Title

Below the 12-vertex: 10-vertex carborane anions as non-corrosive, halide free, electrolytes for rechargeable Mg batteries

Journal

Chemical Communications, 53(32)

ISSN

1359-7345

Authors

McArthur, Scott G
Jay, Rahul
Geng, Linxiao
et al.

Publication Date

2017-04-18

DOI

10.1039/c7cc01570d

Peer reviewed

ChemComm

COMMUNICATION

View Article Online
View Journal | View Issue

Cite this: *Chem. Commun.*, 2017, 53, 4453

Received 28th February 2017,
Accepted 24th March 2017

DOI: 10.1039/c7cc01570d

rsc.li/chemcomm

Below the 12-vertex: 10-vertex carborane anions as non-corrosive, halide free, electrolytes for rechargeable Mg batteries†

Scott G. McArthur,‡[a] Rahul Jay,‡[b] Linxiao Geng,[b] Juchen Guo*[b] and Vincent Lavallo*[a]

The development of practical Mg based batteries is limited by the lack of a library of suitable electrolytes. Recently a 12-vertex *closo*-carborane anion based electrolyte has been shown to be the first electrolyte for Mg based batteries, which is both non-corrosive and has high electrochemical stability (+3.5 V *vs.* $Mg^{0/2+}$). Herein we show that smaller 10-vertex *closo*-carborane anions also enable electrolytes for Mg batteries. Reduction of the trimethylammonium cation of $[HNMe_3^{1+}][HCB_9H_9^{1-}]$ with elemental Mg yields the novel magnesium electrolyte $[Mg^{2+}][HCB_9H_9^{1-}]_2$. The electrolyte displays excellent electrochemical stability, is non-nucleophilic, reversibly deposits and strips Mg, and is halide free. This discovery paves the way for the development of libraries of Mg electrolytes based on more cost effective 10-vertex *closo*-carborane anions.

Due to rapid technological advances in rechargeable portable devices and electric vehicles, there is an urgent need to develop rechargeable batteries that are safer and have greater energy density compared to the current state-of-the-art Li-ion cells.[1] Furthermore, because the cells constructed with pure Li metal are inherently unsafe due to dendrite formation, alternative anode materials are of great interest.

Mg-based batteries[2] are a potentially game changing alternative to Li-ion systems because Mg is far less expensive, more tolerant of air, and does not form dendrites. The fact that Mg does not form dendrites allows the utilization of pure Mg anodes, which significantly increases both the volumetric and gravimetric energy densities of Mg-cells compared to Li-ion batteries. To realize high energy density Mg-cells appropriate cathode materials must be identified. However, the discovery of such cathode materials has been hampered by the lack of suitable electrolytes that facilitate the electrochemical oxidation and reduction reactions. In contrast to Li^+ ions, Mg^{2+} ions cannot reversibly penetrate the solid electrolyte interface (SEI) layer on Mg anodes,[3] therefore suitable electrolytes must feature counter-anions that do not decompose easily. Most of the current Mg electrolytes are composed of simple ethereal solvents and Mg^{2+} organometallic/main-group complexes represented by Grignard reagents and similar compounds like organoborates,[2g,h,4] boro-hydrides,[5] and organohalo-aluminates.[2a,f,i,j] However, these compounds are generally limited by narrow electrochemical stability windows. Another caveat is that the electrolyte cannot contain halide ions, since their oxidation leads to radicals or elemental halogens that corrode non-noble metal current collectors and battery casing materials.[2g]

Recently, we[6] and Mohtadi[7] and coworkers independently reported the synthesis and implementation of the non-corrosive and halide free electrolyte $[Mg^{2+}][HCB_{11}H_{11}^{1-}]_2$ **1**[Mg^{2+}], featuring 12-vertex icosahedral carborane anion[8] **1** (Scheme 1A). The carborane anion **1** ($HCB_{11}H_{11}^{1-}$) is immune to any acids/bases,[8m] is compatible with Mg metal, and does not undergo electrochemical oxidation up to +5.36 V *vs.* $Mg^{0/+2}$.[9] Prior to the discovery of **1**[Mg^{2+}] all other known electrolytes for Mg batteries had high halide content and/or suffered from poor electrochemical stability. In contrast to Mohtadi's route to prepare **1**[Mg^{2+}], which uses a precious metal and results in a material that is difficult to purify, we developed a superior method, namely cation reduction. As depicted in Scheme 1, this cation reduction methodology utilizes magnesium metal to reduce trimethylammonium cations to produce **1**[Mg^{2+}] in high purity and without the consumption of precious metals.

