Supporting information

Sensitizing the phosphorescence of pyromellitic diimide through non-covalent halogen-carbonyl interactions

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Table of Contents

1. General Methods
2. Synthetic Schemes and Procedures
3. Experimental Procedures
4. Supporting Figures
5. Supporting Characterization Original data
6. References

General Methods:

Spectroscopic Measurements: The excitation and emission spectra were recorded on FLS1000 spectrometer, Edinburgh Instruments.

Lifetime and quantum yield measurements: Phosphorescence lifetime ($\lambda_{exc.}$ = 340 nm), gated emission, and time-resolved emission were measured on FLS1000 spectrometer, Edinburgh Instruments equipped with a micro flash-lamp (μF2) set-up. Quantum yields were measured using an integrating sphere in the same instrument. Fluorescence lifetimes were performed on a Horiba Delta Flex time-correlated single-photon-counting (TCSPC) instrument with a 375 nm laser diode as the light source. The instrument response function (IRF) was collected by using a scatterer (Ludox AS40 colloidal silica, Sigma-Aldrich).

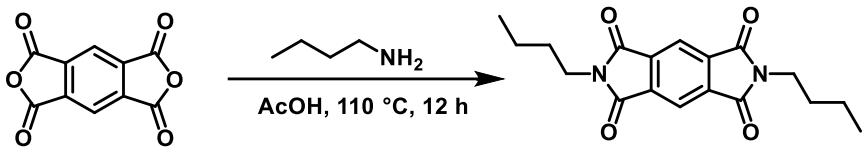
Single Crystal X-ray Crystallography: Suitable single cocrystal of the **PmDI-TBB** and **PmDI-HBB** was mounted on a thin glass fibre with commercially available super glue. Intensity data were collected in Bruker D8 VENTURE diffractometer equipped with a PHOTON detector and graphite-monochromated Mo-Kα radiation (λα = 0.71073 Å, 50 kV, 1mA) at 100 K. APEX III software was used to collect, reduce and integrate the raw data. The direct method was used for solving crystal structure, followed by fullmatrix least-squares refinements against F2 (all data HKLF 4 format) using the SHELXL 2014/7 and difference Fourier synthesis and least-squares refinement revealed the positions of the non-hydrogen atoms. All non-hydrogen atoms were refined anisotropically and remaining hydrogen atoms were placed in geometrically constrained positions and refined with isotropic temperature factors,

generally 1.2 × Ueq of their parent atoms. Molecular structure drawings were prepared using the program Mercury (version 3.1).

There are some B-Alerts in PMDI-TBB upon cif-file check which are generated because the structure has some amount of disorder. C11 and C12 carbon atoms of the butyl chain are modelled isotropically as their contribution to the scattering is affected by the disorder. Dynamically disordered chains (that are tethered to a relatively rigid backbone) may exhibit unusual ratios for NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range.

Synthetic Scheme and Procedure:

Pyromellitic dianhydride (PMDA) was purchased from Sigma Aldrich; 1,2,4,5-Tetrabromobenzene and Hexabromobenzene were purchased from TCI, Acetic acid was purchased from Spectrochem and used without further purification.



Synthetic procedure of PmDI: Compound was synthesized according to the literature procedure.[S1]

Experimental Procedures:

Protocol for co-crystal synthesis: 0.05 M solution of both donor and acceptor in a 1:1 molar ratio in DMF was prepared. Then the mixture was heated at 70 °C until it gets fully dissolved and then kept at room temperature for cocrystallization.

Protocol for sample preparation: The phosphorescence studies of the cocrystal were done by taking a small amount of the cocrystal between two quartz plates. Solution phase studies were done by taking compounds ([c] = 10^{-5} M) in THF. For neat film studies, donor-acceptor 1:1 mixture in DMF was taken and then drop-casted on a clean quartz substrate. The drop-casted films were dried in vacuum oven at 60°C until the DMF was completely removed.

Supporting Figures:

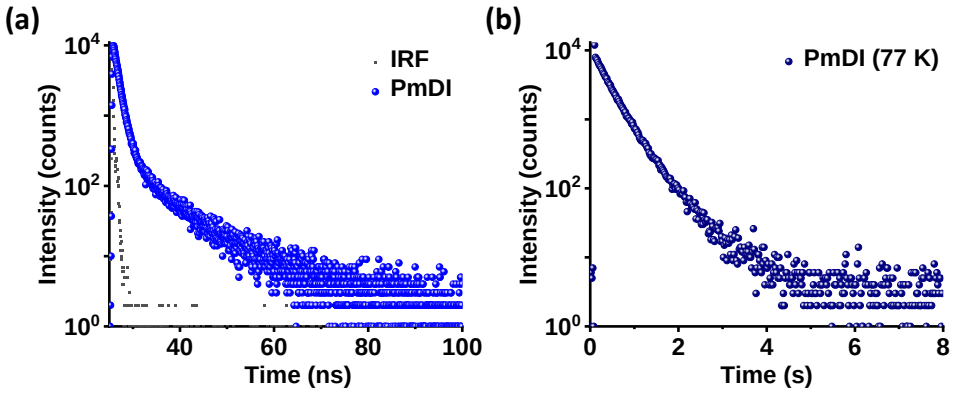


Figure S1. Lifetime decay profiles of **PmDI** ([c] = 10^{-5} M) in THF (a) at room temperature ($\lambda_{exc.}$= 375 nm, $\lambda_{monitored}$ = 450 nm) and (b) at 77 K ($\lambda_{exc.}$= 340 nm, $\lambda_{monitored}$ = 550 nm).

