-7.3759228	3.8267164
H	2.0334260	-6.7203473	2.1599856

H	4.4018854	-5.7967841	2.5157243
H	4.3838919	-6.5293711	4.1565421
H	4.7770843	-4.7945639	3.9539290
H	3.6991643	-1.2352743	-3.2501871
H	2.6701291	-2.6460837	-3.6688778
H	2.2654631	-1.6272584	-2.2370611
N	-2.1451726	6.8564662	0.7828928
C	-4.6390819	2.8061276	2.2735402
N	-4.4971219	-5.6082154	0.6549862
C	-5.7983280	-0.8362754	0.0495841
O	-5.0198814	-5.9142951	-0.4223237
O	-4.2513552	-6.4007844	1.5707241
H	-6.2669165	-1.1629425	-0.8972985
H	-6.6109839	-0.6639395	0.7878888
H	-5.2927285	0.1317912	-0.1262058
O	-2.0387832	7.2527954	1.9487920
O	-2.0410653	7.5726810	-0.2185824
H	-4.5701277	3.2434003	3.2869034
H	-5.6851322	2.9322520	1.9199671
H	-4.4379468	1.7206736	2.3469129

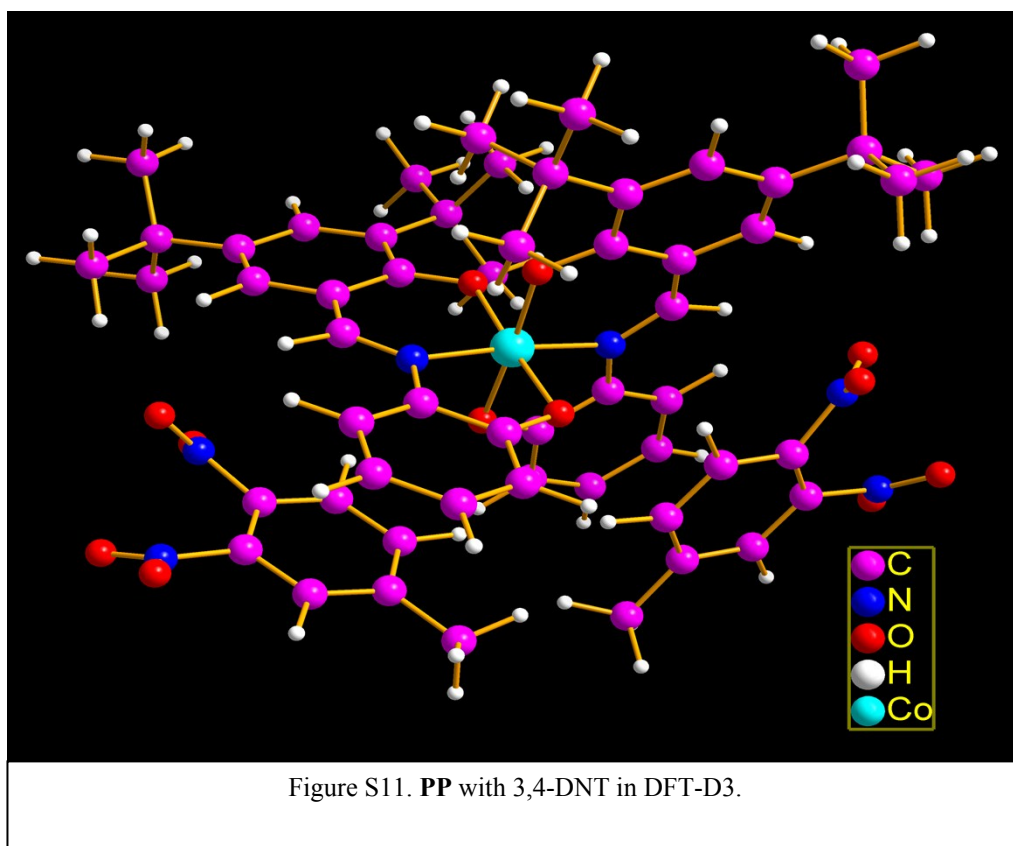


Table S11. Coordinates of geometry optimized file for **PP** with 3,5-DNBA.

C	-0.471747	-4.965077	-3.900542
C	-0.396256	-4.751732	-2.524930
C	-1.392278	-4.013530	-1.781159
C	-2.518337	-3.574513	-2.577559
C	-2.599934	-3.787251	-3.952887
C	-1.572732	-4.475675	-4.605095
N	0.788971	-5.299708	-1.854552

O	0.706245	-5.631696	-0.673194
N	-1.645311	-4.670285	-6.051486
O	-2.578402	-4.129799	-6.658670
O	1.816367	-5.414458	-2.544984
O	-0.765039	-5.352088	-6.590759
C	2.983144	-3.318518	-0.621452
C	1.965718	-2.324418	-0.525269
C	1.707273	-1.673933	0.735167
C	2.504774	-2.053004	1.881617
C	3.464886	-3.051200	1.712141
C	3.727519	-3.716978	0.479459
O	0.802763	-0.750659	0.903636
Co	-0.496887	-0.233237	-0.322145
O	-1.643195	-1.650911	0.279840
C	-2.312482	-1.312274	1.384641
C	-2.068914	-0.005148	1.911716
C	-2.642962	0.379828	3.139872
C	-3.522879	-0.489870	3.795741
C	-3.823990	-1.749884	3.234591
C	-3.218777	-2.169952	2.042848
N	-1.233118	0.781188	1.104680
C	-0.975618	2.053528	1.307724

