How to cite: *Angew. Chem. Int. Ed.* **2025**, *64*, e202519469
doi.org/10.1002/anie.202519469

Zinc-Iodine Batteries

Correspondence on "Confinement of Polyiodides by Dual-Functional Tetrazine Cathodes in Zn–I_2 Batteries"

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Abstract: In a recent research article (doi.org/10.1002/anie.202507497), Chi, Huang, Qu et al. described a multifunctional cathode for Zn–I_2 batteries based on a *s*-tetrazine ligand bearing two morpholine pendants, forming the active $2I_3^-$@BMT complex. In addition to the lack of proper attribution for prior reports by other authors (doi.org/10.1021/acs.inorgchem.6b01138; doi.org/10.1039/c7dt00134g) regarding the design of this ligand as an anion receptor, its synthesis and its ability to form triiodide complexes, the article is affected by serious scientific/technical flaws. The actual composition of the $2I_3^-$@BMT complex was not established, and protonation of morpholine groups in aqueous media, essential to the formation of the triiodide complex, was overlooked, despite prior studies and crystallographic evidence. The 2:1 I_3^-:BMT ratio was investigated in chloroform using a Job plot, while a 1:1 stability constant was determined via UV–vis titration in the same solvent. Both methods raise concerns, their results lack consistency and the extrapolation of data from chloroform to aqueous systems is not justified. Additionally, theoretical calculations yielded a highly positive binding energy, erroneously interpreted as indicative of complex stability, and a questionable complex structure featuring unconvincingly short anion–tetrazine contacts. Nevertheless, functioning of reported cathode for Zn–I_2 batteries is a notable outcome of the study.

In a recent Research Article (Hot Article) (doi.org/10.1002/anie.202507497), Chi, Huang, Qu et al. (hereafter referred to as CHQ) reported the development of a multifunctional cathode for Zn–I_2 batteries, employing a *s*-tetrazine functionalized with two morpholine moieties that forms a triiodide complex, $2I_3^-$@BMT, which is the central species and structural motif around which the study is conceptually and experimentally organized.

Anion coordination chemistry has emerged as a well-defined area of supramolecular chemistry. In line with the characteristics of the broader field, anion complexes are commonly formed through the interplay of various intermolecular forces, primarily electrostatic attractions, hydrogen bonding, and anion–π interactions, both in the solid state and in solution, where solvent effects can play a crucial role in determining their stability.[1–4]

s-Tetrazine-based molecules are interesting ligands for the formation of anion complexes as they can take advantage of all these weak forces to bind anions. They have also proven to be valuable tools for studying anion–π interactions—among the most recently recognized intermolecular forces—arising from the highly positive quadrupole moment of the *s*-tetrazine heterocycle. For the same reason, *s*-tetrazines are also capable of engaging in lone pair–π interactions.[5]

Some years ago, we set out to contribute to the understanding of these emerging weak forces by developing a new series of anion receptors (L1–L4 in Figure 1) capable of forming anion–π interactions in water.[6,7] To this end, the *s*-tetrazine ring was functionalized with two morpholine arms of increasing length, in order to modulate the distance between the heterocyclic ring (responsible for the anion–π interaction) and the morpholine groups capable of introducing additional binding forces such as hydrogen bonds and salt bridges. The two morpholine groups can undergo protonation in water,

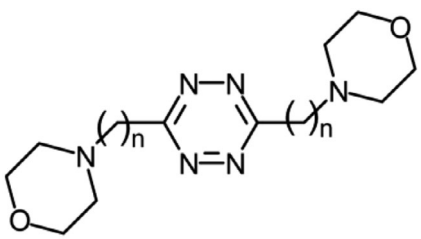

Figure 1. The L1-L4 *s*-tetrazine ligands. L2 = BMT.

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giving rise to mono and diprotonated species. That is, depending on the solution pH, ligand L1-L4 (L) can be present in the three L, HL^+ and H_2L^{2+} forms whose ammonium groups may promote anion binding via the formation of salt-bridges, while potentially hindering anion−π interactions.