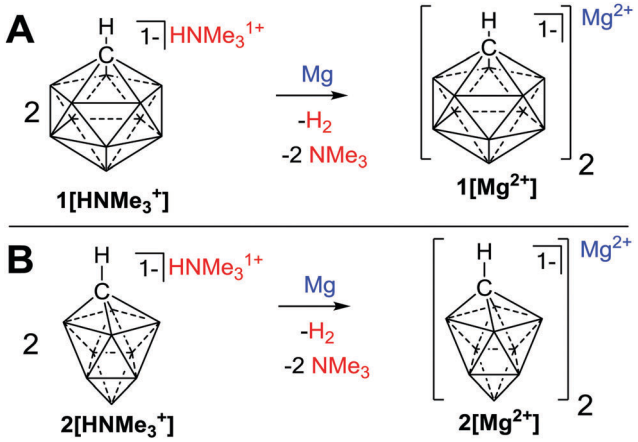
While **1**[Mg^{2+}] meets the basic electrochemical requirements to enable the discovery of novel cathode materials that will result in the development of high capacity Mg batteries, cluster **1** is rather expensive to produce and requires the use of toxic cyanide as well as pyrophoric Na metal.[8m] Furthermore, even if functional high capacity conversion cathodes (*e.g.* sulfur) or moderate capacity high voltage cathodes (*e.g.* certain metal oxides) for Mg cells are discovered, a library of electrolytes will

[a] *Departments of Chemistry, University of California Riverside, Riverside, CA 92521, USA. E-mail: vincent.lavallo@ucr.edu; Web: http://faculty.ucr.edu/~vincentl*

[b] *Department of Chemical and Environmental Engineering, University of California Riverside, Riverside, CA 92521, USA. E-mail: jguo@engr.ucr.edu; Web: http://www.cee.ucr.edu/jguo*

† Electronic supplementary information (ESI) available: Full crystallographic data for **2**[Mg^{2+}]. CCDC 1529836. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c7cc01570d

‡ Denotes equal author contributions.



Scheme 1 Synthesis of **1[Mg^{2+}]** and **2[Mg^{2+}]** *via* cation reduction.

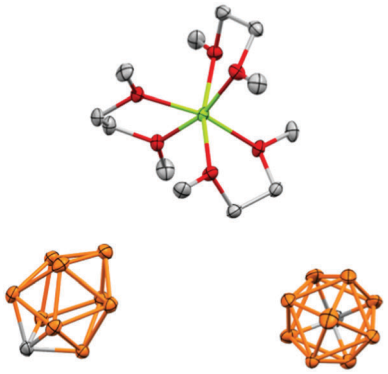


Fig. 1 Solid state-structure of **2[Mg^{2+}]** with 3 coordinated DME molecules to the Mg cation. Hydrogen atoms omitted for clarity (color code: brown = boron; red = oxygen; green = Mg; grey = carbon).

be needed to optimize the performance of the materials. Indeed, each cathode material will display distinct chemical behavior with different electrolytes. Here we report the discovery of a novel, non-corrosive, and air/H_2O stable electrolyte $[Mg^{2+}][HCB_9H_9^{1-}]_2$ **2[Mg^{2+}]** that utilizes a smaller 10-vertex carborane anion **2**[10] (Scheme 1B). This electrolyte is less expensive to prepare due to the facile synthesis of the carborane anion **2**. Anion **2** can be conveniently prepared without cyanide and Na metal, *via* a simple reaction of $B_{10}H_{14}$ with *p*-formaldehyde[10b] followed by oxidation with I_2.[10c]