Note: **PmDI** at room temperature exhibited characteristic fluorescence with maximum at 434 nm and corresponding nanosecond lifetime of 2.17 ns in THF. Upon freezing to 77 K glassy matrix, a red-shifted band was observed at 500 nm with an average decay time of 0.4 s, suggesting it to be **PmDI** phosphorescence. At cryogenic conditions, the triplet state of **PmDI** gets activated because of reduced non-radiative vibrational relaxations.

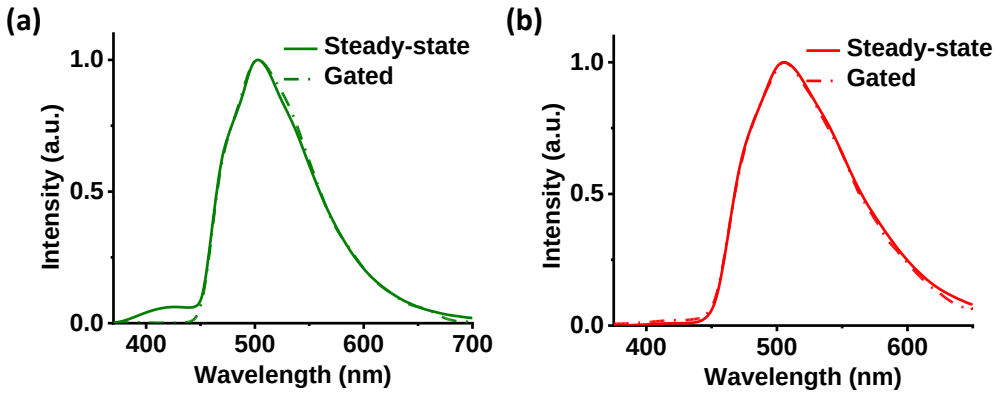


Figure S2. Steady-state and gated emission (1 ms delay) spectra of (a) **PmDI-TBB** (b) **PmDI-HBB**, which prove the presence of a delayed component ($\lambda_{exc.}$= 340 nm).

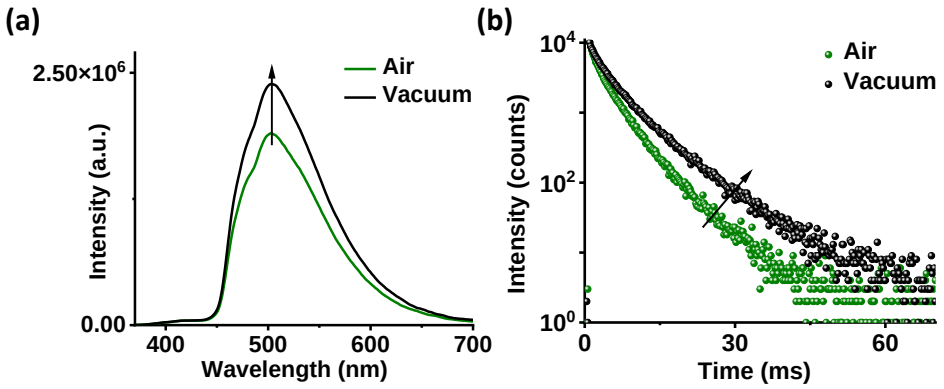


Figure S3. (a) Emission spectra of **PmDI-TBB** in the presence and in absence of air ($\lambda_{exc.}$= 340 nm). (b) Lifetime decay profile of **PmDI-TBB** in the presence and in absence of air ($\lambda_{exc.}$= 340 nm, $\lambda_{monitored}$ = 550 nm).

Note: Reduced emission intensity and lifetime in the presence of air (oxygen) suggested triplet contribution in the emission.

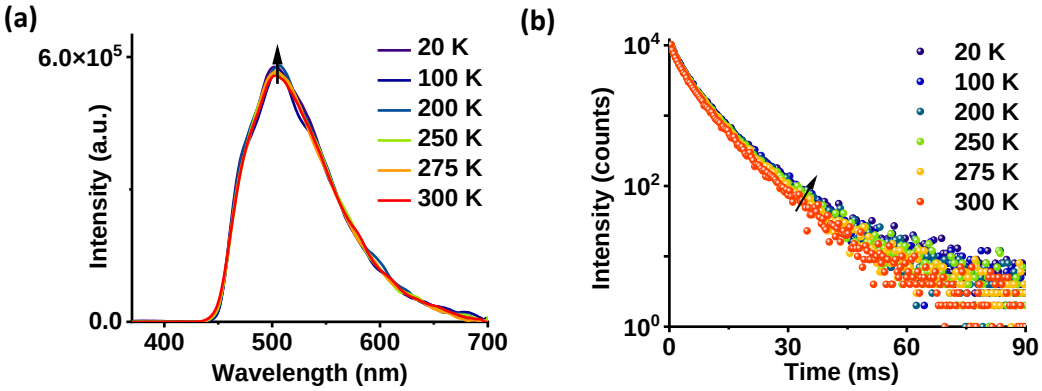


Figure S4. Temperature-dependent (a) gated emission spectra (1 ms delay; $\lambda_{exc.}$= 340 nm) and (b) lifetime decay profiles ($\lambda_{exc.}$ = 340 nm, $\lambda_{monitored}$ = 550 nm) for **PmDI-TBB** cocrystal.

Note: Upon gradually lowering the temperature from 300 K to 20 K, the emission intensity and lifetime enhanced due to reduced thermal vibration that validified the nature of emission to be phosphorescence. However, the changes in emission and lifetime were not so significant at lower temperatures, which is assumed to be due to pre-existing constrained vibrational motion of the molecules within the cocrystal.

