Supporting Information for

Pyromellitic Dihydrazides as Hydrolytically Robust Alternatives to Pyromellitic Diimide

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S1. General Experimental Methods

Reagents were purchased from TCI Chemicals and Ambeed Inc. and used as supplied. Compound **5** was synthesized following previously reported procedures (*J. Chem. Soc., Perkin Trans. 1*, **1999**, 1057–1066). ^{1}H-NMR and ^{13}C-NMR spectra were collected on a Bruker Avance III 400 MHz and referenced to residual solvent as the internal standard ($CDCl_3$: ^{1}H-7.26 ppm and ^{13}C-77.16 ppm; DMSO-d_6: ^{1}H-2.50 ppm). X-Ray analysis was performed on a Bruker-AXS D8 Venture diffractometer purchased through a grant from NSF/MRI (#1229400) and the University of Minnesota. UV-Vis data were collected with an Evolution™ 300 UV-Vis Spectrophotometer. Cyclic voltammetry experiments were performed using a Pine Research WaveNow potentiostat equipped with a Pt working electrode (1.6 mm diameter disk, PCTFE shroud), Pt coil counter electrode (PCTFE shroud), and non-aqueous reference electrode (Ag wire, 0.01 M $AgNO_3$, 0.1 M Bu_4PF_6, MeCN). Electrochemical samples (ca. 1.0 mM analyte, 0.1 M Bu_4PF_6) were deoxygenated by bubbling Ar through the solutions. Ferrocene (Fc) was used as an internal standard and the sample was evaluated both with and without Fc to ascertain that there were no significant interactions between Fc and the analyte. Melting points were obtained using a TA Discovery DSC 25. TGA measurements were performed on a TA Instruments Q5500 TGA. For hydrolytic stability testing, treated samples were heated at 90 °C for 18 hours then fully precipitated by the addition of 1.2 M HCl. The solids were collected and dried by vacuum filtration prior to the IR measurements. The Table of Contents graphic was generated using Google Gemini 3 (Nano Banana).

S2. Synthesis and NMR Spectra

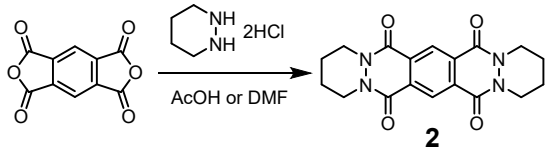

Figure S1. Synthesis of **2**.

Setup A using **AcOH solvent**: A 2–5 mL microwave vial (Biotage) was charged with a stir bar, pyromellitic dianhydride (99.7 mg, 458 µmol, 1.0 equiv) and hexahydropyridazine dihydrochloride (153.1 mg, 963 µmol, 2.1 equiv), and AcOH (4.5 mL). The vial was then sealed and heated in an aluminum heating block set at 120 °C for 5 hr. After the reaction mixture was cooled to room temperature and opened, it was poured into H_2O (10 mL), resulting in a yellow precipitate that was collected by vacuum filtration and left to dry on the vacuum funnel overnight. This solid was identified to be crude **2** (74 mg, 46% yield) that appeared pure by ^{1}H NMR spectroscopy but was found by TLC to consist of three UV-active components.

Purification: Crude **2** was purified by column chromatography over SiO_2 (gradient from 0% to 10% EtOAc / CH_2Cl_2 (v/v)) to yield **2** as a yellow solid (58 mg, 36% yield).

Characterization: **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.16 (s, 2H), 4.23–4.16 (m, 8H), 2.05–1.93 (m, *J* = 4.6, 4.0 Hz, 8H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.02, 132.09, 129.24, 44.63, 21.93. **IR** ν_{max} / cm^{-1} 2946, 2857, 1637, 1644, 1456, 1350, 1265, 1245, 1147, 1108, 988, 937, 695, 621. **mp** (DSC) 394.09 °C (peak).

Note on reaction time: repeat experiments following the same procedure but heating the reaction for 18 hr resulted in an increased yield (100 mg, 62% yield) and purity such that chromatographic purification was no longer required.

Setup B using **DMF solvent**: The reaction was set up as described above using DMF instead of AcOH as solvent and heated to 150 °C for 18 hr. The microcrystalline yellow precipitate formed upon cooling the reaction mixture to room temperature was collected by vacuum filtration and found to be analytically pure **2** (60 mg, 37% yield).

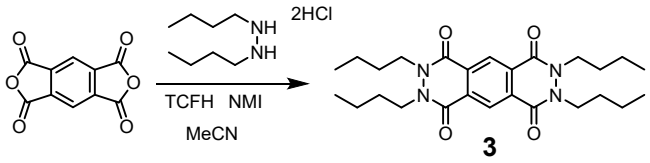

Figure S2. Synthesis of **3**.

Setup: A 2–5 mL microwave vial (Biotage) was charged with a stir bar, pyromellitic dianhydride (50.4 mg, 231 µmol, 1.0 equiv), 1,2-dibutylhydrazine dihydrochloride (100.4 mg, 462 µmol, 2 equiv), N-methylimidazole (0.258 mL, 14.0 equiv), MeCN (0.616 mL), and lastly N,N,N',N'-tetramethylchloroformamidinium hexafluorophosphate (311.2 mg, 1.11 mmol, 4.8 equiv). A color change to yellow was observed. The vial was sealed and stirred at room temperature for 18 h.

Purification: Vacuum filtration of the crude mixture followed by MeOH rinses yielded **3** as a yellow solid (95 mg, 87.4% yield).

Characterization: **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.20 (t, *J* = 1.5 Hz, 2H), 4.18 (t, *J* = 7.4 Hz, 8H), 1.64 (p, *J* = 7.3 Hz, 8H), 1.32 (dp, *J* = 7.7, 7.1 Hz, 8H), 0.93 (t, 12H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.66, 132.19, 129.44, 45.21, 30.06, 19.92, 13.80.**IR** ν_{max} / cm^{-1} 2958, 2931, 2872, 1633, 1376, 1254, 1111, 942, 784, 688. **mp** (DSC) 175.53 °C (peak).

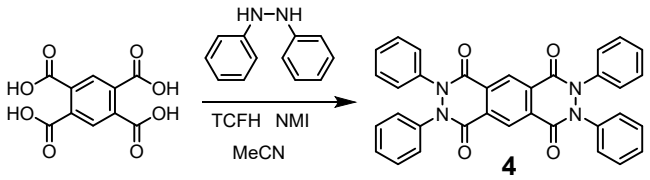

Figure S3. Synthesis of **4**.

Setup: A 50 mL round-bottom flask was charged with a stir bar, pyromellitic tetraacid (1.00 g, 3.94 mmol, 1.0 equiv), hydrazobenzene (1.60 g, 8.66 mmol, 2.2 equiv), N-methylimidazole (2.6 mL, 8.4 equiv), MeCN (10.5 mL), and N,N,N',N'-tetramethylchloroformamidinium hexafluorophosphate (5.30 g, 18.89 mmol, 4.8 equiv). The mixture was stirred for 18 h at RT.

Purification: Vacuum filtration of the reaction mixture followed by MeOH rinses yielded a crude mixture. This crude mixture was then added to EtOH (25 mL), and the resulting mixture was heated overnight at 80 °C. After cooling to room temperature, the precipitate was collected by vacuum filtration to yield **4** as a yellow solid (366 mg, 16.8% yield).

Characterization: **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.43 (s, 2H), 7.34 (d, *J* = 8.0 Hz, 8H), 7.29 (t, *J* = 7.5 Hz, 8H), 7.21 (t, *J* = 7.2 Hz, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.91, 137.21, 133.43, 130.32, 129.12, 128.92, 128.80. **IR** ν_{max} / cm^{-1} 3061, 1645, 1489, 1453, 1326, 1225, 1162, 1074, 1025, 764, 739, 687. **mp** (DSC) 363.51 °C (peak, dec).