As expected, L1-L4 proved to be effective anion receptors, forming complexes with inorganic and organic anions. In these complexes, the ligands could be found in all three protonation states (L, HL^+ and H_2L^{2+}) and the thermodynamic data obtained for the complexation equilibria provided an estimation of the anion−π contribution. Moreover, the numerous crystal structures of anion complexes with L1-L4, determined by X-ray diffraction (XRD) analysis, offered detailed insights into complex conformations and the organization of binding forces.[5–13]

In one of our studies,[8] we investigated the formation of I^- and I_3^- complexes with L2 and reported the crystal structures of $H_2L2I_2{\cdot}H_2O$ and of the highly water-insoluble $H_2L2(I_3)_2{\cdot}2H_2O$ and $(H_2L2)_2(I_3)_3I{\cdot}4H_2O$ compounds. Notably, the latter complex was found to form spontaneously when aqueous solutions of L2 and I^- were left in contact with air. In the case of I_3^-, the formation of solution complexes was modeled using quantum chemical methods, which revealed the anion positioned at a short distance above the tetrazine ring, slightly shifted toward a protonated morpholine nitrogen. Our calculations further suggested that a pair of water molecules likely forms hydrogen-bonded bridges between the two anions and the diprotonated ligand, thereby stabilizing the entire complex and underscoring the crucial role of the solvent in anion binding phenomena.

The relevance of these anion receptors was further highlighted by a recent publication by CHQ who reported the successful application of L2 (referred to as BMT in the article) in the fabrication of cathodes for Zn–I_2 batteries.[14] Although this result strengthened our appreciation for the relevance of our molecules, we were disappointed to find that the article gave the impression that L2 was being reported for the first time.

Statements such as "In this work, we propose a molecularly engineered tetrazine derivative, 3,6-bis(2-morpholinoethyl)-1,2,4,5-tetrazine (BMT), as a multifunctional cathode to address these challenges" (abstract), and "building upon these insights, we introduce a molecularly engineered tetrazine derivative, 3,6-bis(2-morpholinoethyl)-1,2,4,5-tetrazine (BMT), designed specifically for Zn–I_2 battery cathodes" (introduction), appear to be potentially misleading in terms of proper attribution. This impression is reinforced by the absence of an explicit acknowledgment that L2 (BMT) had previously been reported by others who purposefully designed it as an anion receptor.

The paper in which L2 (BMT) was first reported (ref. [31] in the paper by CHQ) was cited in the main article; however, that citation was used in the context of general properties and applications of *s*-tetrazines, rather than in direct acknowledgment of the authorship of L2. The synthesis of L2 is described in detail in the Supporting Information but not explicitly referenced in the main text. In the Discussion section, the preparation of L2 (BMT) is introduced as follows: "*The tetrazine-based ligand BMT was synthesized following a simple two-step modular approach. The intermediate product H_2BMT was obtained* via *classical Pinner synthesis of 3-(morpholin-4-yl)propanenitrile and hydrazine hydrate under an inert atmosphere, which was further oxidized in air to obtain the final product BMT.*[34]" This description closely parallels the procedure we previously reported, although the reference cited ([34] in CHQ) deals with a general Pinner synthesis rather than our original work.

The article by CHQ includes a section titled "Mechanism of BMT Complexation With I_3^-," which presents the study as entirely novel, overlooking our previously published work titled "Iodide and Triiodide Anion Complexes Involving Anion–π Interactions with a Tetrazine-Based Receptor"[8] As mentioned above, in this study we reported, among other results, a detailed structural analysis of the X-ray diffraction data for the $H_2L_2(I_3)_2{\cdot}2H_2O$ complex—most likely corresponding to the species referred to as "$2I_3^-$@BMT" in the title paper—as well as a detailed topological analysis of the electronic charge density in a computed $(H_2L_2^{2+})(I_3^-)_2$ complex. The omission of a direct citation to this prior work in the discussion of I_3^- complexation by CHQ is particularly striking, given that our paper was known to the authors: it is cited in their introduction (ref. [32]) among general references on tetrazine properties and applications. This selective citation pattern gives the impression that our earlier structural and theoretical findings were consciously overlooked.

We conclude our remarks concerning the inadequate recognition of the original authorship of L2 and some related results—a purely ethical issue—and turn to several substantial scientific shortcomings which, in our view, compromise key aspects of the study and are of broader relevance to the scientific community.