While the 10-vertex anion $HCB_9H_9^{1-}$ **2** was discovered by Knoth[10a] in 1967 very little is known about its electrochemical properties. While the reductive stability of **2** is unknown a single report from Hawthorne[11] claims that the anion is oxidatively stable to +1.95 V *vs.* SCE (+4.56 V *vs.* $Mg^{0/2+}$). Therefore, we became interested in exploring the reductive stability of the cluster and its potential use as an electrolyte for Mg batteries. We envisioned utilizing our cation reduction methodology to prepare **2[Mg^{2+}]** from its corresponding trimethylammonium salt **2[$HNMe_3^+$]**. Cation reduction is not only the most efficient way to prepare halide free Mg electrolytes but it is also a chemical test to prove the compatibility of an electrolyte with Mg metal anodes (reductive stability). Thus we treated a solution of **2[$HNMe_3^+$]** in THF with two equivalents of Mg powder (Scheme 1B). The mixture was monitored by ^{1}H NMR spectroscopy until the methyl resonance for $HNMe_3^+$ completely vanished, indicating completion of the reaction. The ^{11}B NMR spectrum does not change during the reaction indicating the presence of a solvent separated ion pair and suggesting that the cluster is compatible with metallic Mg. Indeed, stirring a solution of **2[Mg^{2+}]** with the activated Mg powder for one month results in no decomposition of the electrolyte. Similar to **1[Mg^{2+}]**, salt **2[Mg^{2+}]** precipitates from the THF solution and can be collected by filtration or extraction with DME. The structure of **2[Mg^{2+}]** was unambiguously confirmed by a single crystal X-ray diffraction study. In the solid state the Mg^{2+} ion is coordinated by three chelating DME molecules and the two carborane counteranions do not interact with the metal center (Fig. 1). At room temperature, the ionic conductivity of **2[Mg^{2+}]** in tetraglyme (G4) was measured as a function of concentration (Fig. S5, ESI†) between 0.15 and 0.65 M. A maximum conductivity of 1.57 mS cm^{-1} was achieved at 0.45 M, which is comparable to the optimal conductivity of **1[Mg^{2+}]** in G4 (1.8 mS cm^{-1}) at a much higher concentration of 0.75 M. Cyclic voltammetry (CV) experiments of 0.45 M **2[Mg^{2+}]** in G4 shown in Fig. 2 demonstrate

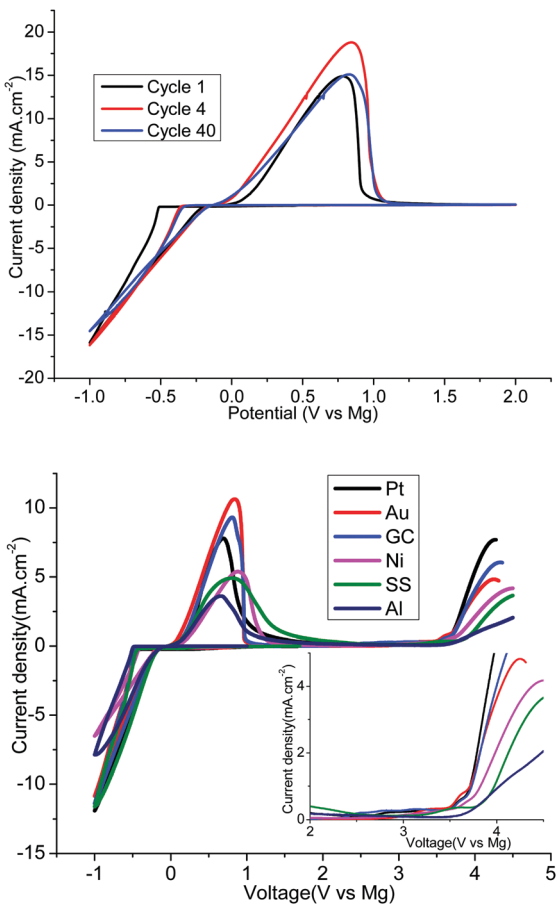


Fig. 2 (top) Selected CV curves of Mg deposition-stripping of 0.45 M **2[Mg^{2+}]** in G4 on Pt WE; (bottom) first CV scan of 0.45 M **2[Mg^{2+}]** in G4 on various WEs at 20 mV s^{-1} (inset – enlargement of 2.0 to 4.5 V region of the anodic scan depicting the oxidative onset potentials).

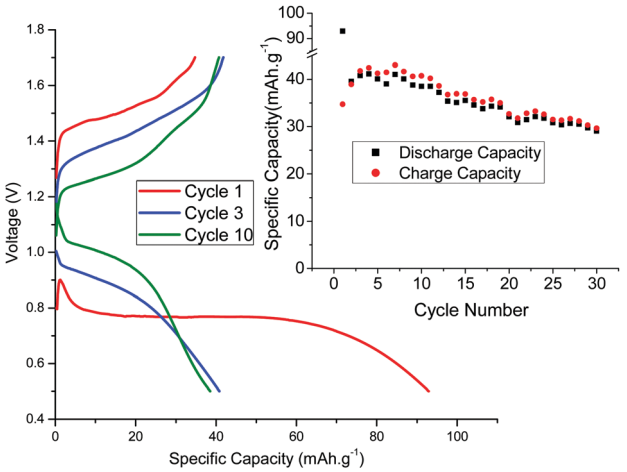


Fig. 3 Charge–discharge profiles of selected cycles of a Mg-ion cell with 0.45 M **2[Mg^{2+}]** in G4 electrolyte and Chevrel phase Mo_6S_8 cathode (inset – cycle stability for a span of 30 cycles).