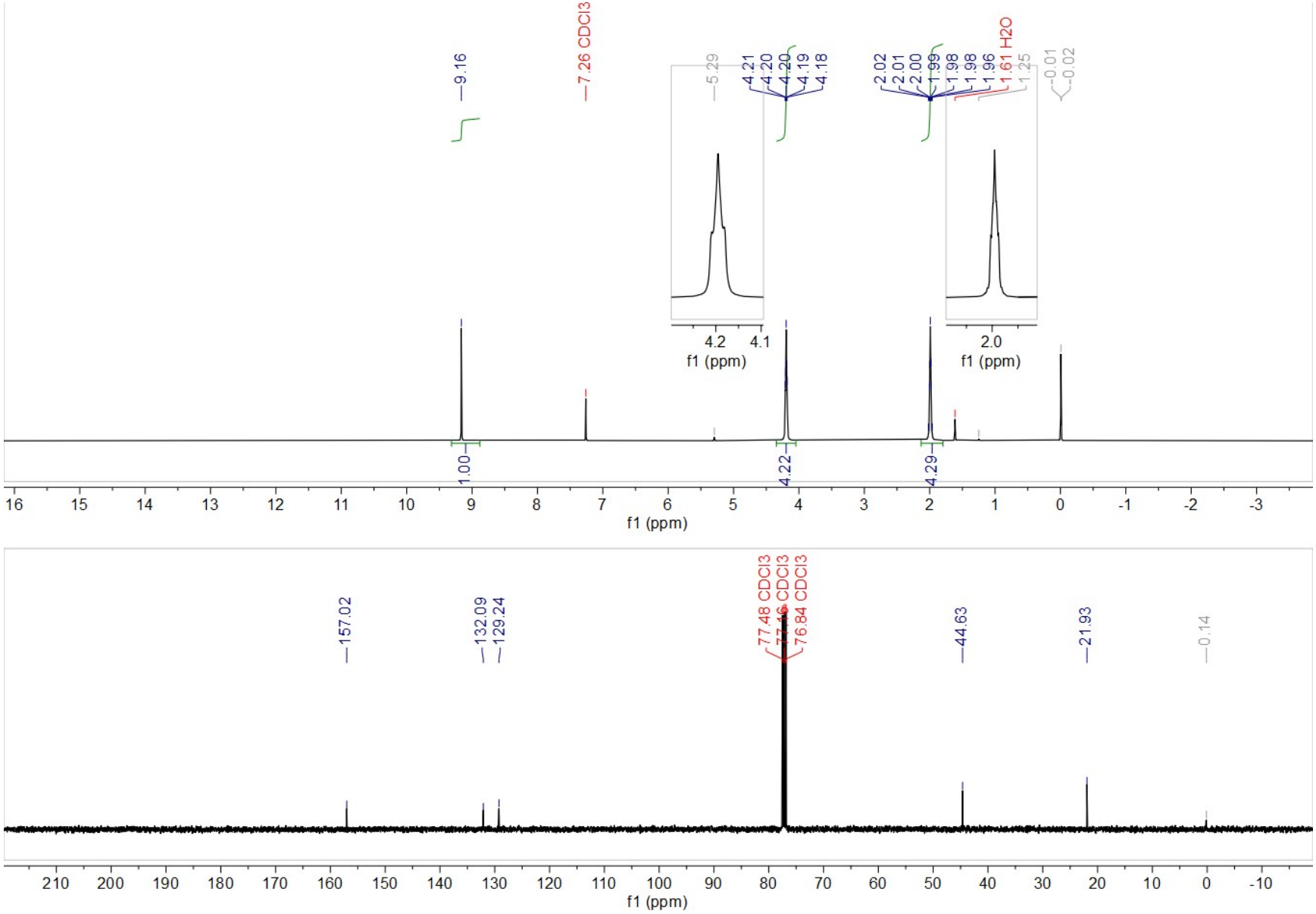

Figure S4.(top) ^{1}H NMR and (bottom) ^{13}C NMR spectra of **2** measured in $CDCl_3$.

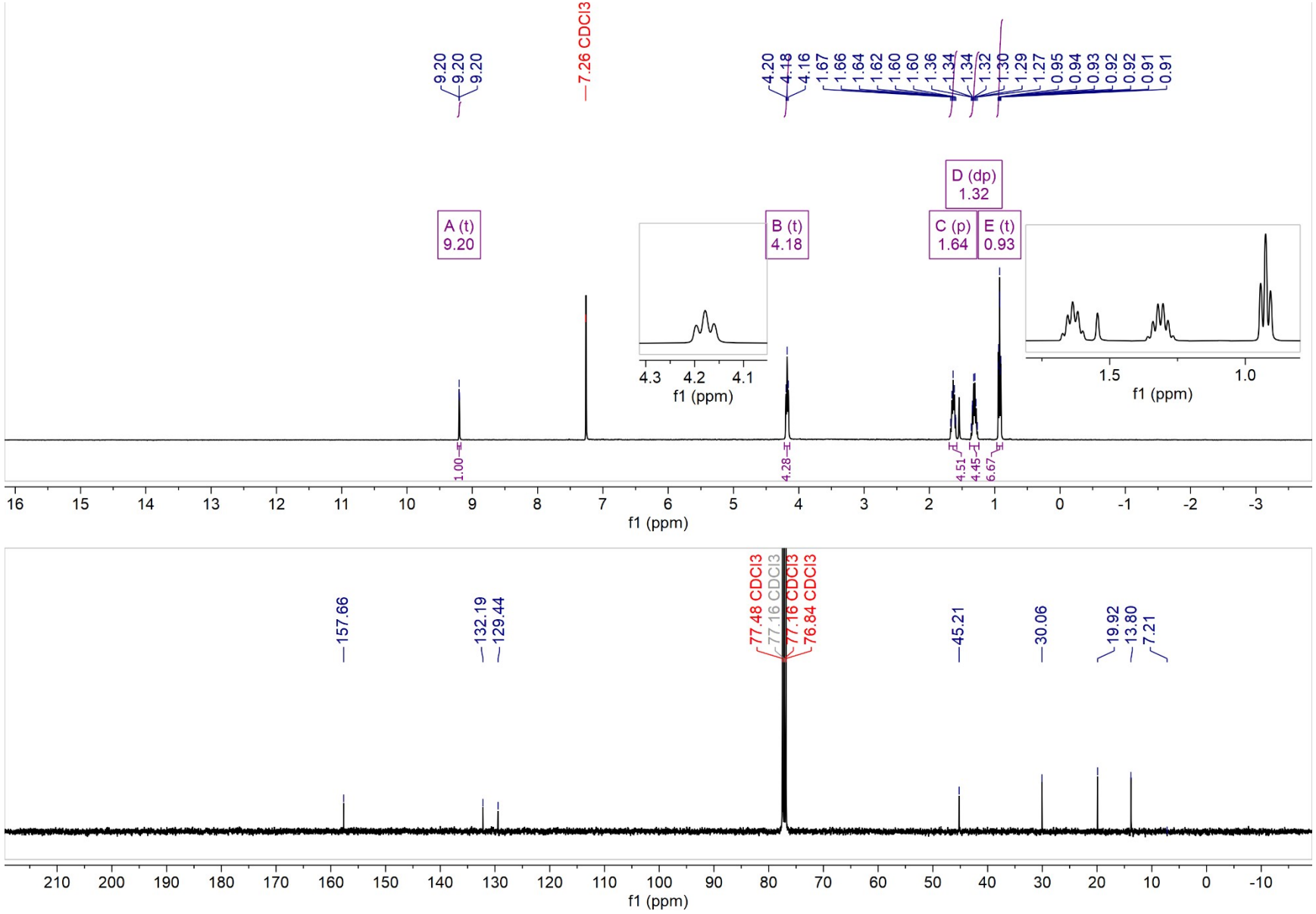

Figure S5.(top) ^{1}H NMR and (bottom) ^{13}C NMR spectra of **3** measured in $CDCl_3$.