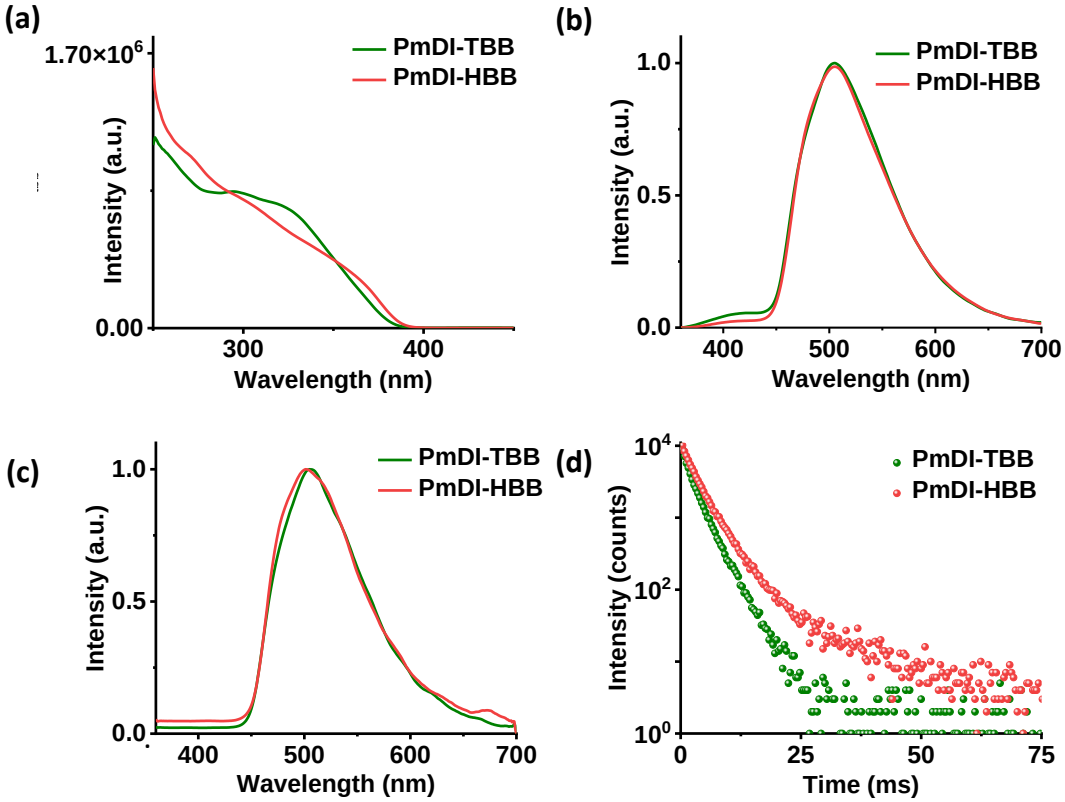


Figure S5. Neat-film studies for **PmDI-TBB** and **PmDI-HBB**: (a) excitation spectra ($\lambda_{monitored}$ = 550 nm), (b) normalized steady-state emission spectra ($\lambda_{exc.}$= 340 nm). (c) Normalized gated emission spectra (1 ms delay time, $\lambda_{exc.}$ = 340 nm), (d) lifetime decay profile ($\lambda_{exc.}$= 340 nm, $\lambda_{monitored}$ = 550 nm).

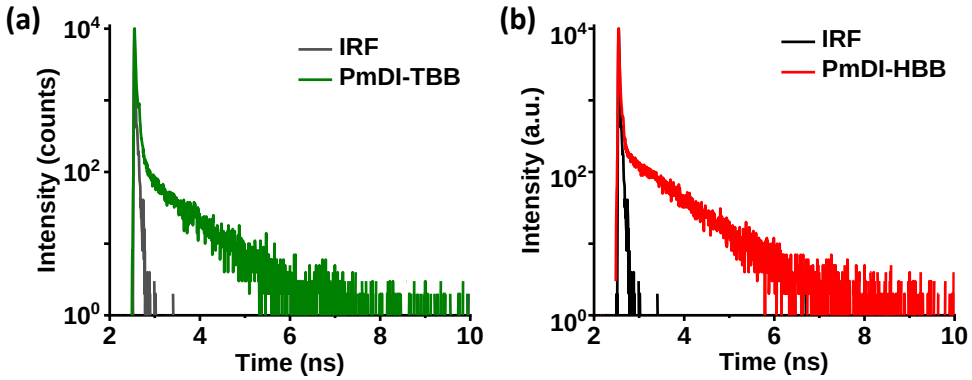


Figure S6. Fluorescence lifetime decay profiles of a) **PmDI-TBB**, and b) **PmDI-HBB** cocrystal ($\lambda_{exc.}$ = 373 nm, $\lambda_{monitored}$ = 420 nm).

	$\lambda_{exc.}$(nm)	$\lambda_{collected}$ (nm)	τ_1	τ_2	τ_3	$<\tau_{avg.}>$
PmDI (rt)	375	450	2.50 ns (16 %)	0.81 ns (73 %)	10.76 ns (11 %)	2.17 ns
PmDI (77 K)	340	550	0.31 s (73 %)	0.66 s (27 %)	-	0.40 s

Table S1. Summary of **PmDI** lifetime decay in 10^{-5} (M) THF solution at different temperatures.

