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Bisphosphonium Benzene Diimides

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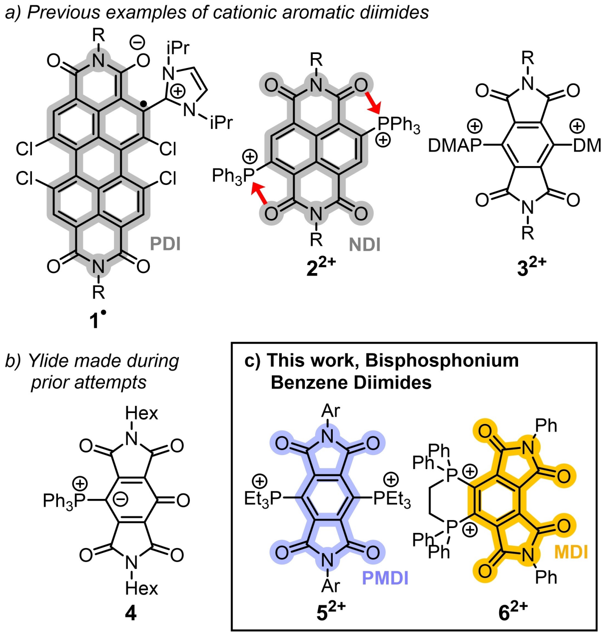
The incorporation of cationic groups onto electron-poor compounds is a viable strategy for achieving potent electron acceptors, as evidenced by reports of air-stable radical forms of large aromatic diimides such as naphthalene and perylene diimides. These ions have also been observed to exhibit anion–π interaction tendencies of interest in molecular recognition applications. The benefits of phosphonium incorporation, however, have not yet been extended to the smallest benzene diimides. Here, we report that dibrominated pyromellitic diimide and mellophanic diimide both readily undergo substitution reactions with phosphine sources to yield bisphosphonium compounds. In the single crystalline form, these dications display anion-π interactions and, in the case of mellophanic diimide, the stabilization of a bromide–water H–bonding ring pattern. The reaction of these dications with chemical reductants readily provides the singly and doubly reduced redox states, which were characterized by UV-vis spectroscopy and found to exhibit intense absorptions extending into the near-IR region. Taken together, this work demonstrates that phosphonium incorporation onto congested aromatic diimide scaffolds is synthetically viable and produces unusual electron-poor compounds.

Electron-accepting compounds are of wide interest as active material in n-type electronic devices,[1–9] partners for (supra)molecular charge-transfer recognition,[10–17] building blocks for optically interesting materials,[7,18–21] and as platforms for stabilizing radical electrons.[22–27] One well-known class of such compounds consists of aromatic diimides, which have been exploited both as single molecules and as building blocks for polymers. In an effort to enhance the electron-accepting nature of these aromatic diimides, one strategy that has emerged is the incorporation of cationic groups directly onto aromatic core (Figure 1a). Würthner et al. described the serendipitous discovery of a perylene diimide (PDI) zwitterionic radical (**1**).[28] Wu et al.[29] and Mukhopadhyay et al.[30–32] have studied phosphonium naphthalene diimides (NDIs, **2**$^{2+}$) for both radical stabilization and anion recognition. We have focused on the benzene diimides and previously reported pyridinium-functionalization of pyromellitic diimide (PMDI, **3**$^{2+}$)[33] in addition to the isolation of an unexpected stable phosphonium ylide (**4**)[34] from our initial attempts to produce a bisphosphonium PMDI.

While in most cases cationic groups exert what can be understood as an inductive stabilization of LUMO levels, Mukhopadhyay et al.[30–32] have demonstrated through NBO calculations that for the bisphophonium NDIs, the phosphonium groups located adjacent to carbonyl groups are additionally stabilized by an unusual O···P$^+$ interaction that can be conceived as a $n_O \rightarrow \sigma^*_{P-C}$ interaction (Figure 1a, red arrows). Remarkably, the singly reduced states of bisphosphonium-NDIs are found to be stable to column chromatography under ambient conditions[30] and the doubly reduced states can be synthesized and characterized in air.[32] With these prior examples in mind, we sought to determine whether the same LUMO-stabilizing effects of phosphoniums could be extended to the smaller benzene diimides, namely pyromellitic diimide (PMDI) and its structural isomer mellophanic diimide (MDI).[35–37]


a) Previous examples of cationic aromatic diimides

b) Ylide made during prior attempts

c) This work, Bisphosphonium Benzene Diimides

Figure 1. a) Previously published examples of cationically modified aromatic diimides. DMAP = 4-(dimethylamino)pyridin-1-yl). b) The structure of an unexpected phosphonium ylide produced in previous attempts to synthesize bisphosphonium PMDIs. c) Structural formula of the compounds described herein. Ar = 2,6-diisopropylphenyl.