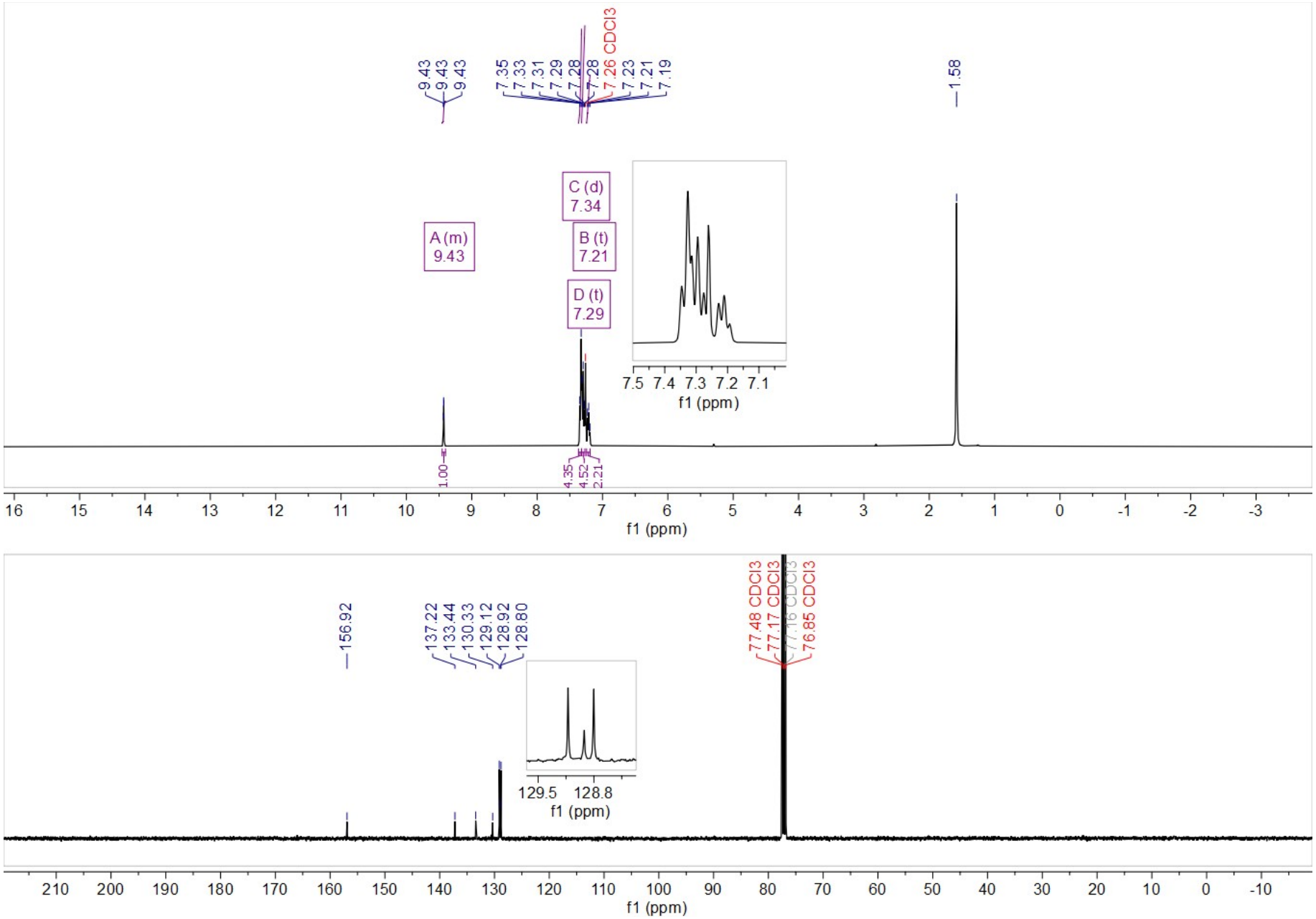

Figure S6.(top) ^{1}H NMR and (bottom) ^{13}C NMR spectra of **4** measured in $CDCl_3$.

S3. X-Ray Crystallography

Compound 2

A crystal (approximate dimensions 0.200 x 0.035 x 0.015 mm3) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a Bruker PHOTON-III CPAD diffractometer for a data collection at 150(2) K.[1] A preliminary set of cell constants was calculated from reflections harvested from three sets of frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced an initial orientation matrix determined from 326 reflections. The data collection was carried out using MoKa radiation (parabolic mirrors) with a frame time of 10 seconds and a detector distance of 6.0 cm. A strategy program was used to assure complete coverage of all unique data to a resolution of 0.75 Å. All major sections of frames were collected with 1.20° steps in ω or ϕ at different detector positions in 2θ. The intensity data were corrected for absorption and decay (SADABS).[2] Final cell constants were calculated from 2976 strong reflections from the actual data collection after integration (SAINT).[3] Please refer to Table S1 for additional crystal and refinement information.

The structure was solved using SHELXT-2018/2 (Sheldrick 2015)[4] and refined using SHELXL-2018/3 (Sheldrick 2015).[4] The space group $P2_12_12$ was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1$ = 0.0552 and $wR2$ = 0.1319 (F^2, obs. data).

The structure is the one suggested. There are four molecules in the asymmetric unit: Z'=4 and Z=16. Unexpectedly, the molecules could have internal two-fold symmetry, but this is not used in the space group symmetry. Also, when the packing diagram is viewed along the *c*-axis, it appears there are two abutted tetragonal cells. Finally, a number of reflections (12) were either omitted due to being behind the beam stop or bad fit.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 192 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs.

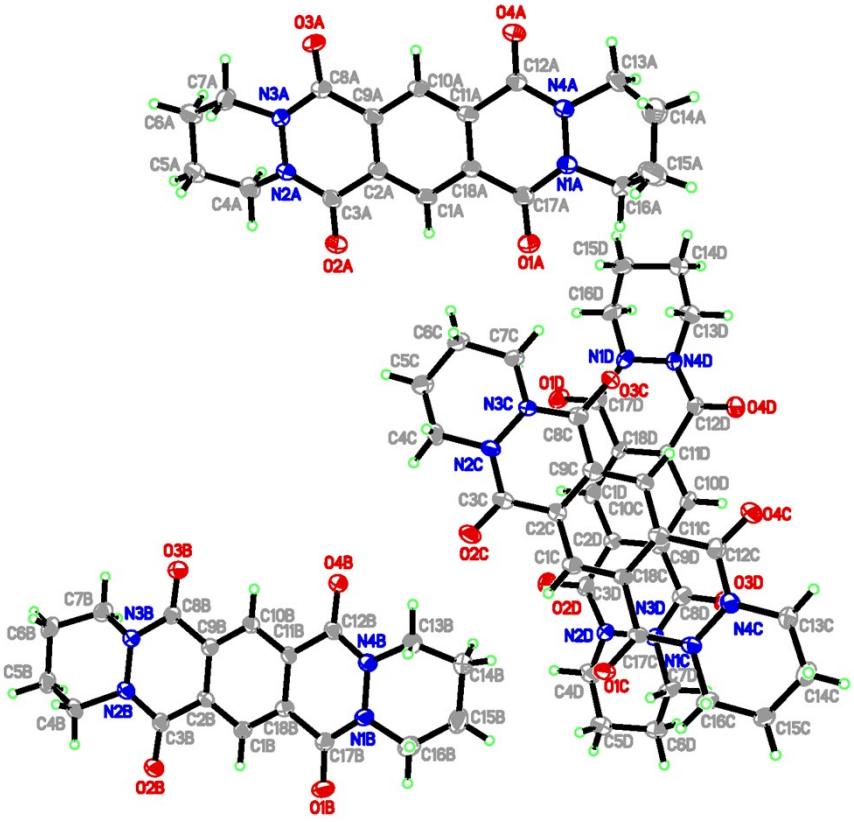

Figure S7. The asymmetric unit of **2**.

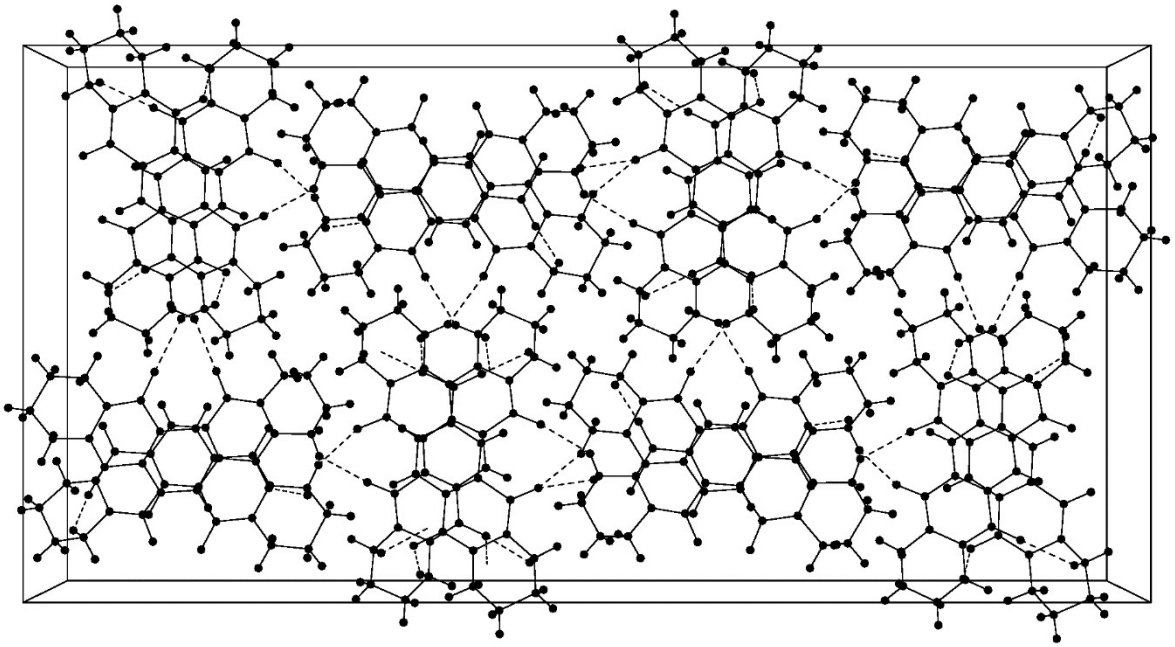

Figure S8. The unit cell of **2**.