	$\lambda_{exc.}$ (nm)	$\lambda_{collected}$ (nm)	τ_1 (ms)	τ_2 (ms)	τ_3 (ms)	$<\tau_{avg.}>$ (ms)
PmDI-TBB (air)	340	550	1.76 ms (36 %)	5.22 ms (64 %)	-	3.97 ms
PmDI-TBB (vacuum)	340	550	2.91 ms (43 %)	7.88 ms (57 %)	-	5.74 ms
PmDI-HBB (air)	340	550	1.26 ms (14 %)	3.17 ms (78 %)	8.41 ms (8 %)	3.32 ms
PmDI-HBB (vacuum)	340	550	1.64 ms (29 %)	3.68 ms (69 %)	17.21 ms (2 %)	3.35 ms

Table S2. Summary of phosphorescence decay for **PmDI-TBB** and **PmDI-HBB** cocrystals under air and vacuum at room temperature.

	$\lambda_{exc.}$ (nm)	$\lambda_{collected}$ (nm)	τ_1 (ms)	τ_2 (ms)	τ_3 (ms)	$<\tau_{avg.}>$ (ms)
PmDI-TBB (20 K)	340	550	2.85 ms (28 %)	7.73 ms (67 %)	25.93 ms (5 %)	7.27 ms
PmDI-TBB (300 K)	340	550	2.86 ms (45 %)	8.26 ms (55 %)	-	5.83 ms
PmDI-HBB (20 K)	340	550	3.99 ms (95 %)	33.32 ms (5 %)	-	5.45 ms
PmDI-HBB (300 K)	340	550	2.35 ms (68 %)	5.32 ms (32 %)	-	3.30 ms

Table S3. Summary of phosphorescence decay of **PmDI-TBB** and **PmDI-HBB** cocrystals at different temperatures.

Cocrystal	k_P^r**(s^{-1})**	k_{nr}**(s^{-1})**	k_{ISC}**(s^{-1})**
PmDI-TBB	136.02	115.86	7.71×10^8
PmDI-HBB	126.50	174.69	1.58×10^8

k_P^r(s^{-1}) = $\Phi_P/<\tau>_P$; k_{nr} = (1- Φ_P)/ $<\tau>_P$; k_{ISC} = $\Phi_P/<\tau>_F$

Table S4. Summary k_P^r(s^{-1}), k_{ISC}(s^{-1}), and k_{nr}(s^{-1}) of **PmDI-TBB** and **PmDI-HBB** .

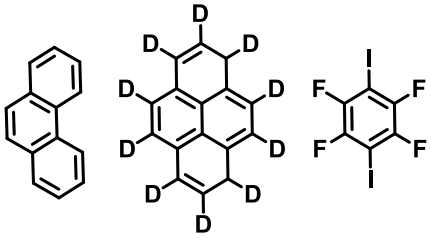
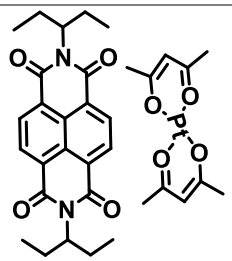
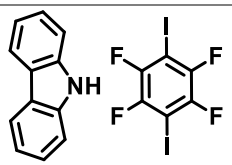
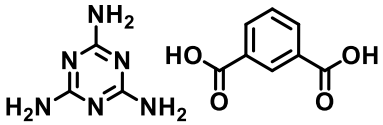
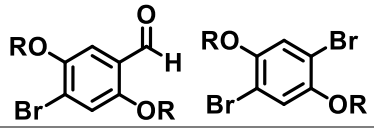
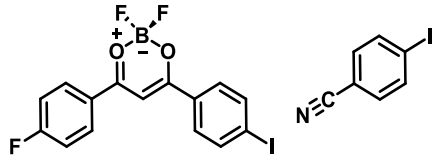
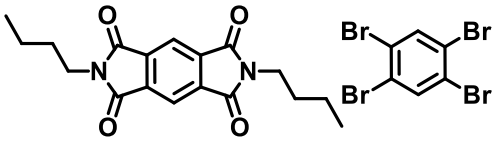
Co-crystals	Phosphorescence QY (Types of crystal)	References
	26 % (Cocrystal)	S2
	25 % (Cocrystal)	S3
	33 % (Cocrystal)	S4
	24 % (Cocrystal)	S5
	55 % (Doped crystal)	S6
	62 % (Doped crystal)	S7
	**54 % (Cocrystal)**	**This work**

Table S5. Summary of existing reported highly efficient cocrystal phosphorescence QY in comparison with this work.