Our first concern relates to the correct identification of the key compound investigated in the study, which is vaguely referred to as "$2I_3^-$@BMT" throughout the article. In the section 1.3., "cathode preparation," of the Supporting Information, the preparation of the BMT-based cathode is described as involving the addition of a KI_3 solution (containing 2 M KI and excess I_2) to a mixture of BMT, activated carbon and Ketjen Black in water: "*The reaction mixture was stirred overnight at room temperature, resulting in the formation of a black precipitate of $2I_3^-$@BMT*." Throughout both the article and the Supporting Information, this key compound is consistently referred to as $2I_3^-$@BMT, without any consideration of the necessary counterions required to balance its overall 2– negative charge. In other words, the complete composition of this compound remains undefined. This lack of compositional clarity not only affects the correct interpretation of the work and most of the results but it also seems to contradict the editorial policy of the journal, which states: "The structure and composition of all compounds and materials central to the manuscript must be disclosed in the main text or in the Supporting Information, including commercial and proprietary products, pure materials, and mixtures. Manuscripts reporting results using undisclosed material compositions may be returned without external review."

It is also somewhat surprising that even the I_3^-:BMT ratio in the $2I_3^-$@BMT solid compound (with counterion not considered) is not supported by any clear experimental evidence. Sentence like "*scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS) mapping demonstrated homogeneous distribution of nitrogen (from BMT) and iodine within the cycled cathode (Figure S4), confirming the formation of a cohesive $2I_3^-$@BMT composite*" cannot be taken as confirmation of the formation of $2I_3^-$@BMT. SEM and EDS merely provide evidence of a homogeneous distribution of nitrogen and iodine, not the composition or the stoichiometry of the compound. Similarly, the statement regarding FT-IR measurements "*in addition, the result from the FT-IR spectrum also confirmed the formation of the $2I_3^-$@BMT complex (Figure 3c)*" does not constitute evidence that this very complex has indeed formed. The FT-IR spectra shown in the cited figure merely suggests an interaction between I_3^- and BMT, again without confirming the compound's composition or stoichiometry.

Instead, the I_3^-:BMT ratio of a possible complex formed in solution was investigated through the Job's plot reported in Figure 3a of the title paper, which suggested the formation of a complex with 2:1 stoichiometry. Furthermore, a quantitative analysis of the complexation equilibrium performed with a separated spectrophotometric titration afforded the stability constant of a 1:1 complex ($K_a = 6.28 \times 10^3$ M^{-1}). Since the solvent used for these experiments was not specified either in the paper or in the Supporting Information, we initially assumed it to be water, consistent with the rest of the study. Yet, the possible use of water for equilibrium study involving I_3^- seemed questionable, given that it is well known that I_3^- undergoes dissociation into I_2 and I^- in aqueous solution. We therefore contacted the authors directly, and we were informed that these solution studies had actually been carried out in chloroform.

While this clarification resolves the issue of I_3^- stability (I_3^- is stable in chloroform), three main concerns regarding solution data still remain.

The first relates to the appropriateness of using equilibrium data obtained in chloroform to describe phenomena that are hypothesized to occur in water. Given the significant differences in polarity, dielectric constant, and solvation behavior between these two solvents, extrapolating results from chloroform to aqueous conditions is highly questionable, especially in the context of anion binding, which is dominated by weak forces which sometime are weaker than solvation forces. As a matter of fact, in our earlier work, we reported on the effect of the solvent on anion binding equilibria with L2, showing that the addition of as little as 20% ethanol to water caused significant changes in both the nature of the complex species formed and their stability constants.[6]

The second concern arises from the inconsistency between the results obtained from the Job's plot and those derived from the determination of the complex stability constant. In the Job plot, the experimental data (absorbance values) lie almost perfectly along two straight lines that intersect at $R = [I_3^-]/([I_3^-] + [BMT]) = 0.68$, which is very close to the 0.67 value expected for the formation of a complex with 2:1 I_3^-:BMT stoichiometry, while no inflection is observed at $R = 0.5$, which would be indicative of a 1:1 complex. This Job plot suggests the formation of a very stable 1:2 species, which hinders the formation of the 1:1 species. Considering the negative charge accumulation on the complex (two anions interacting with a charge-neutral ligand), it is hard to understand why this should occur in the present case. Nevertheless, caution is advised when applying this method in systems where both 1:1 and 1:2 species may form as the Job plot has been shown to be more sensitive to the K_1/K_2 ratio and the host concentration than to the actual stoichiometry.[15]