Table S1. Crystal data and structure refinement for **2**.

CCDC Deposition No.	2303924	
Empirical formula	$C_{18}\ H_{18}\ N_4\ O_4$	
Formula weight	354.36	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12$	
Unit cell dimensions	a = 20.9907(7) Å	α = 90°
	b = 42.5286(15) Å	β = 90°
	c = 6.9390(2) Å	γ = 90°
Volume	6194.5(3) Å^3	
Z	16	
Density (calculated)	1.520 Mg/m^3	
Absorption coefficient	0.110 mm^{-1}	
***F*(000)**	2976	
Crystal color, morphology	yellow needle	
Crystal size	0.200 x 0.035 x 0.015 mm^3	
Theta range for data collection	1.999 to 28.314°	
Index ranges	$-28 \le h \le 28$, $-56 \le k \le 56$, $-9 \le l \le 8$	
Reflections collected	41725	
Independent reflections	15366 [R(int) = 0.0450]	
Observed reflections	10783	
Completeness to theta = 25.242°	99.7%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7457 and 0.6621	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15366 / 0 / 937	
Goodness-of-fit on F^2	1.018	
Final R indices [$I>2\sigma(I)$]	$R1$ = 0.0552, $wR2$ = 0.1319	
R indices (all data)	$R1$ = 0.0880, $wR2$ = 0.1477	
Absolute structure parameter	–0.1(7)	
Largest diff. peak and hole	0.361 and –0.235 e Å^{-3}	

Compound 3

A crystal (approximate dimensions 0.200 x 0.200 x 0.120 mm^3) was placed onto the tip of a 200 µm diameter MiTeGen dual-thickness micro-loop and mounted on a Bruker VENTURE D8 diffractometer for a data collection at 100(2) K. A preliminary set of cell constants was calculated from reflections harvested from three sets of frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced an initial orientation matrix determined from 199 reflections. The data collection was carried out using MoKa radiation (parabolic mirrors) with a frame time of 20 seconds and a detector distance of 5.0 cm. A strategy program was used to assure complete coverage of all unique data to a resolution of 0.77 Å. All major sections of frames were collected with 1.20° steps in w or f at different detector positions in 2q. The intensity data were corrected for absorption and decay (SADABS).[2] Final cell constants were calculated from 2995 strong reflections from the actual data collection after integration (SAINT).[3] Please refer to Table 2 for additional crystal and refinement information.

The structure was solved using SHELXT-2018/2 (Sheldrick, 2018)[4] and refined using SHELXL-2019/2 (Sheldrick, 2019).[4] The space group *C*2/c was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0451$ and $wR2 = 0.1235$ ($F2$, obs. data).

The structure is the one suggested. The molecule is on an inversion making ½ molecule unique. There is solvent located on the two-fold axis, but the resulting carbon positions made little chemical sense for a putative hexane molecule. PLATON/SQUEEZE was applied. The void space provides room for about 4 *n*-hexane (or hexanes) molecules.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 192 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs.

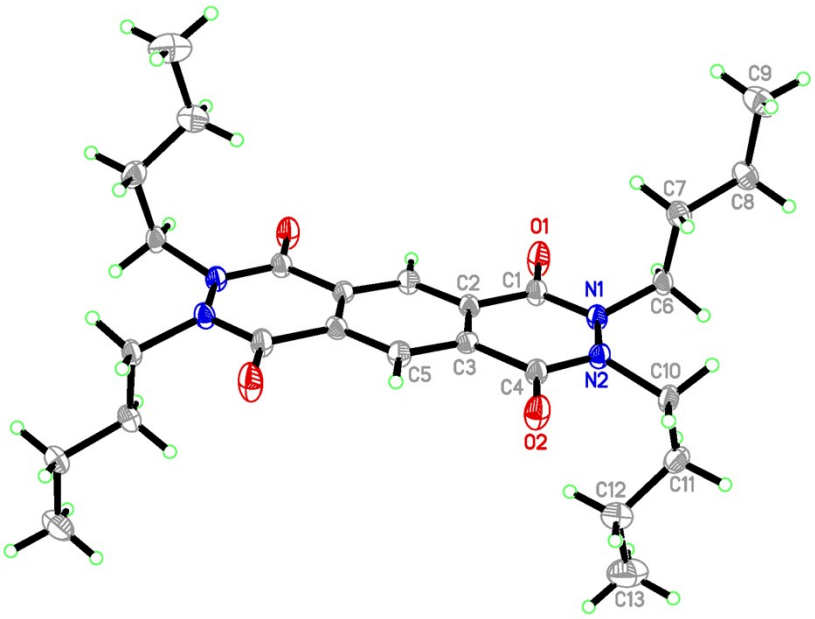

Figure S9. The labeled asymmetric unit of **3**.

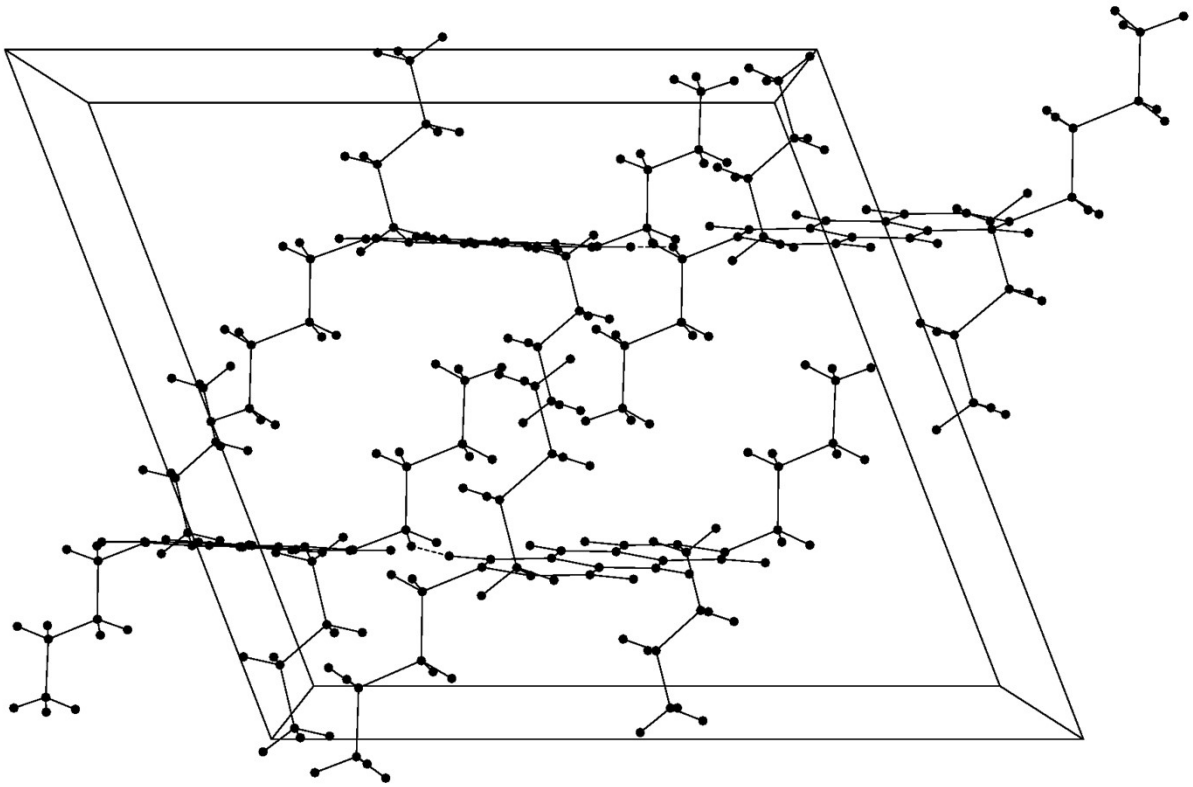

Figure S10. The unit cell of **3**.

Table S2. Crystal data and structure refinement for **3**.