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Our previous efforts began with the reaction of dibromo-PMDI with triphenylphosphine. It was from those initial attempts that we discovered the unexpected formation of **4** (Figure 1b) through what we presume to be a hydrolytic process.[34]

We began our efforts toward the preparation of bisphosphonium benzene diimides (Figure 1c) by evaluating the reaction of smaller phosphine nucleophiles with halogenated PMDIs. Gratifyingly, heating $Et_3P^{\bullet}HBF_4$ and dibromominated PMDI **7** in THF at 125 °C in a microwave reactor produced **5·2BF$_4$** (Figure 2a), which precipitated out of the reaction mixture in 73 % yield. The identity of the counteranion as BF_4^- and not Br^- was definitively assigned through a combination of ^{19}F NMR spectroscopy and single crystal X-ray crystallography (*vide infra*). Presumably, HBr is generated as a byproduct of the reaction. When planning the preparation of a bisphosphonium-MDI, we were inspired by our success with using 1,2-dinucleophiles for the synthesis of azaacenes[38–40] and thus evaluated (diphenylphosphino)ethane (dppe) as the nucleophilic phosphine source. Heating dibromo-MDI **8** and dppe either in refluxing MeCN or at 125 °C under microwave conditions successfully yielded **6·2Br** (Figure 2b). The compound precipitated out of solution as an orange solid upon cooling of the reaction mixture to room temperature and excess reactants were triturated away by rinsing with CH_2Cl_2.

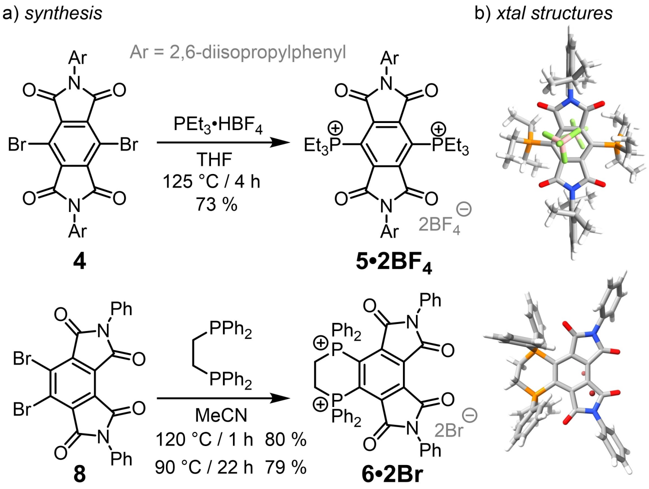

Figure 2. a) Synthesis and b) single-crystal X-ray structures of compounds **5·2BF$_4$** and **6·2Br**.

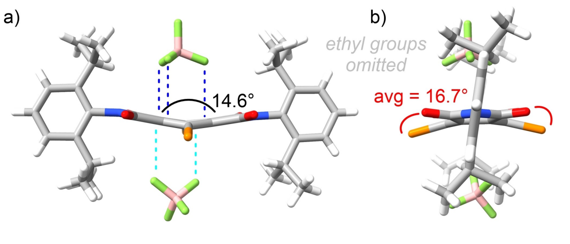

Figure 3. Crystal structure of **5·2BF$_4$** with ethyl groups removed. a) An edge-on view shows the bending of the central benzene ring. F···π close contacts are indicated by blue and teal dashed lines. b) Viewing along the N–N axis reveals torsion between C═O and C–P$^+$. Colors: C = gray, H = white, F = green, N = blue, O = red, P = orange, B = pink.

The identity of the bisphosphoniums was confirmed by single crystal X-ray crystallography (Figure 2b). Single crystals of **5·2BF$_4$** were grown from a supersaturated THF solution. The compound crystallizes in the $P2_1/n$ space group. For **5·2BF$_4$**, the steric demand of the triethylphosphoniums is evidenced by the significant distortions of the PMDI core away from planarity. The central benzene ring is substantially puckered into a cyclohexane boat-like shape, with a puckering angle of 14.6° when measuring between the two planes defined by either edge and the aft/bow carbons of the "boat" (Figure 3a). The curved nature of the core is further demonstrated by the fact that the planes defined by the cyclic imide rings are 19.8° with respect to each other. The triethylphosphoniums deflect the carbonyls with an average torsional angle of 16.7° (Figure 3b). This deflection occurs in a manner that places the two triethylphosphonium groups on the same side of the PMDI core, which then results in two different modes of anion–π interaction between the BF_4 anion and the central benzene ring. The BF_4^- located on the concave side of the PMDI engages three fluorine atoms with the plane defined by all 6 atoms of the central benzene ring at an average distance of 3.034 Å. On the convex side, the BF_4^- is rotated to place only two fluorines in contact with the central benzene ring, with an average anion-π distance of 2.955 Å. When viewed from above, the anions appear to sit within an alkyl pocket that is defined by the ethyl groups of the phosphoniums and the isopropyl groups on the 2,6-diisopropylphenyl group (Figure 2b). Unlike the quinoid form observed in the phosphonium ylide we reported previously,[34] **5·2BF$_4$** maintains a benzenoid core with the six C–C bond lengths being between 1.390 and 1.404 Å in length.