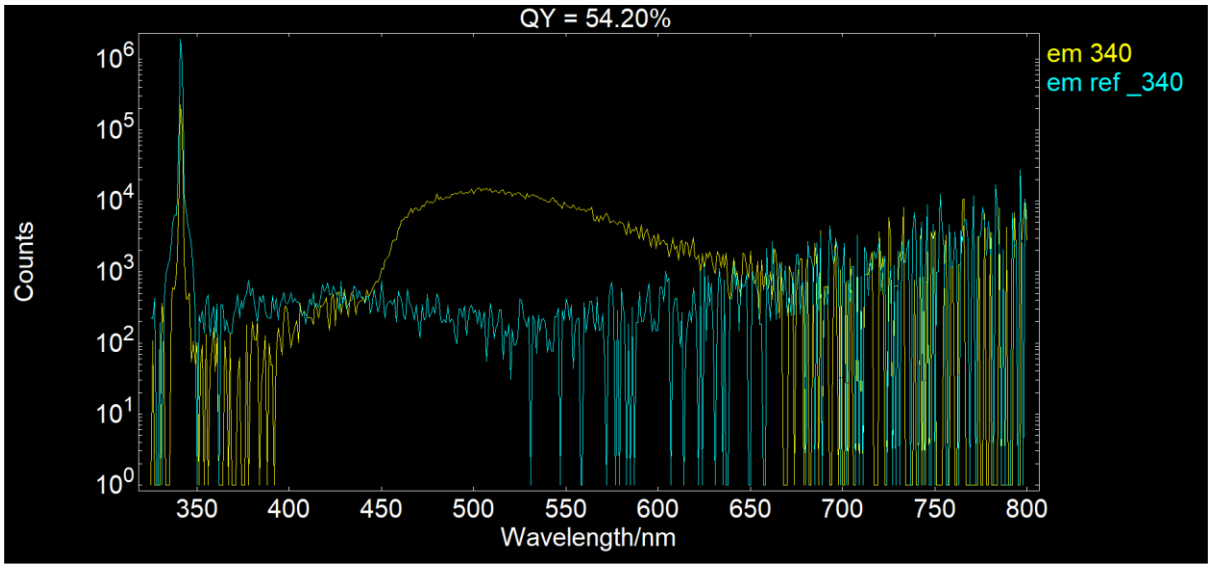


Figure S7. Screenshot of phosphorescence quantum yield for **PmDI-TBB** cocrystal.

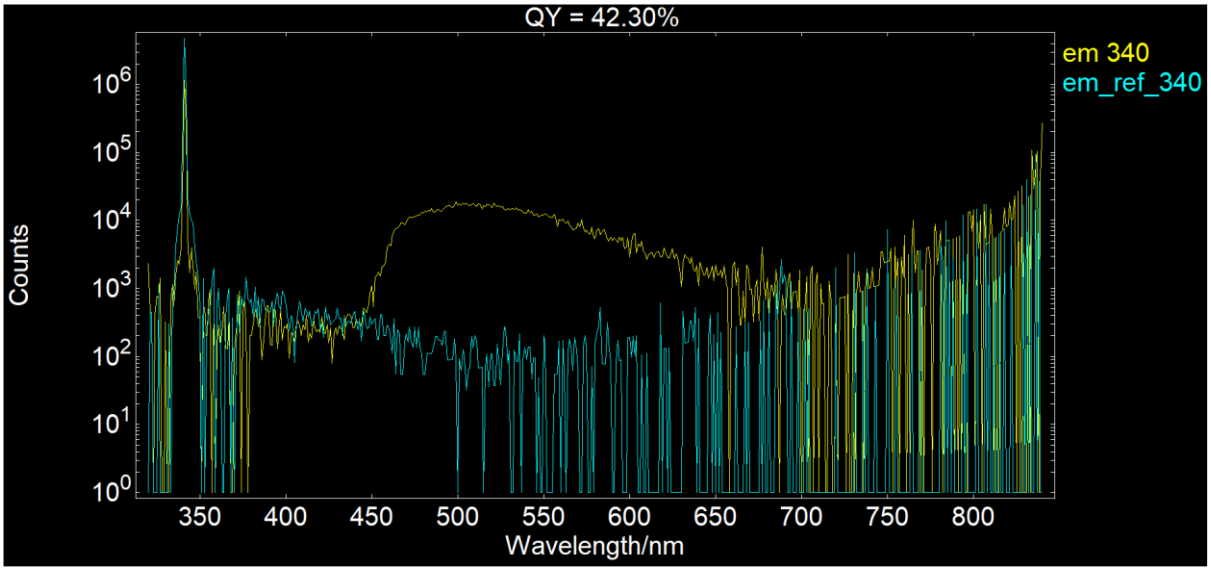


Figure S8. Screenshot of phosphorescence quantum yield for **PmDI-HBB** cocrystal.

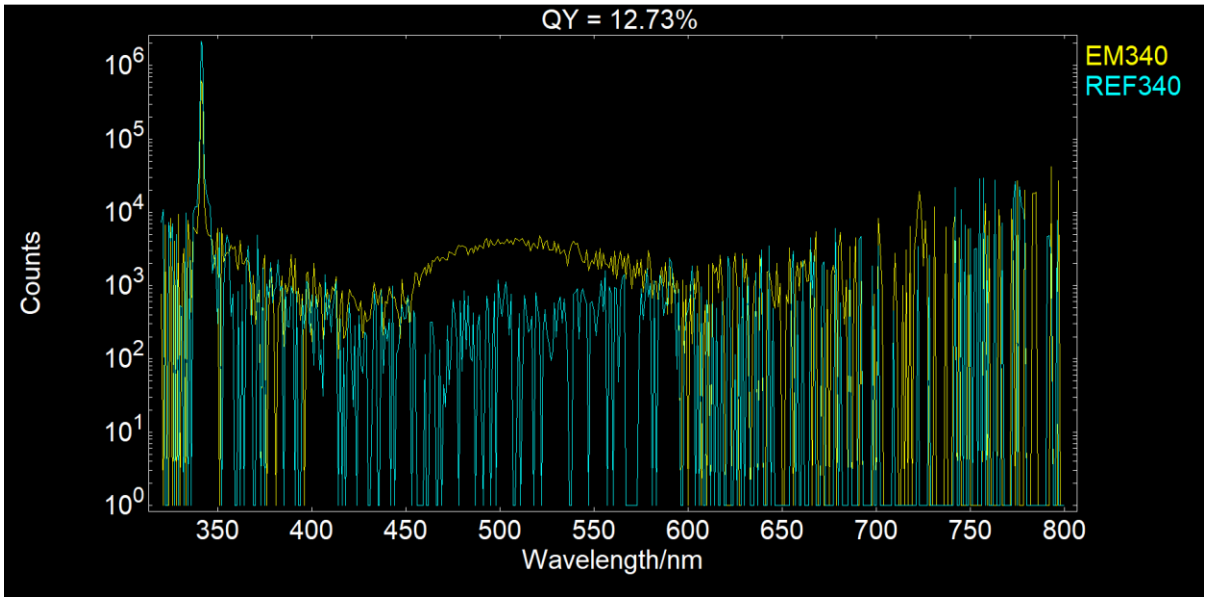


Figure S9. Screenshot of phosphorescence quantum yield for **PmDI-TBB** neat film.