CCDC Deposition No.	2521161	
Empirical formula	C26 H38 N4 O4	
Formula weight	470.60	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	*a* = 16.2995(9) Å	α = 90°
	b = 11.1901(5) Å	β = 111.166(2)°
	c = 17.9213(9) Å	γ = 90°
Volume	3048.2(3) Å^3	
Z	4	
Density (calculated)	1.025 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
***F*(000)**	1016	
Crystal color, morphology	yellow block	
Crystal size	0.200 x 0.200 x 0.120 mm^3	
Theta range for data collection	2.260 to 27.513°	
Index ranges	$-18 \le h \le 21$, $-14 \le k \le 12$, $-23 \le l \le 22$	
Reflections collected	17810	
Independent reflections	3494 [*R*(int) = 0.0305]	
Observed reflections	2954	
Completeness to theta = 25.242°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7456 and 0.6373	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3494 / 0 / 156	
Goodness-of-fit on F^2	1.037	
Final *R* indices [$I>2\sigma(I)$]	*R*1 = 0.0451, *wR*2 = 0.1235	
***R* indices (all data)**	*R*1 = 0.0529, *wR*2 = 0.1303	
Largest diff. peak and hole	0.326 and –0.235 e Å^{-3}	

Compound 4

A yellow, plate-shaped crystal was mounted on a MiTeGen micromount with perfluoroether oil. Data were collected from a shock-cooled single crystal at 100(2) K on a Bruker D8 VENTURE dual wavelength Mo/Cu three-circle diffractometer with a microfocus sealed X-ray tube using a mirror optics as monochromator and a Bruker PHOTON III detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used Mo*Kα* radiation (λ = 0.71073 Å). All data were integrated with SAINT and a Multi-scan absorption correction using SADABS Bruker was applied.[2,3] The structure was solved by direct methods with SHELXT 2018/2 and refined by full-matrix least-squares methods against *F*2 using SHELXL-2019/2.[5,6] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined isotropic on calculated positions using a riding model with their *U*iso values constrained to 1.5 times the *U*eq of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[7] This report and the CIF file were generated using FinalCif.[8]

The compound crystallizes as yellow plates in a monoclinic system. Four molecules fit in a P 2_1/n space group with two solvent molecules in the asymmetric unit . Hydrogen bonds can be observed between one of the solvent molecules with one of the hydrogens in the phenyl ring, and another hydrogen bond between the two TPPMDH molecules.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 192 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs.

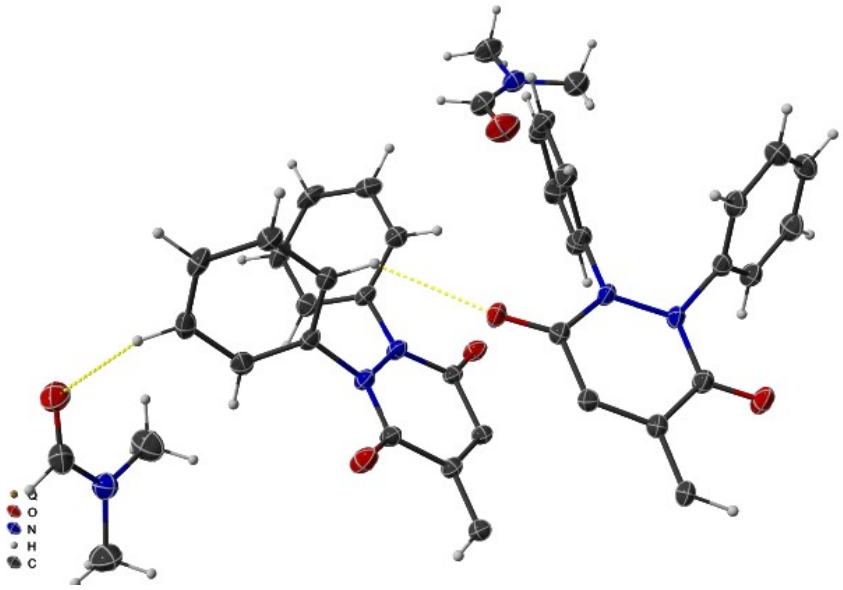

Figure S11. Asymmetric unit of the crystal structure of **4**. Hydrogen bonds are shown in dashed yellow lines.

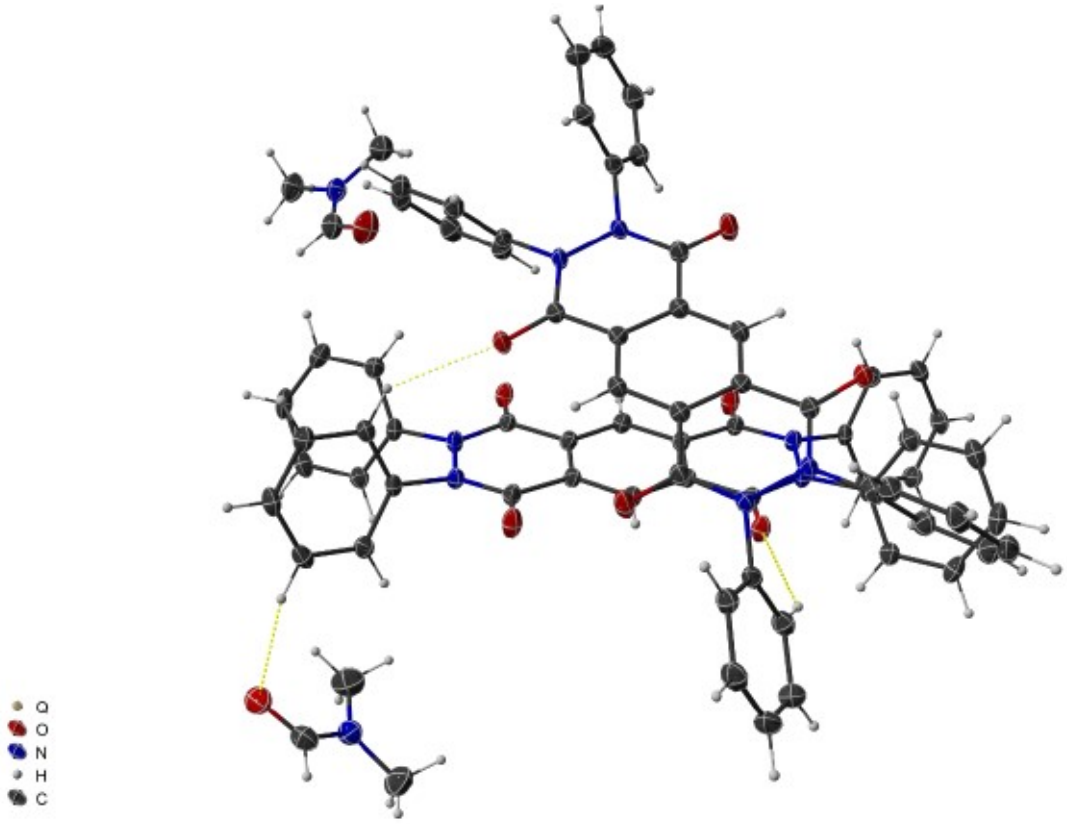

Figure S12. Full view of the crystal structure of **4**. Hydrogen bonds are shown in dashed yellow lines.

Table S3. Crystal data and structure refinement for **4**.

CCDC Deposition No.	2521160	
Empirical formula	C40 H36 N6 O6	
Formula weight	696.75	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	*a* = 7.6117(9) Å	α = 90°
	b = 28.606(4) Å	β = 95.126(3)°
	c = 15.887(2) Å	γ = 90°
Volume	3445.3(8) Å^3	
Z	4	
Density (calculated)	1.343 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
***F*(000)**	1464	
Crystal color, morphology	yellow plate	
Crystal size	0.090 x 0.190 x 0.390 mm^3	
Theta range for data collection	3.84 to 55.06°	
Index ranges	$-8 \le h \le 9$, $-37 \le k \le 37$, $-20 \le l \le 20$	
Reflections collected	43686	
Independent reflections	7904 [*R*(int) = 0.0382]	
Completeness to theta = 25.242°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.6643 and 0.7456	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7904 / 0 / 473	
Goodness-of-fit on F^2	1.035	
Final *R* indices [$I>2\sigma(I)$]	*R*1 = 0.0419, *wR*2 = 0.1017	
***R* indices (all data)**	*R*1 = 0.0576, *wR*2 = 0.1122	
Largest diff. peak and hole	0.59 and –0.29 e Å^{-3}	

Crystallography References

[1]APEX3, Bruker Analytical X-ray Systems, Madison, WI (2014).
[2]SADABS, Bruker Analytical X-ray Systems, Madison, WI (2014).
[3]SAINT Bruker Analytical X-ray Systems, Madison, WI (2014).
[4]SHELXTL 2014, Bruker Analytical X-Ray Systems, Madison, WI (2013); G. M. Sheldrick, *Acta Cryst.* **A64**, 112-122 (2008).
[5]G. M. Sheldrick, *Acta Cryst.* **2015**, *A71*, 3–8, doi:10.1107/S2053273314026370.
[6]G. M. Sheldrick, *Acta Cryst.* **2015**, *C71*, 3–8, doi:10.1107/S2053229614024218.
[7]C. R. Groom, I. J. Bruno, M. P. Lightfoot, S. C. Ward, *Acta Cryst.* **2016**, *B72*, 171–179, doi:10.1107/S2052520616003954.
[8]D. Kratzert, *FinalCif*, *V155*, https://dkratzert.de/finalcif.html.