C	-0.140944	2.876961	0.489053
C	0.631833	2.351455	-0.608827
C	1.489830	3.254743	-1.344109
C	1.463086	4.607597	-1.003411
C	0.647770	5.162342	0.025750
C	-0.114448	4.274221	0.772542
O	0.615616	1.101534	-0.976354
C	2.374107	2.712485	-2.483390
C	3.241924	3.821971	-3.108494
C	0.632552	6.681675	0.263066
C	0.385486	7.413970	-1.077628
C	1.203039	-2.054483	-1.703547
N	0.154009	-1.266910	-1.775745
C	-0.593690	-1.040489	-2.941020
C	-1.750404	-0.225270	-2.732107
C	-2.658190	-0.025042	-3.794511
C	-2.386041	-0.583518	-5.049718
C	-1.202442	-1.319568	-5.274917
C	-0.301522	-1.538582	-4.225901
C	4.739390	-4.872474	0.433925
C	4.195373	-6.023878	1.315407
C	2.263108	-1.373682	3.243197

C	0.816386	-1.663028	3.717765
O	-1.904291	0.311069	-1.519874
C	3.229127	-1.899721	4.322590
C	2.482894	0.155270	3.114383
C	6.109131	-4.402151	0.974354
C	4.927884	-5.407185	-0.997735
C	3.324841	1.618441	-1.933622
C	1.478765	2.121718	-3.602539
C	-0.494389	7.079631	1.235332
C	1.996660	7.120724	0.845016
C	-5.710466	0.633281	1.822118
C	-4.973178	0.749850	0.645616
C	-4.152239	1.901192	0.346422
C	-4.212613	2.943394	1.345472
C	-4.936595	2.827334	2.530874
C	-5.679436	1.668399	2.760582
N	-3.459614	4.190105	1.175070
O	-3.043766	4.737157	2.209997
N	-6.413846	1.520104	4.015513
O	-6.988973	0.444536	4.222447
O	-6.404963	2.470275	4.808092
O	-3.295943	4.636111	0.040111

H	-1.341476	-3.757900	-0.712481
C	-3.706455	-3.020911	-1.957557
H	-3.534997	1.914951	-0.563975
C	-5.188206	-0.294387	-0.337152
H	3.128349	-3.796727	-1.599014
H	-3.568327	0.561330	-3.613963
H	-3.101469	-0.436476	-5.872704
H	0.615593	-2.117426	-4.402716
H	-0.990160	-1.727734	-6.272962
H	4.051251	-3.354377	2.590111
H	1.516703	-2.590416	-2.618349
H	4.894382	-6.886561	1.311143
H	3.212346	-6.366450	0.932738
H	4.059083	-5.702832	2.368139
H	0.631482	-1.176632	4.698452
H	0.657012	-2.754304	3.839277
H	0.072850	-1.281523	2.996583
H	6.040635	-4.042568	2.020841
H	6.514192	-3.574471	0.356355
H	6.841226	-5.236292	0.955565
H	5.646887	-6.251616	-0.992997
H	5.329763	-4.625311	-1.674685

H	3.972399	-5.770851	-1.424605
H	4.290544	-1.714923	4.057871
H	3.102866	-2.987162	4.501447
H	3.027671	-1.379318	5.280864
H	-3.431279	-3.155290	1.608310
H	-3.977195	-0.190275	4.751007
H	-4.530347	-2.419943	3.747345
H	-2.409359	1.359231	3.580243
H	-0.752305	4.632900	1.591379
H	2.102838	5.294153	-1.574003
H	-1.460559	2.551553	2.168281
H	3.920387	4.288445	-2.364997
H	2.627536	4.624422	-3.565666
H	3.871837	3.387527	-3.911009
H	3.959303	1.219954	-2.753080
H	2.755921	0.782488	-1.487614
H	3.995473	2.040353	-1.156521
H	2.109332	1.732936	-4.429603
H	0.810861	2.902968	-4.020906
H	0.852848	1.295198	-3.222384
H	1.184913	7.211205	-1.817975
H	0.352788	8.511633	-0.916669

H	-0.580604	7.101914	-1.524855
H	-1.474114	6.729630	0.853041
H	-0.529294	8.182637	1.345240
H	-0.346833	6.646742	2.245063
H	2.188935	6.620596	1.816334
H	2.019864	8.218565	1.010182
H	2.830247	6.863141	0.159829
H	3.526132	0.373594	2.805213
H	2.305603	0.647603	4.093633
H	1.797600	0.594162	2.366847
H	0.331480	-5.501866	-4.418367
H	-3.483847	-3.437241	-4.496174
H	-4.905686	3.631450	3.275311
H	-6.325566	-0.258020	1.983778
O	-4.781135	-2.604059	-2.752099
O	-3.769605	-2.918379	-0.743515
H	-5.474704	-2.268880	-2.196116
O	-5.988092	-1.399072	-0.021156
O	-4.672084	-0.210331	-1.439401
H	-6.026938	-1.985720	-0.767370