Compound **6·2Br** crystallized from a supersaturated MeCN solution in the $P2_1/c$ space group. The aromatic core in **6·2Br** is more planar than that of **5·2BF$_4$** (Figure 4a), indicating that there is less steric hindrance in the MDI derivative. The asymmetric unit contains two $\mathbf{6^{2+}}$ dications, four Br^- anions,

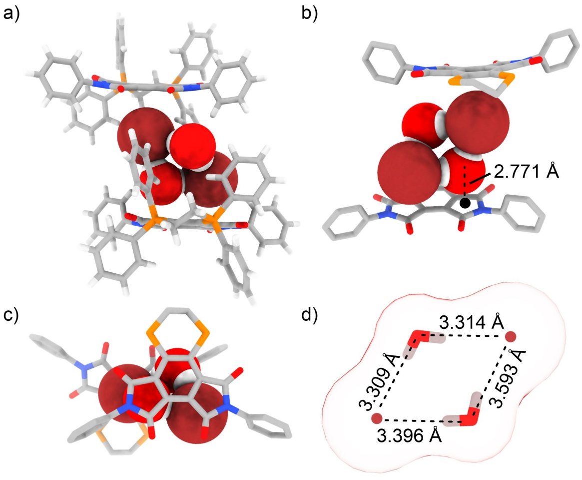

Figure 4. Crystal structure of **6·2Br**. a–c) Different views of the bromide-H_2O tetrad sandwiched between $\mathbf{6^{2+}}$ molecules. d) Isolated plan view of the bromide-H_2O $R_4^2(8)$ ring pattern. In (b) and (c), some phenyl groups and all H are omitted for clarity. Colors: C = gray, H = white, Br = maroon, N = blue, O = red.

and four H_2O molecules. The water molecules are engaged in an interesting halogen/hydrogen bonding arrangement with two bromide ions to form an alternating water/bromide hydrogen-bonding tetrad in a so-called $R_4^2(8)$ ring pattern.[41–44] This tetrad is sandwiched between two molecules of **6**$^{2+}$ (Figure 4a), but the bromides are not centered over the nearby rings as would be expected of typical anion-π interactions, and are instead located over the aromatic C–C bonds (Figure 4b,c). The water O atoms are engaged in clear polar-π interactions with the neighboring cyclic imide, with the closest O to imide centroid distance being 2.771 Å (Figure 4b). The average Br···O distance (3.40 Å) is roughly equal to the expected van der Waals distance of 3.37 Å despite the interceding H atom, confirming that the H-bonding interaction is significant. In hindsight, this binding of water had been foreshadowed by the presence of larger-than-normal water signals in ^{1}H NMR spectra of **6·2Br**. We attempted to obtain dehydrated crystals by heating them under vacuum or by adding molecular sieves to solutions of redissolved **6·2Br** crystals, all to no avail.