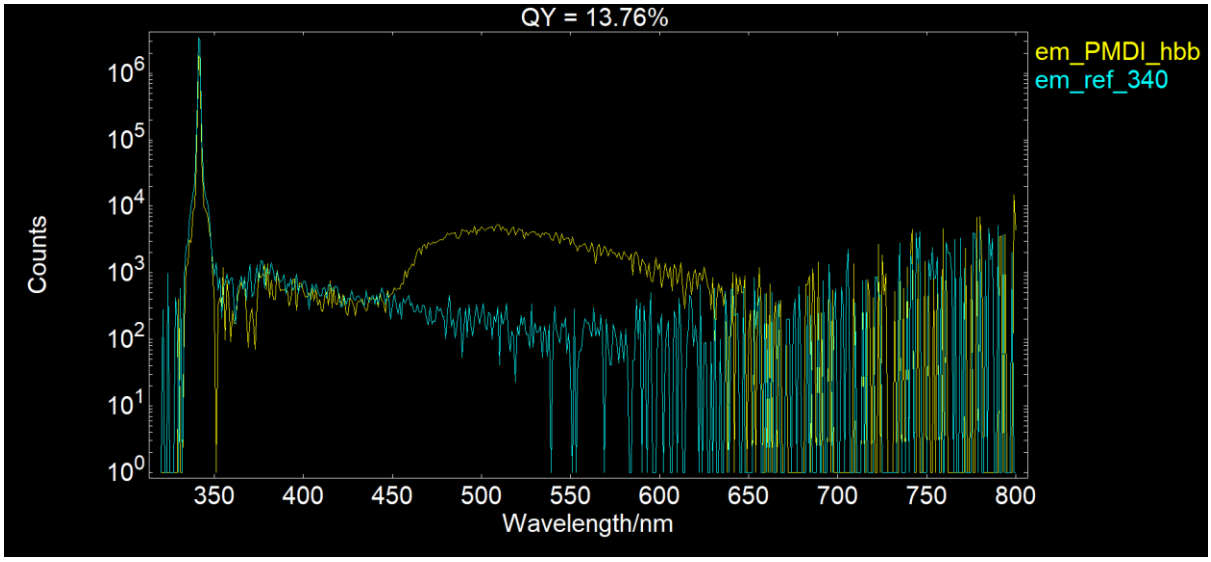


Figure S10. Screenshot of phosphorescence quantum yield for **PmDI-HBB** neat film.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

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Bond precision:   C-C = 0.0039 A          Wavelength=0.71073

Cell:           a=5.3021(3)       b=10.5026(8)      c=12.7532(9)
                alpha=76.068(3)   beta=80.338(3)    gamma=84.483(3)
Temperature:    301 K

                Calculated                  Reported
Volume          678.35(8)                   678.35(8)
Space group     P -1                        P -1
Hall group      -P 1                        -P 1
Moiety formula  C18 H20 N2 O4, C6 Br6       ?
Sum formula     C24 H20 Br6 N2 O4           C3 H2.50 Br0.75 N0.25 O0.50
Mr              879.82                      109.98
Dx,g cm-3       2.154                       2.154
Z               1                           8
Mu (mm-1)       8.912                       8.912
F000            420.0                       420.0
F000'           418.58
h,k,lmax        6,12,15                     6,12,15
Nref            2395                        2392
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Tmin'           0.371

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test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

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PLAT431_ALERT_2_B Short Inter HL..A Contact  Br01     ..O1       .       3.05 Ang.
                                          2-x,1-y,1-z  =      2_766 Check
PLAT431_ALERT_2_B Short Inter HL..A Contact  Br02     ..O2       .       3.02 Ang.
                                          x,y,z  =      1_555 Check
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Alert level C

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PLAT218_ALERT_3_C Constrained U(i,j) Components(s) for O2                   6 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
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Alert level G

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          3 Note
            Br01    Br02    Br03
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         78% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
              0   1   0,    0   0   1,
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
             -1   2   0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
              0   1   0,
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged      Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..        50.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       2.123 Note
            Predicted wR2: Based on SigI**2  2.85 or SHELX Weight  6.29
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          6 Info
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```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  12 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 15/07/2024; check.def file version of 15/07/2024