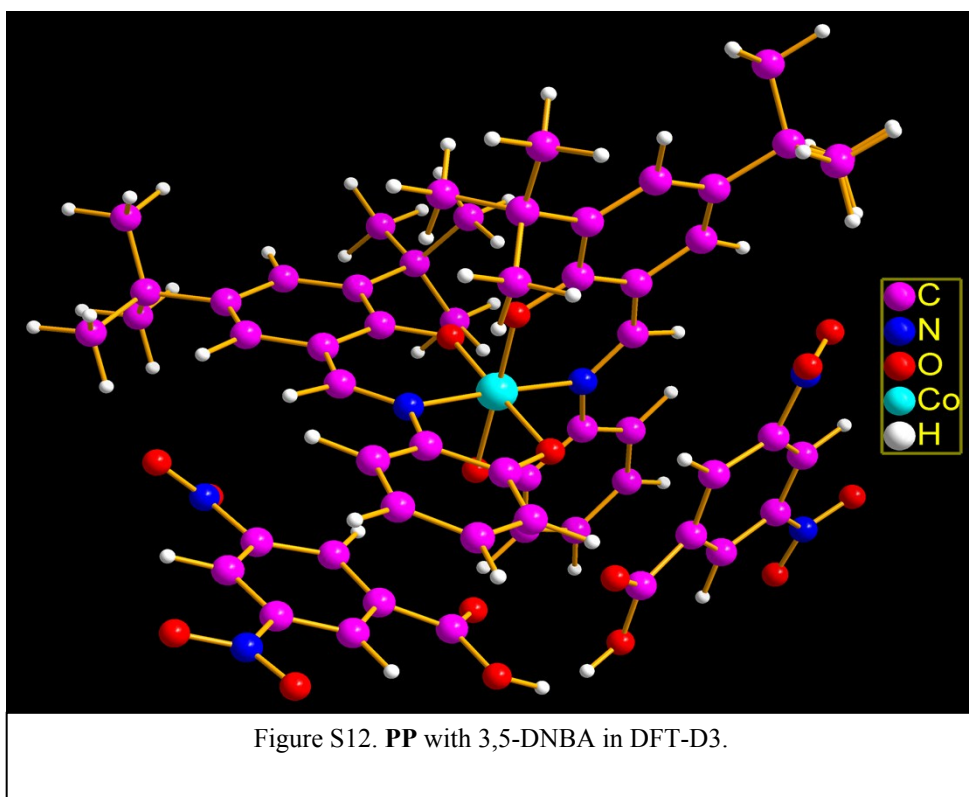


Table S12. Coordinates of geometry optimized file for **PP** with NB.

C	5.6787759	0.5484195	-2.0635071
C	5.1856020	0.8711111	-0.7897648
C	4.0797191	1.7244136	-0.6985036
C	3.4945836	2.2536801	-1.8607638
C	4.0184684	1.9365058	-3.1283496
C	5.1113334	1.0689057	-3.2397037
N	6.8105858	-0.3775543	-2.1712574
O	7.1565383	-0.7527346	-3.3008456
O	7.3771807	-0.7365181	-1.1301079

C 4.2287797 -2.3377462 -2.2455766

C 3.1240338 -1.5125492 -2.5014856

C 2.4038109 -0.9548655 -1.4289544

C 2.7620509 -1.2465141 -0.0704001

C 3.8957334 -2.0697405 0.1650499

C 4.6124421 -2.6038024 -0.9128966

O 2.0388259 -0.7330467 0.8988096

Co 0.5072726 0.1748606 0.1848482

O 1.2855584 1.9231393 0.3094185

C 0.8529041 2.5439524 1.3833946

C 0.0339207 1.8229029 2.3150199

C -0.4854568 2.4550811 3.4598646

C -0.1742408 3.7982534 3.7165957

C 0.6590046 4.5086115 2.8249086

C 1.1701681 3.8981092 1.6730389

N 1.3020072 -0.0936763 -1.5170885

C 0.8899437 0.4868582 -2.6176374

C -0.2812436 1.3049936 -2.7435478

C -1.2131126 1.5035417 -1.6563302

C -2.4053076 2.2863115 -1.9194005

C -2.5748232 2.8333451 -3.1923818

C -1.6562112 2.6688670 -4.2697145

C -0.5277469 1.8966209 -4.0175373
O -1.0522579 1.0083669 -0.4646610
C -3.4391307 2.5054581 -0.7980886
C -2.7792841 3.2792531 0.3706839
C -1.9489283 3.3311931 -5.6264374
C -3.2950298 2.8018459 -6.1771283
N -0.1627213 0.4894386 1.9318933
C -0.7052252 -0.4351138 2.6861319
C -0.9979852 -1.7792875 2.2810119
C -1.5457751 -2.6512226 3.2676450
C -1.9170309 -3.9591589 2.9765516
C -1.7388769 -4.3920125 1.6302687
C -1.2101402 -3.5999929 0.6096891
C -0.8006056 -2.2454012 0.9269087
O -0.2907776 -1.5186276 -0.0232235
C -1.0420114 -4.1322760 -0.8264621
C -1.8329354 -3.2348999 -1.8122458
C -2.5043149 -4.9287348 4.0159038
C -2.6111118 -4.2811937 5.4087809
C -4.6507620 3.3242248 -1.2845818
C -3.9635361 1.1361932 -0.2955428
C -2.0395435 4.8647615 -5.4372825