S4. Thermal Gravimetric Analysis (TGA)

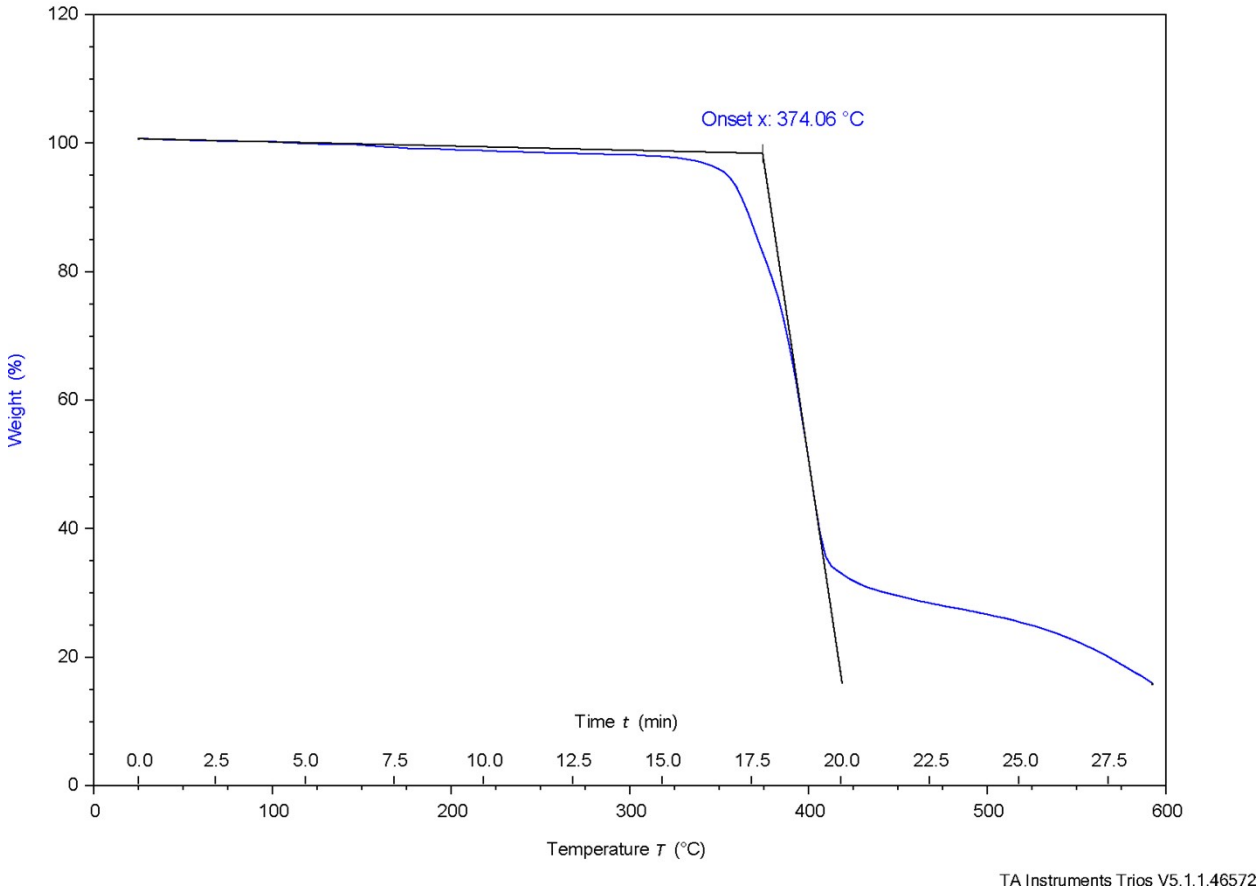

Figure S13. TGA trace and determination of onset temperature for **2**.

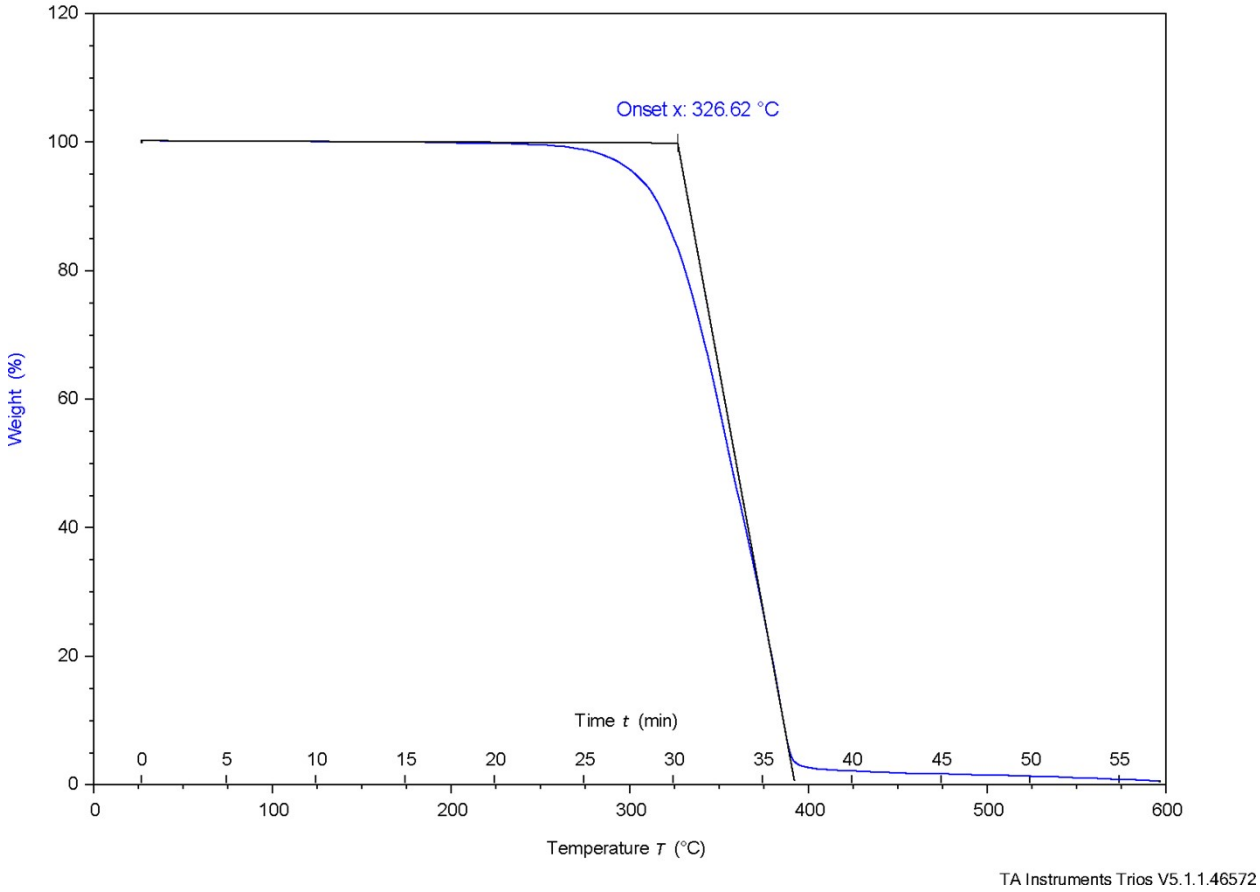

Figure S14. TGA trace and determination of onset temperature for **3**.