In sharp contrast to the Job plot results, spectrophotometric titration data indicated the exclusive formation of a highly stable 1:1 complex ($K_a = 6.28 \times 10^3$ M^{-1}), even when I_3^- was added to BMT in up to a fourfold excess. Remarkably and surprisingly the spectrophotometric titration data were fitted using an equation that assumes only 1:1 complex formation (see Supporting Information of the paper by CHQ). Obviously, species not included in the fitting model cannot be detected. However, given the good quality of the fit shown in Figure 4b, there appears to be little room for the formation of an additional 2:1 complex of high stability.

It is very hard to reconcile these results. It is also difficult to suggest a way to resolve this inconsistency. Perhaps, a clearer picture could emerge if: 1) the Job plot were constructed using absorbance values corrected for the baseline absorbance expected in the absence of complexation, as commonly recommended in analytical chemistry textbooks,[16] thus isolating the absorbance contribution attributable to complex formation, 2) the entire spectra recorded for the spectrophotometric titration, instead of data at a single wavelength, were analyzed for the speciation of I_3^- complexes and the determination of their stability constants by using one of the available computer programs (e.g., the HypSpec software[17]), which allow for simultaneous fitting of multiple equilibria.

The third concern relates to the complete oversight of the fact that L2 (BMT) contains two amine groups, which undergo protonation in aqueous solution, even in the absence of added acid, leading to the formation of HL^+ and H_2L^{2+} species.[6] Considering the procedure reported for the preparation of the $2I_3^-$@BMT complex (see Supporting Information for the paper by CHQ), which resembles the condition we used for the preparation of $H_2L2(I_3)_2{\cdot}2H_2O$,[8] it is very plausible that the protonated ligand is the missing counterion in $2I_3^-$@BMT and this complex is identical to $H_2L_2(I_3)_2{\cdot}2H_2O$. Elemental analysis of $2I_3^-$@BMT would be particularly helpful in clarifying this point.

Chloroform offers a different situation as this solvent is not capable to transfer protons to L2 (BMT); in other worlds, the ligand does not undergo protonation, as it does in water, unless the chloroform has been contaminated with protolytic substances. Accordingly, in chloroform, the scenario differs significantly from the aqueous conditions under which the $2I_3^-$@BMT-based cathode was prepared and utilized. In practical terms, it is as if two different ligands were involved: a neutral one in chloroform and a positively charged one in water. This adds another critical element against the extrapolation of results from one medium to the other. This issue is equally relevant for NMR and, likely (solvent not

specified), for FT-IR analysis of the interaction of BMT (L2) with I_3^- in solution.

Similar considerations apply to density functional theory (DFT) calculations and electrostatic potential (ESP) mapping, which were performed under the assumption that BMT (L2) is in its neutral, nonprotonated form. Since this condition is highly unlikely under the experimental conditions used for preparing the $2I_3^-$@BMT cathode material, such calculations, related comments and considerations are not directly relevant to the actual system studied.

Nevertheless, it appears that far more serious flaws affect the DFT calculations. First of all, we noted that the energy calculated for the interaction between I_3^- and BMT (E_{int} = 512.6 kcal mol^{-1}) is positive, which, according to standard conventions, implies that the complexation reaction is endergonic, —i.e., the complex is not stable. Since this E_{int} value is repeatedly used throughout the text to emphasize the high stability of the $2I_3^-$@BMT complex, we initially suspected a misinterpretation on our part. We therefore inspected Table S2 of the Supporting Information, which reports the BSSE-corrected binding energy of all species involved in the complexation reaction, and readily confirmed that this E_{int} value is indeed positive. Unless there are details or assumptions which are not disclosed in the paper, data in Table S2 clearly indicate that the complex $2I_3^-$@BMT is not stable, rather, it is very unstable because 512.6 kcal mol^{-1} is an extraordinarily large value when compared to binding energies (B_e) such as those reported by us for the 1:1 complex of I_3^- and *s*-tetrazine which, depending on the orientation of the anion, range from 1.6 to 3.6 kcal mol^{-1} (note that we evaluated $B_e = -E_{int}$),[8] or those typically found for this type of interaction.[18] Even if we had misinterpreted the positive sign of this energy (512.6 kcal mol^{-1}), a value of such magnitude should have raised serious concerns, as it is exceedingly high for an interaction between a ligand and two anions, even assuming the formation of fully covalent bonds. For comparison, the dissociation energies of the triple bonds in N_2 and CO—among the strongest covalent bonds known—are 225.8 and 257.3 kcal mol^{-1}, respectively.[19]