C	-0.8480635	3.0320240	-6.6605504
C	-1.5942612	-6.1759750	4.1246307
C	-3.9204230	-5.3643039	3.5680354
C	0.4603199	-4.1357749	-1.2053477
C	-1.5710749	-5.5724439	-0.9716762
C	2.2857412	-0.1669104	3.9342669
C	1.6728635	0.1102085	5.1708620
C	1.7348906	1.3995989	5.7122360
C	2.4376333	2.3918134	5.0065376
C	3.0746432	2.1295476	3.7837573
C	2.9853942	0.8394036	3.2479334
N	2.4901420	3.7503557	5.5557405
O	1.8226935	3.9997346	6.5700506
O	3.2063231	4.5862780	4.9880824
H	1.1239506	-0.6781569	5.7069602
H	3.5587881	2.3506461	-4.0379800
H	2.1933122	-1.1572040	3.4686557
H	3.4080752	0.6101522	2.2616794
H	2.6005723	2.8841051	-1.7631008
H	3.6182028	1.9450623	0.2721434
H	-1.6707947	-2.2426356	4.2812092
H	1.8152310	4.4487643	0.9716198

H	0.9131512	5.5586345	3.0376025
H	-1.1361771	1.9000396	4.1511716
H	-0.5727399	4.2914815	4.6150385
H	-2.0371969	-5.4196335	1.3821538
H	-0.9775919	-0.1664654	3.7242270
H	-2.0044736	-6.8965737	4.8629714
H	-0.5730269	-5.8905573	4.4507234
H	-1.5045714	-6.7041469	3.1539515
H	0.5932041	-4.5158280	-2.2404954
H	1.0329209	-4.7978646	-0.5233275
H	0.8918134	-3.1212824	-1.1467437
H	-3.9010238	-5.8668034	2.5799758
H	-4.5950741	-4.4871712	3.4890568
H	-4.3611615	-6.0749570	4.2984779
H	-3.0329998	-5.0081071	6.1322939
H	-3.2750663	-3.3929048	5.3991881
H	-1.6192724	-3.9640288	5.7906496
H	-2.6510949	-5.6467900	-0.7283609
H	-1.0223225	-6.2864968	-0.3237270
H	-1.4406383	-5.9082681	-2.0207004
H	4.1871983	-2.2786691	1.2055998
H	4.7976981	-2.7679001	-3.0825879

H	5.4897405	-3.2393901	-0.7160616
H	2.8218391	-1.3047564	-3.5382803
H	0.2167198	1.7129823	-4.8061335
H	-3.4753608	3.4341321	-3.3784036
H	1.4822489	0.3346347	-3.5395436
H	-5.1860517	2.8231375	-2.1173720
H	-4.3601070	4.3397163	-1.6238764
H	-5.3705874	3.4466458	-0.4496626
H	-4.7019230	1.2872894	0.5203170
H	-3.1326901	0.5126731	0.0816082
H	-4.4698074	0.5880422	-1.1173450
H	-3.5147214	3.4397515	1.1872947
H	-2.4257286	4.2740767	0.0292915
H	-1.9154427	2.7278914	0.7809270
H	-2.8397660	5.1425438	-4.7219526
H	-2.2618040	5.3661807	-6.4026715
H	-1.0826382	5.2704574	-5.0493721
H	0.1400116	3.4116142	-6.3294163
H	-1.0910123	3.5239685	-7.6243311
H	-0.7506992	1.9442793	-6.8535256
H	-3.2540802	1.7034056	-6.3270654
H	-3.5324448	3.2753959	-7.1529317

H -4.1343626 3.0184303 -5.4859454

H -2.9161421 -3.2523063 -1.5705826

H -1.7083358 -3.6082163 -2.8509441

H -1.4793635 -2.1891141 -1.7603758

H 1.2448139 1.6555152 6.6599659

H 3.5990497 2.9403209 3.2643900

H 5.5259573 0.7794169 -4.2134080

H 5.6538576 0.4287347 0.0975134

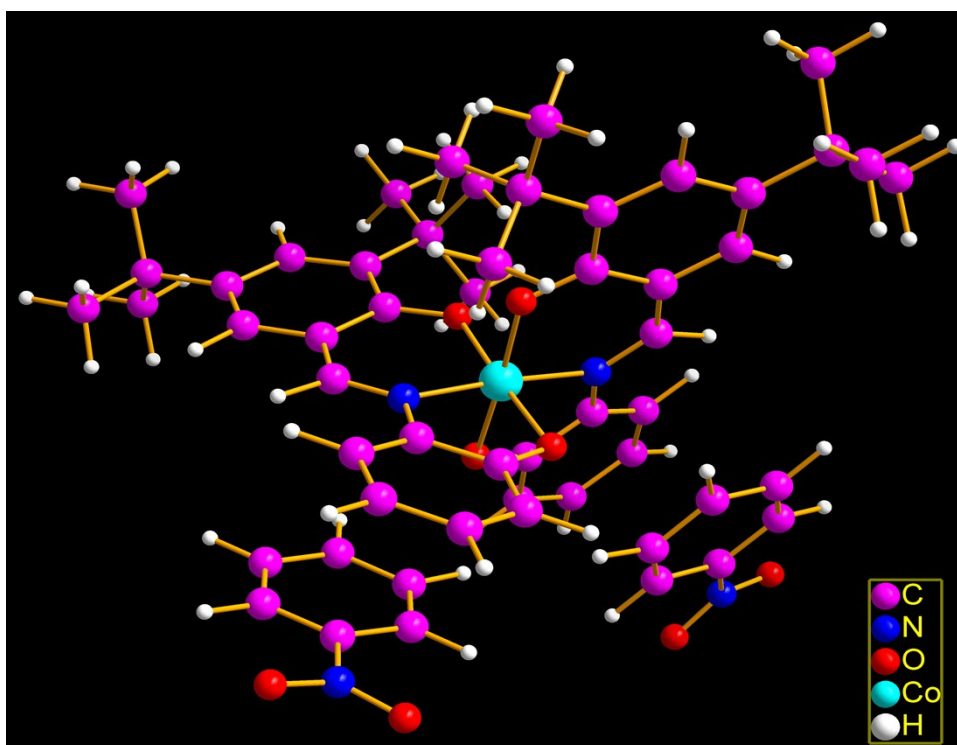


Figure S13. **PP** with NB in DFT-D3.