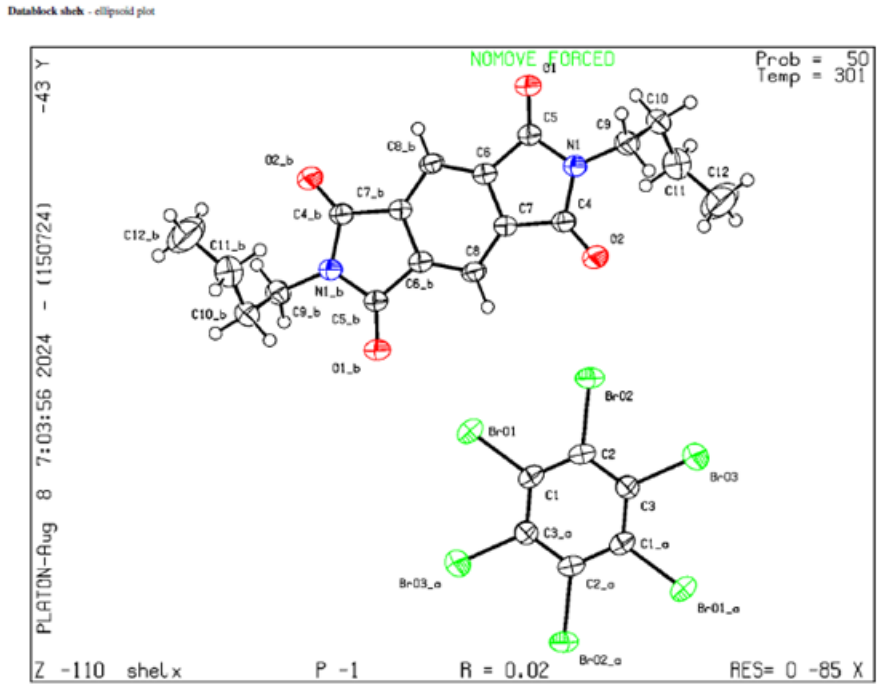

Figure S11. Check CIF documents for **PmDI-HBB** cocrystal.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

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                alpha=71.087(3)   beta=81.499(3)    gamma=86.355(3)
Temperature:    214 K
```

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Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H20 N2 O4, C6 H2 Br4	?
Sum formula	C24 H22 Br4 N2 O4	C3 H2.75 Br0.50 N0.25 O0.50
Mr	722.04	90.26
Dx,g cm-3	1.798	1.798
Z	1	8
Mu (mm-1)	6.067	6.067
F000	352.0	352.0
F000'	351.05	
h,k,lmax	6,12,14	6,12,14
Nref	2337	2328
Tmin,Tmax	0.804,0.886	0.518,0.746
Tmin'	0.483	

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                                                 0.1061( 2328)
S = 1.088                 Npar= 137
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Click on the hyperlinks for more details of the test.

Alert level B

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            C11     C12
PLAT220_ALERT_2_B NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        7.2 Ratio
PLAT431_ALERT_2_B Short Inter HL..A Contact  Br01     ..O1       .        3.02 Ang.
                                                   x,y,z  =      1_555 Check
PLAT431_ALERT_2_B Short Inter HL..A Contact  Br02     ..O2       .        3.03 Ang.
                                          2-x,1-y,1-z  =      2_766 Check
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Alert level C

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C11 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00855 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C10      - C11      .        1.35 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C11      - C12      .        1.41 Ang.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4     Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595          7 Report
              -1  2  0,   0  3  0,   1 -2  1,   1  1  1,   0  3  1,   1  3  1,
               0  0  3,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          4 Note
              -1  2  0,   1 -2  1,   1  1  1,   0  0  3,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
PLAT977_ALERT_2_C Check Negative Difference Density on H10B      .      -0.32 eA-3
```

Alert level G

```
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.125 Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.003 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          2 Note
            Br01    Br02
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         71% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
               0  1  0,   0  0  1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
               0  1  0,
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..        50.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       4.852 Note
            Predicted wR2: Based on SigI**2  2.19 or SHELX Weight  9.76
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          3 Info
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

```
  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
  2 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 15/07/2024; check.def file version of 15/07/2024

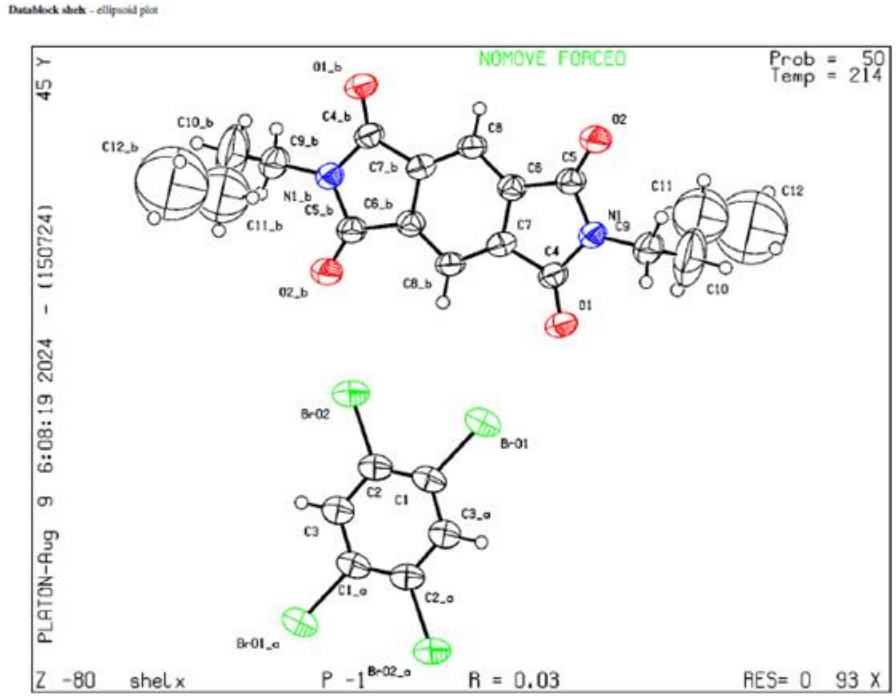

Figure S12. Check CIF documents for **PmDI-TBB** cocrystal.