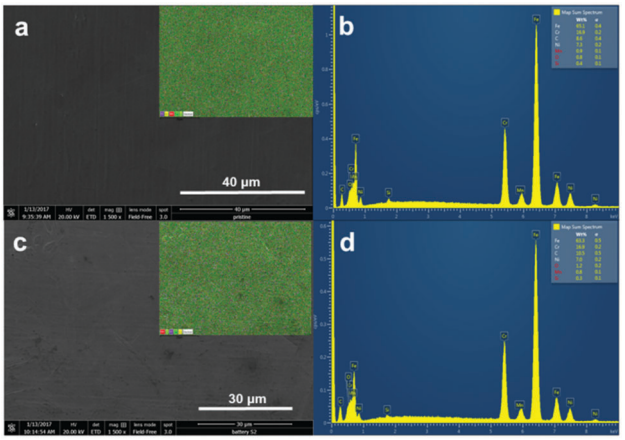


Fig. 4 Pristine SS coin cell inner surface on the cathode side: (a) SEM image with EDS mapping and (b) EDS spectrum; the same surface after 30 cycles with 0.45 M **2[Mg^{2+}]** in the G4 electrolyte: (c) SEM image with EDS mapping and (d) EDS spectrum.

reversible Mg deposition/stripping and excellent anodic(oxidative) stability on a variety of metal working electrodes (WE) including platinum (Pt), gold (Au), glassy carbon (GC), nickel (Ni), 316 stainless steel (SS) and aluminum (Al). Oxidative onset occurs at around 3.5 V *vs.* $Mg^{0/2+}$ on all current collectors, which is at the solvents' oxidative stability limit. In other words, similar to **1[Mg^{2+}]**, the solvent in **2[Mg^{2+}]** is oxidized before the carborane anion **2**.

We next sought to test the electrolytes' performance in a prototype Mg battery. Due to the limited number of suitable electrolytes, the only reliable cathode material yet discovered for such applications is the Chevrel phase Mo_6S_8. Coin cell Mg-ion battery performance was demonstrated with a Mg anode and Mo_6S_8 cathode using 0.45 M **2[Mg^{2+}]** in G4 as the electrolyte. The prepared cells were cycled at a current density of 12.9 mA g^{-1} (0.1 C). The initial discharge capacity of 93 mA h g^{-1} was achieved in the first discharge, but the capacity of the subsequent cycles decreases to approximately 40 mA h g^{-1} (Fig. 3). While the observed performance of this Mg/Mo_6S_8 battery is slightly lower than that of the analogous cell utilizing **1[Mg^{2+}]** as an electrolyte, these results serve as proof of principle that smaller carborane anions are viable alternatives. Furthermore, while the mechanism of the irreversible capacity and the capacity fade is currently under investigation, it is conceivable that chemical modifications to the tunable cluster 2's surface might lead to improved performance. Importantly, one must realize that cathode materials other than Mo_6S_8 materials may behave completely different, thus **2[Mg^{2+}]** would be a good candidate to include in any screens of novel high capacity/voltage cathode materials being developed.

It is also important to note that like **1[Mg^{2+}]**, **2[Mg^{2+}]** is air/H_2O stable and non-corrosive. After 30 cycles in the Mg–Mo_6S_8 coin cell, no pitting was observed on the SS casing surface *via* scanning electron microscopy (SEM) as shown in Fig. 4. Elemental analysis by energy-dispersive X-ray spectroscopy (EDX) also demonstrated almost identical elemental contents on the SS surface before and after battery cycling.

This manuscript introduces a new paradigm in the development of Mg batteries, by showing that *closo*-carborane anions having less than 12 vertices are enabling electrolytes. These 10-vertex anions are less expensive to produce than their larger cousins and thus should be more amenable to commercialization if high capacity secondary Mg batteries are realized. We are currently developing a library of chemically modified clusters **1** and **2** that feature improved chemical properties as well as attempting to identify novel high capacity and high voltage cathode materials for Mg batteries.