Table S13. Coordinates of geometry optimized file for **PP** with PA.

C	-2.4772336	-3.6080290	-2.5108389
C	-1.3762471	-4.0420958	-1.6728343
C	-0.3638530	-4.7985135	-2.3811701
C	-0.4050342	-5.0369899	-3.7533461
C	-1.4888304	-4.5611092	-4.4938625
C	-2.5295940	-3.8581098	-3.8800015
O	-1.2243379	-3.7943258	-0.4153930
N	0.8054940	-5.3306314	-1.6725225
O	0.6985746	-5.6350763	-0.4856450
N	-1.5253669	-4.7793570	-5.9374589
O	-0.6206194	-5.4537174	-6.4460552
N	-3.6807628	-2.9892626	-1.9306384
O	-4.6092080	-2.7106584	-2.6931876
O	1.8494906	-5.4589668	-2.3366570
O	-2.4520178	-4.2634838	-6.5753567
O	-3.7142040	-2.8246761	-0.7085455
C	-0.9612544	-1.3892480	-5.0731614
C	-0.1139935	-1.6006661	-3.9786940
C	-0.4677414	-1.0894830	-2.7142473
C	-1.6424038	-0.2901746	-2.5688073
C	-2.4952114	-0.0941806	-3.6741995

C -2.1553752 -0.6538429 -4.9130278
N 0.2402963 -1.2756782 -1.5166809
Co -0.4590550 -0.1962256 -0.1146072
O -1.8643315 0.2392518 -1.3601883
C 1.2858408 -2.0599197 -1.3865667
C 2.0170827 -2.2814861 -0.1788882
C 1.7508333 -1.5511989 1.0350508
C 2.5405849 -1.8551787 2.2087964
C 3.4875940 -2.8759193 2.1153876
C 3.7450632 -3.6320633 0.9347783
C 3.0186269 -3.2958765 -0.1984767
O 0.8462345 -0.6179478 1.1387311
C 2.3053275 -1.0740705 3.5159050
C 3.2651558 -1.5286769 4.6326067
C 4.7467311 -4.7966214 0.9752508
C 4.2201260 -5.8579531 1.9722633
O 0.5945230 1.1557524 -0.8264641
C 0.6240101 2.4036074 -0.4495435
C -0.0588010 2.9076014 0.7154817
C 0.0520746 4.2840461 1.0689499
C 0.7653737 5.1861087 0.2933478
C 1.4313301 4.6658161 -0.8545191

C	1.3997311	3.3277135	-1.2474105
C	-0.9084253	2.0926816	1.5244193
N	-1.2267830	0.8409480	1.2850307
C	-2.0862949	0.0731068	2.0881878
C	-2.2927758	-1.2540796	1.6047555
C	-3.2116983	-2.1022216	2.2553370
C	-3.8764633	-1.6456273	3.4009559
C	-3.6199606	-0.3592076	3.9221570
C	-2.7211035	0.4960748	3.2726319
C	0.7790616	6.6978570	0.5678458
C	-0.0349463	7.3871340	-0.5556172
C	2.1391847	2.8258795	-2.5023937
C	1.1131021	2.2640416	-3.5187810
O	-1.5744748	-1.6215662	0.5375471
C	2.9194570	3.9593780	-3.1963110
C	3.1551899	1.7231119	-2.1093424
C	2.2285430	7.2335149	0.5729881
C	0.1220528	7.0371553	1.9186950
C	2.5430720	0.4383485	3.2725321
C	0.8554457	-1.3094565	4.0099794
C	4.8986525	-5.4623272	-0.4048881
C	6.1308027	-4.2868723	1.4390286

O	-3.1948910	2.1513588	-0.7652706
C	-3.9776836	2.1089208	0.2610623
C	-4.0096864	3.2228745	1.1855398
C	-4.7383845	3.2092154	2.3727107
C	-5.5121976	2.0889079	2.6844150
C	-5.5808389	0.9949726	1.8170213
C	-4.8443128	1.0086708	0.6349111
N	-3.2383644	4.4445267	0.9184655
O	-2.9976697	4.7522786	-0.2477178
N	-6.2501918	2.0533493	3.9441935
O	-6.2202205	3.0601420	4.6634349
N	-5.1158161	-0.1020928	-0.2946792
O	-5.8552626	-1.0085718	0.0936018
O	-2.8938933	5.1141552	1.9065371
O	-6.8529627	1.0109394	4.2304843
O	-4.6362190	-0.0355462	-1.4295558
H	-0.4937549	4.6198335	1.9603633
H	-3.3904263	-3.1071052	1.8509610
H	-4.5973437	-2.3060604	3.9060563
H	-2.5313049	1.4997629	3.6773586
H	-4.1298977	-0.0251870	4.8368883
H	2.0001448	5.3700362	-1.4764084