Supporting Characterization Original data:

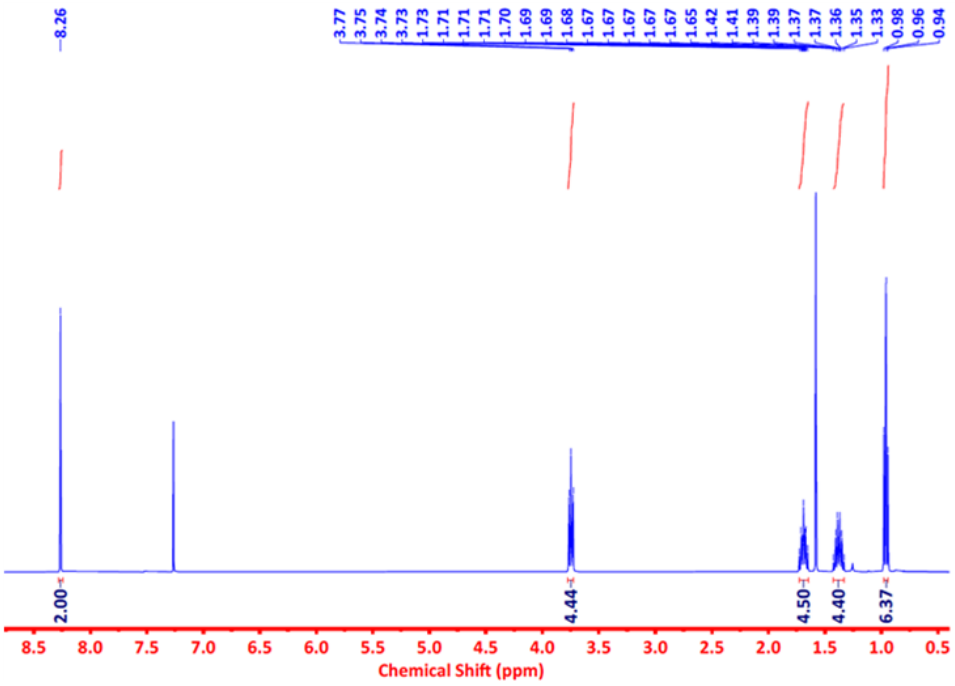

Figure S13. ^{1}H NMR spectrum of **PmDI** in $CDCl_3$.

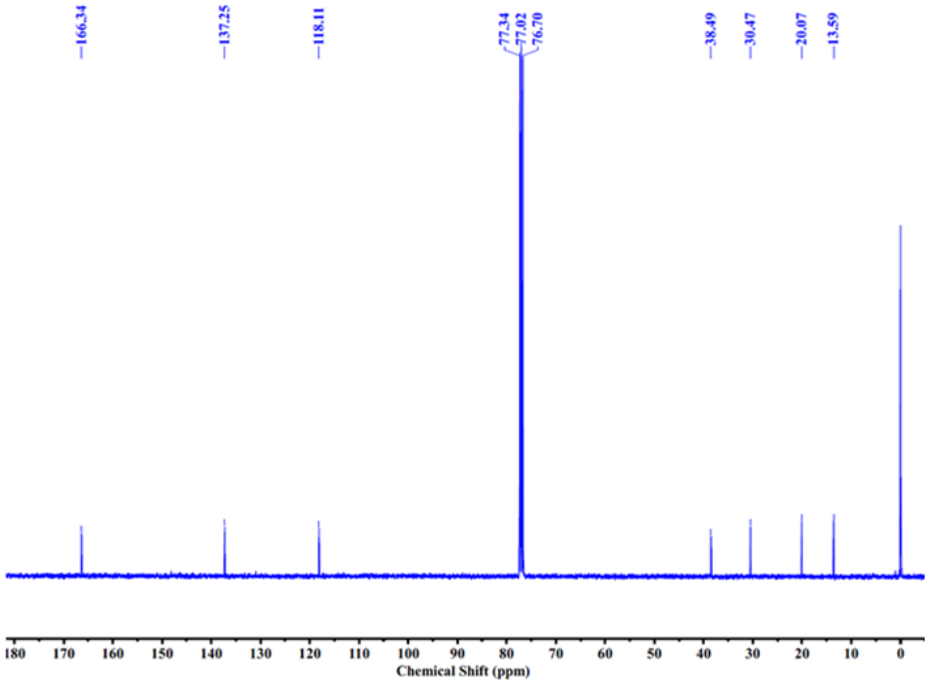

Figure S14. ^{13}C NMR spectrum of **PmDI** in $CDCl_3$.

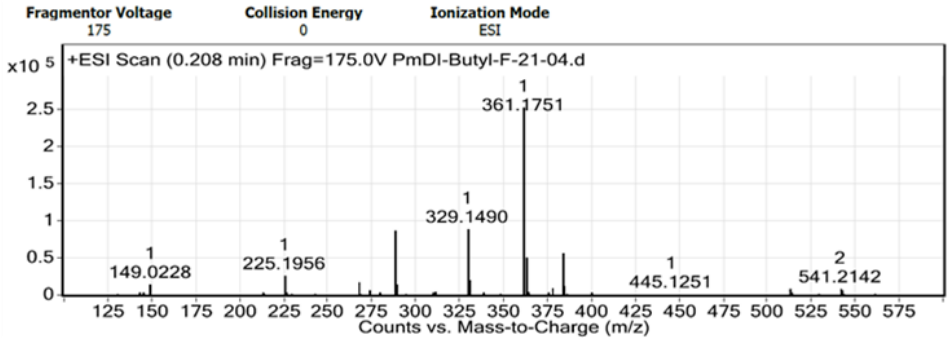

Figure S15. ESI-HRMS spectrum of **PmDI**.

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