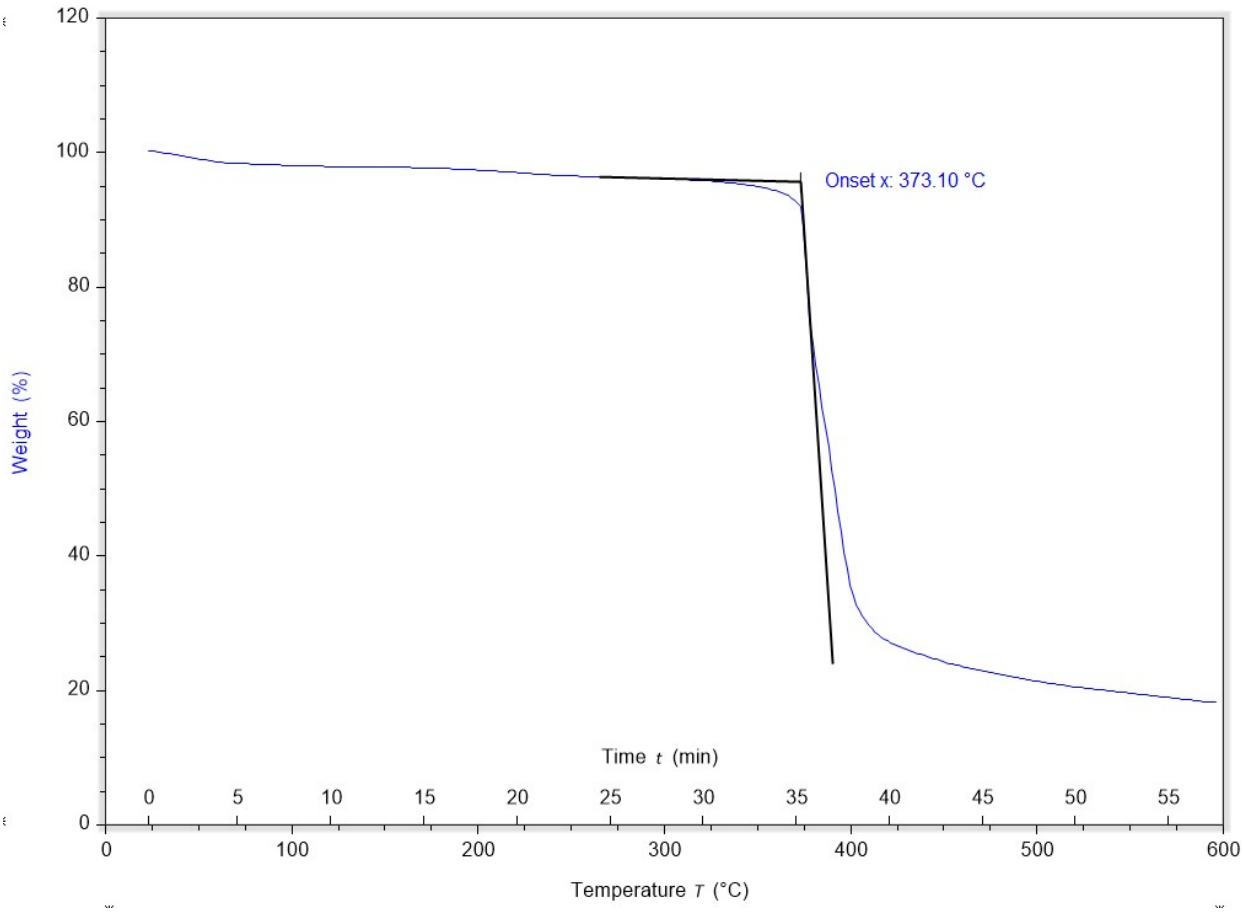

Figure S15. TGA trace and determination of onset temperature for **4**.

S5. NMR Pre and Post-alkaline Treatment

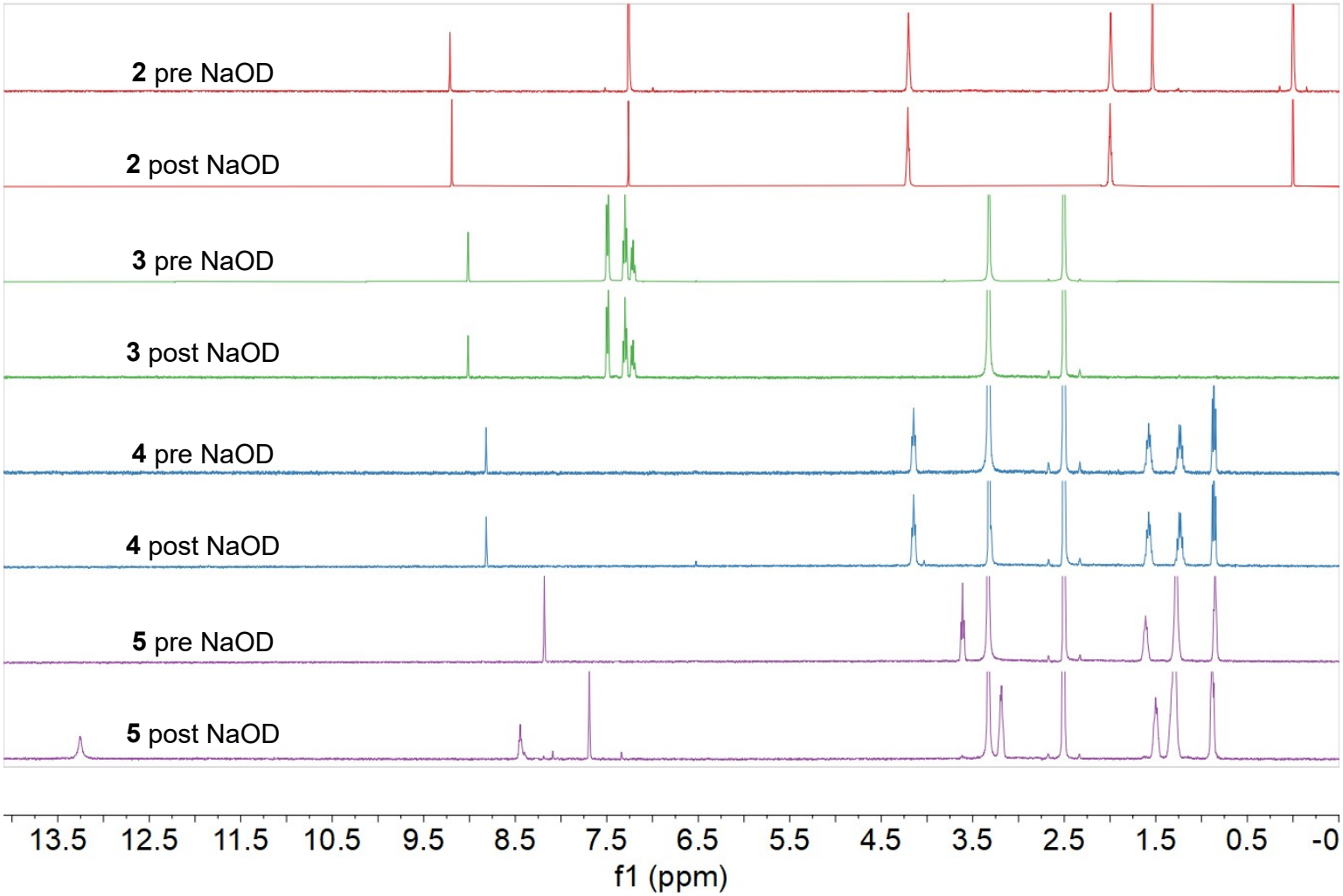

Figure S16. ^{1}H NMR spectrum of compounds **2–5** pre- and post NaOD treatment. $CDCl_3$ was used as solvent for **2**. DMSO-d_6 was used as solvent for **3**–**5**.

S6. Computational Data

Table S4. Summary of calculated energies and frequencies (M062X/6-311+G(2d,p)).

Molecule	Number of Imaginary Frequencies	Calculated Total Energy (Hartree)
N,N′-dimethylpyromellitic diimide	0	–1061.71764908
N,N′,N″,N‴-tetramethylpyromellitic dihydrazide	0	–872.493804913
N,N′-diphenylpyromellitic diimide	0	–1255.9177082
N,N′,N″,N‴-tetraphenylpyromellitic dihydrazide	0	–1828.57122895

Table S5. Cartesian Coordinates for N,N′-dimethylpyromellitic diimide

Atom	X	Y	Z
C 6	0.00000000	0.00000000	0.00000000
N 7	0.00826300	0.00065300	1.44813400
C 6	1.16172900	0.03007200	2.22979300
C 6	0.68997600	0.01885300	3.65144400
C 6	1.43298000	0.03803000	4.81908600
C 6	0.67824600	0.01963300	5.97924900
C 6	-0.71109200	-0.01519900	5.97193000
C 6	-1.45409600	-0.03437600	4.80428800
C 6	-0.69936200	-0.01597900	3.64412500
C 6	-1.15137700	-0.02803700	2.21666200
O 8	-2.27035600	-0.05630100	1.78454500
H 1	-2.53631400	-0.06156600	4.79921100
C 6	-1.18284500	-0.02641800	7.39358100
N 7	-0.02937900	0.00300100	8.17524000
C 6	1.13026100	0.03169100	7.40671200
O 8	2.24924000	0.05995500	7.83882900
C 6	-0.02111600	0.00365400	9.62337400
H 1	0.51658600	-0.86826900	9.99326600
H 1	0.46788900	0.90392100	9.99299100
H 1	-1.05545900	-0.02465000	9.95789200
O 8	-2.31008600	-0.05464000	7.80242100
H 1	2.51519800	0.06522000	4.82416300
O 8	2.28897000	0.05829400	1.82095300
H 1	-0.53770200	0.87192300	-0.36989200
H 1	1.03434300	0.02830400	-0.33451800
H 1	-0.48900500	-0.90026700	-0.36961700