H	-1.3543120	2.5831955	2.4094630
H	-0.0754879	8.4855651	-0.3975690
H	-1.0707018	6.9911156	-0.5687143
H	0.4137752	7.2030044	-1.5531297
H	1.6361979	1.8968363	-4.4264617
H	0.3990234	3.0547325	-3.8280881
H	0.5381699	1.4261616	-3.0878685
H	2.7411631	7.0580649	-0.3941105
H	2.8277766	6.7454962	1.3691730
H	2.2356610	8.3277216	0.7586944
H	0.1519941	8.1329441	2.0873349
H	0.6513473	6.5496335	2.7632929
H	-0.9379557	6.7166620	1.9428360
H	3.6881533	4.4041450	-2.5313456
H	2.2513471	4.7737994	-3.5438236
H	3.4411458	3.5542197	-4.0870319
H	-3.4121297	0.4941782	-3.5431876
H	-0.6935703	-1.7959928	-6.0587501
H	-2.8232247	-0.5034175	-5.7745265
H	0.8161050	-2.1713231	-4.1069371
H	3.1688898	-3.8370087	-1.1420599
H	4.0676194	-3.1221700	3.0151149

H	1.6230927	-2.6288274	-2.2729246
H	4.3284889	-1.3768808	4.3551870
H	3.1258921	-2.5978705	4.8930639
H	3.0699312	-0.9351783	5.5486749
H	2.3706042	1.0054987	4.2113496
H	1.8640780	0.8291677	2.4928909
H	3.5892896	0.6211157	2.9503865
H	0.6777560	-0.7493996	4.9519919
H	0.6825148	-2.3862505	4.2144026
H	0.1162009	-0.9751792	3.2614088
H	4.1142895	-5.4426786	2.9949680
H	4.9147616	-6.7222906	2.0280139
H	3.2258597	-6.2291860	1.6499632
H	3.9278082	-5.8361761	-0.7861467
H	5.5969506	-6.3210103	-0.3344036
H	5.3088859	-4.7553195	-1.1551887
H	6.5273442	-3.5268797	0.7347206
H	6.8575982	-5.1244993	1.4876522
H	6.0850207	-3.8256476	2.4463072
H	3.9135183	2.1257565	-1.4061169
H	3.6864197	1.3567668	-3.0129320
H	2.6483705	0.8688164	-1.6253224

H	-2.7229599	1.1923430	-1.1159519
H	-4.6911478	4.0654130	3.0554611
H	-6.2196874	0.1346138	2.0424650
H	-1.5737769	-2.8005275	0.0127042
H	0.4120190	-5.5803956	-4.2417978
H	-3.3951928	-3.5145961	-4.4558166

Table S14. Coordinates of geometry optimized file for **PP_{ox}** with PA.

C	-2.4741061	-3.5486293	-2.6363194
C	-1.3697585	-4.0226075	-1.8443816
C	-0.3772955	-4.7619227	-2.5764729
C	-0.4366661	-4.9561050	-3.9556937
C	-1.5243273	-4.4408098	-4.6625025
C	-2.5495285	-3.7494022	-4.0140571
O	-1.1828181	-3.8158425	-0.5661628
N	0.7971285	-5.3167708	-1.8891499
O	0.6768165	-5.7035674	-0.7286445
N	-1.5808950	-4.6056576	-6.1194151
O	-0.7024003	-5.2884435	-6.6552207
N	-3.6477103	-2.9222091	-2.0059443
O	-4.6019937	-2.6313653	-2.7244329

O 1.8509475 -5.3650685 -2.5439488
O -2.4963967 -4.0369817 -6.7230283
O -3.6162933 -2.7584629 -0.7813995
C -0.8686573 -1.2652602 -5.0586546
C -0.0306548 -1.5038400 -3.9680999
C -0.4055637 -1.0256991 -2.6935912
C -1.5906895 -0.2335041 -2.5310327
C -2.4434891 -0.0286983 -3.6417402
C -2.0783060 -0.5463967 -4.8867369
N 0.2680750 -1.2566953 -1.4923672
Co -0.4294477 -0.1774916 -0.0964380
O -1.8311381 0.2643292 -1.3266163
C 1.2771687 -2.0908108 -1.3542476
C 1.9833802 -2.3433690 -0.1415282
C 1.7722187 -1.5590759 1.0603174
C 2.5771047 -1.8462726 2.2338086
C 3.4616478 -2.9177080 2.1603366
C 3.6576811 -3.7282243 0.9990316
C 2.9357109 -3.3973388 -0.1421620
O 0.9169699 -0.5885456 1.1339575
C 2.4136491 -1.0028839 3.5102622
C 3.3923788 -1.4529004 4.6123466

C	4.6023969	-4.9332209	1.0649433
C	4.0238891	-5.9399744	2.0913497
O	0.6516903	1.1815638	-0.7970262
C	0.6499864	2.4348686	-0.4746190
C	-0.0974044	2.9662075	0.6506231
C	-0.0424529	4.3547840	0.9434764
C	0.6780381	5.2405453	0.1504910
C	1.4246929	4.6923324	-0.9389618
C	1.4573899	3.3422976	-1.2712606
C	-0.9110916	2.1500308	1.4889237
N	-1.1785402	0.8747226	1.2950465
C	-1.9948479	0.1074175	2.1278533
C	-2.2168408	-1.2204731	1.6295180
C	-3.1445764	-2.0626355	2.2896211
C	-3.7620002	-1.6123070	3.4577189
C	-3.4717909	-0.3325328	3.9962465
C	-2.5907042	0.5263569	3.3379746
C	0.6451822	6.7579203	0.3610031
C	-0.0837437	7.3850625	-0.8551302
C	2.2819343	2.8089800	-2.4556550
C	1.3306578	2.2037599	-3.5190076
O	-1.5335081	-1.5937685	0.5605050