If the above reasoning is correct, the extensive derivations (e.g., HOMO-LUMO gap, ESP, etc.) based on the DFT calculations performed by CHQ would be substantially meaningless.

Given the large positive interaction energy, it is difficult to understand how the triiodide anions could freely approach the tetrazine ring atoms of BMT so closely as observed in the structure of $2I_3^-$@BMT calculated by CHQ (see Figure 4a in ref. 14). Indeed, the central iodine atoms of the two triiodide anions are engaged in eight N–I contacts within 2.24–2.72 Å and four C–I contacts within 2.25–2.62 Å. The external iodine atoms of the triiodide anions are also interacting with the tetrazine ring atoms, although at slightly longer distances (I–N 2.52–3.20 Å).

A survey of N—I and C—I bond distances in the Cambridge Structural Database[20] reveals sharp maxima at 2.27(4) Å (N–I) and 2.10(3) Å (C–I), indicating that many of the N—I interactions should be fully covalent. As a result, the *s*-tetrazine ring would be expected to deviate from planarity and bond distances within the ring should also change appreciably compared to those of the free *s*-tetrazine. On the contrary, the tetrazine ring of the calculated structure is perfectly planar and calculated bond distances show only negligible differences compared to those observed in the crystal structure of free L2 (BMT).[6] In other words, calculations by CHQ predict covalent interactions between the triiodide anions and the tetrazine ring, yet the structure of this ligand moiety remains essentially unchanged.

In conclusion, the paper by Chi, Huang, Qu et al. reports noteworthy results in the development of an efficient cathode for Zn–I_2 batteries. However, beyond our justified concerns regarding the lack of proper attribution of authorship for the design of L2 (BMT) as an anion receptor, its synthesis, and its ability to form complexes with triiodide (I_3^-), the study suffers from serious flaws, mainly due to the failure to determine the actual composition of $2I_3^-$@BMT, the compound at the centre of this work, and an overreliance on theoretical calculations on structure and binding energy of this complex, whose results appear to be scientifically unsound. The assumption that in this material the BMT ligand is in its neutral form appears unfounded, given that it is almost certainly protonated (and thus positively charged) under the experimental conditions, as demonstrated by our previous studies.[6,8] Consequently, we believe that the entire investigation refers to a material different from the one actually employed, and that the related discussion develops around this fundamental misconception. Moreover, the theoretical calculations fail to clarify the nature of this compound as they depict the triiodide anions as covalently bound to the *s*-tetrazine atoms of BMT, while simultaneously yielding a strongly positive (unfavourable) binding energy.

Additional concerns arise from the solution studies carried out to assess the binding ability of BMT toward I_3^-, which were conducted in chloroform rather than in the aqueous medium used for the synthesis and application of $2I_3^-$@BMT. While the anion-binding capability of BMT (L2) required no further confirmation in light of our previous studies,[5–13] and despite the aforementioned limitations of extrapolating data from chloroform to water, particularly given the different protonation states of the ligand in the two solvents, the reported equilibrium data exhibit internal inconsistencies.

Acknowledgements

The authors have nothing to report.

Conflict of Interests

The authors declare no conflict of interest.

Keywords: Density functional calculations · Electrochemistry · Tetrazine ligands · Triiodide anion complexes · Zn–iodine batteries

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Manuscript received: September 05, 2025
Revised manuscript received: October 14, 2025
Manuscript accepted: October 14, 2025
Version of record online: October 26, 2025