Table S6. Cartesian Coordinates for N,N′,N″,N‴-tetramethylpyromellitic dihydrazide

Atom	X	Y	Z
C 6	0.00000000	0.00000000	0.00000000
N 7	-1.22778100	-0.64504200	-0.44641800
N 7	-1.22778100	-2.04884300	-0.35469900
C 6	-2.37583200	-2.79695400	-0.29166700
C 6	-3.65025600	-2.03805100	-0.30952700
C 6	-4.84513900	-2.73672800	-0.22336300
C 6	-6.04002200	-2.03805100	-0.30953100
C 6	-6.04002100	-0.65583200	-0.49158200
C 6	-4.84513800	0.04284600	-0.57774700
C 6	-3.65025600	-0.65583200	-0.49157900
C 6	-2.37583200	0.10307000	-0.50943700
O 8	-2.34619100	1.31764600	-0.52580700
H 1	-4.84513800	1.11861800	-0.69385400
C 6	-7.31444500	0.10307100	-0.50943900
N 7	-8.46249700	-0.64504100	-0.44642600
N 7	-8.46249600	-2.04884200	-0.35471400
C 6	-7.31444600	-2.79695300	-0.29167900
O 8	-7.34408600	-4.01153000	-0.27531600
C 6	-9.69027200	-2.69388500	-0.80114500
H 1	-9.48018700	-3.75611100	-0.86910300
H 1	-10.5009790	-2.53297200	-0.09233200
H 1	-9.97447600	-2.30334300	-1.78026700
C 6	-9.69027600	-0.00000100	0.00000000
H 1	-10.5009820	-0.16092700	-0.70881000
H 1	-9.97447700	-0.39053400	0.97912700
H 1	-9.48019800	1.06222700	0.06794700
O 8	-7.34408400	1.31764800	-0.52579500
H 1	-4.84514000	-3.81250100	-0.10725700
O 8	-2.34619300	-4.01153100	-0.27534300
C 6	-0.00001000	-2.69388700	-0.80114500
H 1	0.28417900	-2.30334900	-1.78027300
H 1	0.81070500	-2.53297000	-0.09234400
H 1	-0.21009600	-3.75611300	-0.86909600
H 1	-0.21008300	1.06222600	0.06795800
H 1	0.28421300	-0.39054000	0.97911900
H 1	0.81070000	-0.16091500	-0.70882100

Table S7. Cartesian Coordinates for N,N′-diphenylpyromellitic diimide

Atom	X	Y	Z
N 7	0.00000000	0.00000000	0.00000000
C 6	-0.00182100	1.16215100	0.79129500
C 6	0.00000000	0.69376800	2.21056300
C 6	0.00031600	1.44416500	3.37379500
C 6	0.00000000	0.69376800	4.53702700
C 6	-0.00000000	-0.69376800	4.53702700
C 6	-0.00031600	-1.44416500	3.37379500
C 6	-0.00000000	-0.69376800	2.21056300
C 6	0.00182100	-1.16215100	0.79129500
O 8	0.00388400	-2.29153900	0.39397500
H 1	-0.00016700	-2.52669300	3.37379500
C 6	0.00182100	-1.16215100	5.95629500
N 7	0.00000000	0.00000000	6.74759000
C 6	-0.00182100	1.16215100	5.95629500
O 8	-0.00388400	2.29153900	6.35361500
C 6	-0.00000000	-0.00000000	8.17237000
C 6	0.82560900	-0.88221500	8.85877100
C 6	0.81678100	-0.88090200	10.2454580
C 6	-0.00000000	-0.00000000	10.9414070
C 6	-0.81678100	0.88090200	10.2454580
C 6	-0.82560900	0.88221500	8.85877100
H 1	-1.45713600	1.56736900	8.31096300
H 1	-1.45518500	1.57074200	10.7819970
H 1	-0.00000000	-0.00000000	12.0237760
H 1	1.45518500	-1.57074200	10.7819970
H 1	1.45713600	-1.56736900	8.31096300
O 8	0.00388400	-2.29153900	6.35361500
H 1	0.00016700	2.52669300	3.37379500
O 8	-0.00388400	2.29153900	0.39397500
C 6	-0.00000000	-0.00000000	-1.42478000
C 6	0.82560900	-0.88221500	-2.11118100
C 6	0.81678100	-0.88090200	-3.49786800
C 6	-0.00000000	-0.00000000	-4.19381700
C 6	-0.81678100	0.88090200	-3.49786800
C 6	-0.82560900	0.88221500	-2.11118100
H 1	-1.45713600	1.56736900	-1.56337300
H 1	-1.45518500	1.57074200	-4.03440700
H 1	-0.00000000	-0.00000000	-5.27618600
H 1	1.45518500	-1.57074200	-4.03440700
H 1	1.45713600	-1.56736900	-1.56337300

Table S8. Cartesian Coordinates for N,N′-tetramethylpyromellitic dihydrazide

N	7	0.00000000	0.00000000	0.00000000
N	7	0.00000300	1.37192500	0.31083800
C	6	-1.15138300	2.13845700	0.29919000
O	8	-1.13103700	3.33130100	0.49768200
C	6	-2.42309100	1.38286600	0.16057300
C	6	-3.61781800	2.08672700	0.15510000
C	6	-4.81258800	1.38289600	0.15002200
C	6	-6.08428000	2.13847600	0.01115500
N	7	-7.23574900	1.37205400	0.00006500
N	7	-7.23572300	0.00010600	0.31095700
C	6	-6.08431700	-0.76636700	0.29986300
C	6	-4.81260200	-0.01084200	0.16094200
C	6	-3.61785200	-0.71471000	0.15588400
C	6	-2.42310900	-0.01089200	0.15040900
C	6	-1.15141300	-0.76652500	0.01179100
O	8	-1.13109500	-1.95938900	-0.18660400
H	1	-3.61788400	-1.79678100	0.15617200
O	8	-6.10466500	-1.95912500	0.49894700
C	6	-8.40166500	-0.45982100	1.01109800
C	6	-8.98505100	0.36017800	1.97004700
C	6	-10.1151600	-0.07490700	2.64406800
C	6	-10.6591300	-1.32235100	2.36712200
C	6	-10.0701780	-2.13144900	1.40577000
C	6	-8.94476500	-1.70290000	0.71583300
H	1	-8.48086200	-2.32711600	-0.03339500
H	1	-10.4907570	-3.10326100	1.18166600
H	1	-11.5410650	-1.65972300	2.89597500
H	1	-10.5689690	0.56422700	3.39041800
H	1	-8.55909100	1.33307700	2.17896500
C	6	-8.40149300	1.83189000	-0.70047900
C	6	-8.98456800	1.01183100	-1.65956500
C	6	-10.1144440	1.44687600	-2.33400300
C	6	-10.6584860	2.69435700	-2.05736400
C	6	-10.0698380	3.50351100	-1.09587800
C	6	-8.94466900	3.07499600	-0.40551400
H	1	-8.48105900	3.69925800	0.34387000
H	1	-10.4904400	4.47536700	-0.87200800
H	1	-11.5402330	3.03170300	-2.58654200
H	1	-10.5680220	0.80768000	-3.08044300
H	1	-8.55854400	0.03891500	-1.86826400
O	8	-6.10460400	3.33125900	-0.18782600
H	1	-3.61782600	3.16880000	0.15482300
C	6	1.16577600	1.83177200	1.01126300
C	6	1.70871200	3.07509600	0.71668200
C	6	2.83397300	3.50351600	1.40698300
C	6	3.42298500	2.69410700	2.36800300
C	6	2.87920600	1.44640500	2.64423400

C	6	1.74927700	1.01142500	1.96987500
H	1	1.32353600	0.03832400	2.17829600
H	1	3.33304400	0.80696100	3.39030600
H	1	4.30478200	3.03138400	2.89713700
H	1	3.25434300	4.47553100	1.18335000
H	1	1.24487300	3.69963000	-0.03231300
C	6	1.16559400	-0.45983300	-0.70074500
C	6	1.70864900	-1.70312200	-0.40622800
C	6	2.83369200	-2.13158400	-1.09684400
C	6	3.42238800	-1.32223900	-2.05812300
C	6	2.87851300	-0.07457200	-2.33427800
C	6	1.74878900	0.36044500	-1.65959200
H	1	1.32298200	1.33352800	-1.86795600
H	1	3.33209700	0.56482200	-3.08054400
H	1	4.30402900	-1.65955300	-2.58749700
H	1	3.25416000	-3.10357200	-0.87327200
H	1	1.24506100	-2.32759000	0.34297400