We next assessed the redox features of these bisphosphoniums through cyclic voltammetry (Figure 5). Despite the difference in substitution pattern between **5**$^{2+}$ and **6**$^{2+}$, they display surprisingly similar electron accepting ability. The LUMOs of both compounds are not spatially affected by the phosphonium substitution pattern, suggesting that the inductive effects of imide and phosphonium substitution affect the electronic structure of the two scaffolds to a similar extent (Figure S7). Both compounds undergo two reversible one-electron reduction processes in MeCN solution with 0.1 M of Bu_4NPF_6 electrolyte. For **5**$^{2+}$, these take place at $E_{1/2} = -0.52$ V and -1.17 V, while for **6**$^{2+}$, the reductions are at $E_{1/2} = -0.52$ V and -1.12 V (all voltages vs. Fc/Fc$^+$). These potentials are shifted substantially from the parent unfunctionalized PMDI ($E_{1/2} = -1.35$ V)[45] and MDI ($E_{1/2} = -1.56$ V)[38] as measured in CH_2Cl_2 solution. The onset of the first reduction waves can be used to estimate the LUMO level to be *ca.* -4.35 eV for both **5**$^{2+}$ and **6**$^{2+}$. With the caveat that they are measured in different solvents, these shifts in first reduction potential of **5**$^{2+}$ and **6**$^{2+}$ are comparable in magnitude to the equivalent shift in reduction potential between unmodified NDI compounds ($E_{1/2} = -1.10$ V)[8] and bisphosphonium NDIs such as **2**$^{2+}$ ($E_{1/2} = -0.20$ V).[30] This similarity indicates that the stabilization afforded by the non-covalent P$^+$···O interaction is minimally affected when the relationship between the C–P$^+$ and C=O bonds changes from being parallel in NDI compounds to being non-parallel in **5**$^{2+}$ and **6**$^{2+}$ (average displacement of 22.5° and 15.1°, respectively). It is also worth noting that while on paper it may appear as though PMDI **5**$^{2+}$ is capable of twice as many P$^+$···O interactions as MDI **6**$^{2+}$ (and NDI **2**$^{2+}$), the electrochemical data confirm that the extent of LUMO stabilization in **5**$^{2+}$ is not greater than that of **6**$^{2+}$. This observation can be rationalized by noting that because of the tetrahedral geometry of the phosphonium center, P$^+$···O interactions can only take place with one of the two flanking carbonyls at any given time.

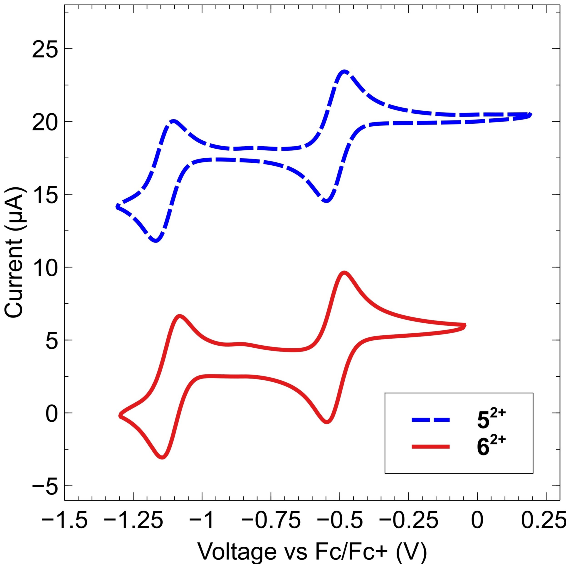

Figure 5. Cyclic voltammograms of **5**$^{2+}$ and **6**$^{2+}$ (*ca.* 1 mM in MeCN, 0.1 M Bu_4NPF_6, 100 mV/s). The major *y*-axis tick marks correspond to 5 μA increments.

The mild reduction potentials needed to reach the singly and doubly reduced states of **5**$^{2+}$ and **6**$^{2+}$ presented us the opportunity to characterize the UV-Vis profiles of these redox states under chemical reduction conditions. The titration spectra are presented in Figure 6 and the spectroscopic features are summarized in Table 1. The addition of single electron reductant cobaltocene ($CoCp_2$) to solutions of **5·2BF$_4$** or **6·2Br** in MeCN provided the respective reduced forms. The singly reduced form **5**$^{\bullet+}$ exhibits a long wave-length absorption band in the near-IR region ($\lambda_{max} = 821$ nm). This absorption is red-shifted by 100 nm compared to the analogous absorption in unfunctionalized PMDI[46,47] and pyridinium-modified PMDI.[33] The doubly reduced form **5**$^{2\bullet}$ appears teal-colored in solution, with absorption maxima at 611 and 720 nm. The molar absorptivities of both redox states are slightly lower, but still in the same order of magnitude as the unfunctionalized parent compounds generated by electrochemical methods in DMF solvent.[46,47]

We were particularly interested in the absorption features of MDI reduced states because they have not been reported to date. Despite the significant structural differences between **5**$^{2+}$ and **6**$^{2+}$, the reduced forms of MDI derivative **6**$^{2+}$ have UV-vis signatures similar to their PMDI counterparts. Unrestricted DFT calculations reveal that in both compounds, the spin densities in the radical cations are similarly concentrated on the imide O atoms and a subset of the central benzene carbons (Figure S7). Titration of 1 equiv. of $CoCp_2$ into a solution of **6·2Br** in MeCN led to formation of a nearly colorless solution of radical species **6**$^{\bullet+}$ with $\lambda_{max} = 728$ nm. Upon titration of an additional equivalent of $CoCp_2$, the formation of the doubly reduced **6**$^{2\bullet}$ is observed ($\lambda_{max} = 639$ nm). The molar absorptivities of the reduced forms of **6**$^{2+}$ are in the 10^4 M^{-1}cm^{-1} regime and are slightly lower than those measured for **5**$^{\bullet+}$ and **5**$^{2\bullet}$.