C	3.0919214	3.9334099	-3.1300121
C	3.2840545	1.7348284	-1.9590352
C	2.0861548	7.3126366	0.4517468
C	-0.1191032	7.1398503	1.6418156
C	2.7054893	0.4872980	3.1953066
C	0.9728741	-1.1614575	4.0584031
C	4.7244843	-5.6370080	-0.2989230
C	6.0076144	-4.4729192	1.5202876
O	-3.2667888	2.1700412	-0.5732890
C	-4.0603584	2.0511724	0.4582923
C	-4.1128802	3.1176296	1.4227853
C	-4.8484454	3.0374044	2.6045220
C	-5.5933763	1.8850676	2.8599642
C	-5.6285017	0.8273927	1.9489199
C	-4.8872264	0.9141894	0.7714499
N	-3.3467044	4.3552052	1.2160957
O	-3.1448493	4.7420419	0.0671346
N	-6.3390989	1.7734188	4.1182640
O	-6.3604342	2.7581678	4.8634837
N	-5.1057363	-0.1649530	-0.2093601
O	-5.8291623	-1.1027989	0.1204241
O	-2.9578504	4.9434950	2.2381118

O	-6.8873495	0.6938129	4.3634479
O	-4.5868003	-0.0375221	-1.3227208
H	-0.6229014	4.7174448	1.8014885
H	-3.3494578	-3.0597312	1.8782328
H	-4.4750871	-2.2686532	3.9780838
H	-2.3729974	1.5188351	3.7554797
H	-3.9439368	-0.0166107	4.9369504
H	2.0054494	5.3885832	-1.5574429
H	-1.3701821	2.6498286	2.3608385
H	-0.1375459	8.4878161	-0.7435067
H	-1.1164800	6.9892651	-0.9322372
H	0.4414165	7.1650035	-1.8064968
H	1.9189087	1.8274876	-4.3811833
H	0.6240586	2.9718697	-3.8940508
H	0.7447866	1.3619861	-3.1109748
H	2.6705247	7.1123347	-0.4683323
H	2.6302113	6.8641431	1.3079300
H	2.0607246	8.4120958	0.5965382
H	-0.1261060	8.2421375	1.7581194
H	0.3582308	6.7080022	2.5452203
H	-1.1706727	6.7927187	1.6097431
H	3.8042201	4.4120900	-2.4274018

H	2.4380348	4.7224326	-3.5536950
H	3.6814689	3.5070122	-3.9660529
H	-3.3704951	0.5430818	-3.5071479
H	-0.5869387	-1.6318266	-6.0556151
H	-2.7352560	-0.3785609	-5.7529516
H	0.9083665	-2.0575954	-4.1036487
H	3.0643378	-3.9681729	-1.0709516
H	4.0462333	-3.1642092	3.0560334
H	1.6020003	-2.6648131	-2.2409413
H	4.4502783	-1.3599119	4.2925278
H	3.2147626	-2.5016882	4.9256154
H	3.2547510	-0.8120706	5.5060098
H	2.6003295	1.0924826	4.1192705
H	2.0092938	0.8847619	2.4350159
H	3.7422321	0.6119079	2.8206970
H	0.8543624	-0.5647135	4.9861465
H	0.7612809	-2.2222227	4.3036480
H	0.2190389	-0.8166649	3.3294519
H	3.9366347	-5.4929803	3.1020853
H	4.6832550	-6.8289932	2.1695453
H	3.0159777	-6.2796818	1.7779957
H	3.7420018	-5.9915160	-0.6681452

H	5.3942683	-6.5154241	-0.2075624
H	5.1552128	-4.9637157	-1.0680567
H	6.4363452	-3.7431271	0.8036236
H	6.6925787	-5.3435866	1.5786382
H	5.9865851	-3.9979472	2.5215067
H	3.9818548	2.1668357	-1.2127456
H	3.8847754	1.3611499	-2.8136386
H	2.7632490	0.8781529	-1.4950996
H	-2.9112121	1.2764519	-0.9726076
H	-4.8251401	3.8634269	3.3252017
H	-6.2447366	-0.0595193	2.1331057
H	-1.6266124	-2.9651404	-0.1758519
H	0.3679333	-5.4919482	-4.4732127
H	-3.4192417	-3.3764232	-4.5660124

Table S15. Coordinates of geometry optimized file for **dtHBAP** with PA.

C	-2.4327491	-0.6851674	0.0000000
C	-2.3187611	-2.1274769	0.0000000
C	-1.2758823	0.1548752	0.0000000
C	-1.4272208	1.5732933	0.0000000
C	-2.7379395	2.0723835	0.0000000
C	-3.9091912	1.2725487	0.0000000

C	-3.7293173	-0.1087416	0.0000000
O	-0.0576418	-0.4135934	0.0000000
C	-0.2039835	2.5117054	0.0000000
H	-2.8677872	3.1564964	0.0000000
C	-5.2925034	1.9485567	0.0000000
H	-4.5832404	-0.7930007	0.0000000
N	-1.1792112	-2.7678831	0.0000000
H	-3.2805932	-2.6697619	0.0000000
C	-1.1102897	-4.1721213	0.0000000
C	0.1896345	-4.7644262	0.0000000
C	0.3262297	-6.1684235	0.0000000
C	-0.8004676	-6.9944109	0.0000000
C	-2.0888491	-6.4257131	0.0000000
C	-2.2335153	-5.0365438	0.0000000
O	1.3278689	-4.0387068	0.0000000
H	1.3391338	-6.5863765	0.0000000
H	-0.6759617	-8.0836519	0.0000000
H	-2.9780460	-7.0663374	0.0000000
H	-3.2428679	-4.6136147	0.0000000
C	-0.6110554	3.9994041	0.0000000
C	0.6350100	2.2624030	1.2789235
C	0.6350100	2.2624030	-1.2789235