As discussed previously, compound **6·2Br** associates with H_2O to form a hydrate. The presence of this water does not seem to affect the (electro)chemical generation of **6**$^{\bullet+}$ or **6**$^{2\bullet}$, which suggests the potential for future iterations of these

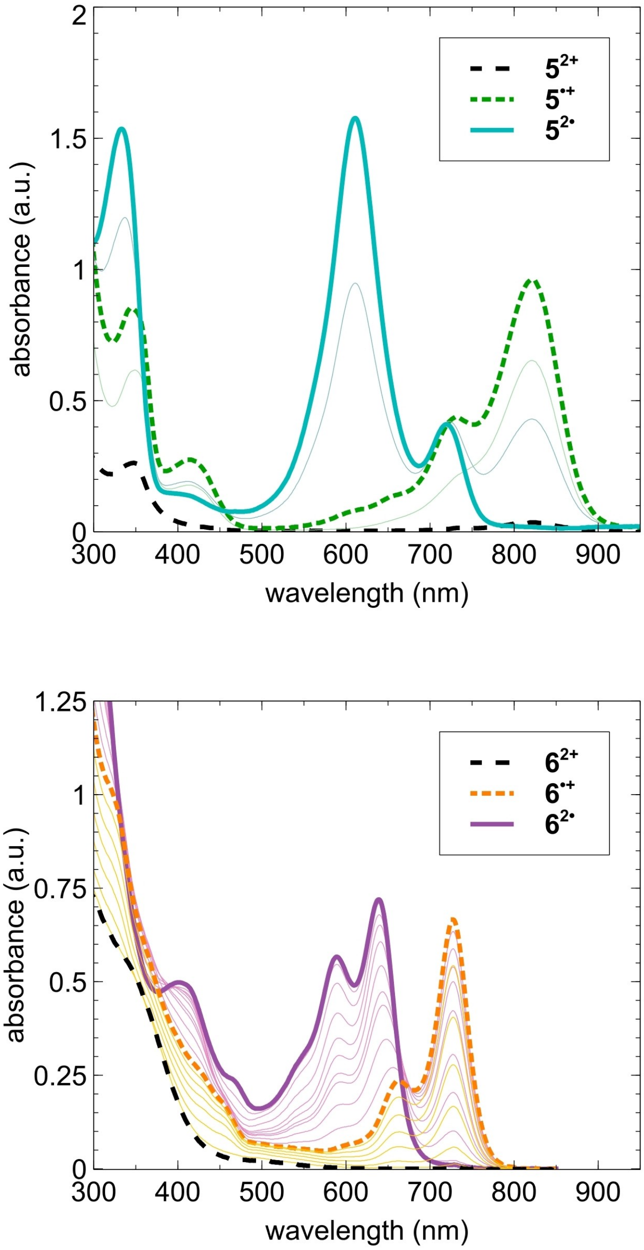

Figure 6. UV-vis absorption spectra of $\mathbf{5}^{2+}$ and $\mathbf{6}^{2+}$ and their reduced forms as produced by titration with $CoCp_2$.

cations to have utility in aqueous solution if adequate stability to O_2 can be achieved. We expended significant effort attempting to prepare single crystals of $\mathbf{5}^{\bullet+}$ and $\mathbf{6}^{\bullet+}$ suitable for X-ray structure determination, but unfortunately have not been successful to date.

In conclusion, we have demonstrated that phosphonium incorporation into benzene diimide is feasible despite the steric constraints of performing substitution chemistry on a fully substituted benzene core. The extent of cationic LUMO stabilization achieved in these bisphosphonium benzene diimides is comparable to those observed for bisphosphonium naphthalene diimide, showing that placing a phosphonium and carbonyl group skewed apart from each other, instead of parallel as described in previous literature, does not reduce the extent of stabilization gained. This stabilization further enables the chemical generation and spectroscopic characterization of the singly and doubly reduced states of both pyromellitic diimide and mellophanic diimide, the latter having been completely uncharacterized to date. Efforts to bring these minimal core benzene diimide radical species into the realm of complete air stability are underway currently.

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Conflict of Interests

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available in the supplementary material of this article.

Keywords: Radical ions · Phosphorus · Electron-deficient compounds · Aromatic substitution · Strained molecules

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