C	-6.4370585	0.9176502	0.0000000
C	-5.4297081	2.8310867	1.2644488
C	-5.4297081	2.8310867	-1.2644488
H	1.5403635	2.8941236	1.2691603
H	0.0412375	2.5153438	2.1762746
H	0.9524673	1.2130175	1.3621745
H	1.5403635	2.8941236	-1.2691603
H	0.9524673	1.2130175	-1.3621745
H	0.0412375	2.5153438	-2.1762746
H	0.3003900	4.6228516	0.0000000
H	-1.1988683	4.2689486	-0.8955093
H	-1.1988683	4.2689486	0.8955093
H	-7.4094800	1.4410070	0.0000000
H	-6.4040694	0.2709582	-0.8947056
H	-6.4040694	0.2709582	0.8947056
H	-6.4176284	3.3270097	1.2823586
H	-5.3336413	2.2199221	2.1800933
H	-4.6581217	3.6199754	1.2997363
H	-6.4176284	3.3270097	-1.2823586
H	-4.6581217	3.6199754	-1.2997363
H	-5.3336413	2.2199221	-2.1800933
H	-0.2117229	-1.4156714	0.0000000

H	1.1298315	-3.0853509	0.0000000
H	2.8060933	0.1558872	0.0000000
O	3.3630373	0.9964768	0.0000000
C	4.6126973	0.6124072	0.0000000
C	5.6952338	1.5520517	0.0000000
C	7.0223243	1.1329681	0.0000000
C	7.3227078	-0.2328824	0.0000000
C	6.3183218	-1.1972434	0.0000000
C	4.9885487	-0.7767836	0.0000000
N	5.4603947	3.0183831	0.0000000
H	7.8199723	1.8773165	0.0000000
N	8.7353480	-0.6615164	0.0000000
H	6.5584534	-2.2618312	0.0000000
N	3.9579245	-1.8132326	0.0000000
O	2.7625254	-1.4366060	0.0000000
O	4.2849541	-2.9824249	0.0000000
O	6.4538885	3.7406599	0.0000000
O	4.3083091	3.4299398	0.0000000
O	8.9630070	-1.8668276	0.0000000
O	9.5944241	0.2138820	0.0000000

Water Specimens:

Specimen- (I) Bardhaman development authority supplied water (rural area) (Central-western area of West Bengal, India).^{ref 2}

Specimen- (II) Dubrajpur hand pump water (an area of Birbhum district) (North western part of West Bengal, India).^{ref 3}

Specimen- (III) Digba hand pump water (nearby area of '*Bay of Bengal*') (Southern part of West Bengal, India).
^{ref 4}

Specimen- (IV) Raniganj hand pump water (coal area)(Western part of West Bengal, India).^{ref 5}

Specimen- (V) Darjeeling tap water (Mountain '*The Kanchengjunga*' adjacent area)(Northmost district of West Bengal, India).^{ref 6}

Specimen- (VI) Bankura hand pump water (land of red soil) (Western part of West Bengal, India).^{ref 7}

Specimen- (VII) Howrah tap water (an area alongside of river '*The Ganges*' in central part of West Bengal, India).^{ref 8}

Cell culture, imaging details:

Imaging System:

The imaging system was comprised of an inverted fluorescence microscope (Leica DM 1000 LED), digital compact camera (Leica DFC 420C), and an image processor (Leica Application Suite v3.3.0). The microscope was equipped with a mercury 50 watt lamp.

Preparation of Cell image:

Candida albicans cells (IMTECH No. 3018) have been collected from exponentially growing culture in yeast extract glucose broth medium (pH 6.0 and incubation temperature 37°C). First they were washed by suspending them in normal saline and centrifuged at 3000 rpm for 15 minutes. Then, cells were washed twice with 0.1 M HEPES buffer (pH 7.4). Then cells were treated with **PP** solution (10 µM) for 1hr. After incubation, the cells were again washed with HEPES buffer and then incubated with picric acid (10 µM) for another 40 minutes. Cells obtained this way are mounted on a grease free glass slide and observed under a Leica DM 1000 Fluorescence microscope with UV filter. Cells treated with **PP** are used as control.^{ref 9}

Preparation of pollen grains to detect intracellular F⁻:

Pollen grains of *Techoma stans* (Family: Bignoniaceae) are collected from fresh buds and then washed twice with 0.1 M HEPES buffer at pH 7.4. Pollens are treated with 10 µM **PP** for 1hr in 0.1 M HEPES buffer (pH 7.4) containing 0.01% Triton X100 as a permeability enhancing agent. After incubation the pollens are washed again with HEPES buffer at pH 7.4 and incubated with picric acid (10 µM) for 40 minutes. Picric acid treated pollens are washed by centrifugation (3000 rpm for 5 minutes) using HEPES buffer and are mounted on a grease free glass slide and observed under a Leica DM 1000 fluorescence microscope equipped with a UV filter. Cells treated with **PP** are used as control.^{ref 9}

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