We gratefully acknowledge the National Science Foundation (DMR-1508537) for support of this work.

Notes and references

1 R. V. Noorden, *Nature*, 2014, **507**, 26.
2 For recent reviews on Mg batteries, see: (*a*) J. W. Choi and D. Aurbach, *Nat. Rev. Mater.*, 2016, **1**, 16013; (*b*) J. Song, E. Sahadeo, M. Noked and S. B. Lee, *J. Phys. Chem. Lett.*, 2016, **7**, 1736; (*c*) Y. Cheng, H. J. Chang, H. Dong, D. Choi, V. L. Sprenkle, J. Liu, Y. Yao and G. Li, *J. Mater. Res.*, 2016, **31**, 3125; (*d*) C. B. Bucur, T. Gregory, A. G. Oliver and J. Muldoon, *J. Phys. Chem. Lett.*, 2015, **6**, 3578; (*e*) R. Mohtadi and F. Mizuno, *Beilstein J. Nanotechnol.*, 2014, **5**, 1291; (*f*) H. D. Yoo, I. Shterenberg, Y. Gofer, G. Gershinsky, N. Pour and D. Aurbach, *Energy Environ. Sci.*, 2013, **6**, 2265; (*g*) J. Muldoon, C. B. Bucur, A. G. Oliver, J. Zajicek, G. D. Allred and W. C. Boggess, *Energy Environ. Sci.*, 2013, **6**, 482; (*h*) J. Muldoon, C. B. Bucur, A. G. Oliver, T. Sugimoto, M. Matsui, H. S. Kim, G. D. Allred, J. Zajicek and Y. Kotani, *Energy Environ. Sci.*, 2012, **5**, 5941; (*i*) D. Aurbach, G. S. Suresh, E. Levi, A. Mitelman, O. Mizrahi, O. Chusid and M. Brunelli, *Adv. Mater.*, 2007, **19**, 4260; (*j*) N. Amir, Y. Vestfrid, O. Chusid, Y. Gofer and D. Aurbach, *J. Power Sources*, 2007, **174**, 1234; for select recent advances in Mg battery design, see: (*k*) B. Pan, Z. Feng, N. Sa, S.-D. Han, Q. Ma, P. Fenter, J. T. Vaughey, Z. Zhang and C. Liao, *Chem. Commun.*, 2016, **52**, 9961; (*l*) Y. Shao, T. Liu, G. Li, M. Gu, Z. Nie, M. Engelhard, J. Xiao, D. Lv, C. Wang, J.-G. Zhang and J. Liu, *Sci. Rep.*, 2013, **3**, 3130; (*m*) H. S. Kim, T. S. Arthur, G. D. Allred, J. Zajicek, J. G. Newman, A. E. Rodnyansky, A. G. Oliver, W. C. Boggess and J. Muldoon, *Nat. Commun.*, 2011, **2**, 427; for the first example of a secondary Mg battery, see: (*n*) D. Aurbach, Z. Lu, A. Schechter, Y. Gofer, H. Gizbar, R. Turgeman, Y. Cohen, M. Moshkovich and E. Levi, *Nature*, 2000, **407**, 724.
3 T. D. Gregory, R. J. Hoffman and R. C. Winterton, *J. Electrochem. Soc.*, 1990, **137**, 775.
4 Y.-s. Guo, F. Zhang, J. Yang, F.-f. Wang, Y. NuLi and S.-i. Hirano, *Energy Environ. Sci.*, 2012, **5**, 9100.

5 R. Mohtadi, M. Matsui, T. S. Arthur and S.-J. Hwang, *Angew. Chem., Int. Ed.*, 2012, **51**, 9780.
6 S. G. McArthur, L. Geng, J. Guo and V. Lavallo, *Inorg. Chem. Front.*, 2015, **2**, 1101.
7 O. Tutusaus, R. Mohtadi, T. S. Arthur, F. Mizuno, E. G. Nelson and Y. V. Sevryugina, *Angew. Chem., Int. Ed.*, 2015, **54**, 7900.
8 For recent examples and reviews of applications of carboranes and related molecules, see: (*a*) M. S. Messina, J. C. Axtell, Y. Wang, P. Chong, A. I. Wixtrom, K. O. Kirlikovali, B. M. Upton, B. M. Hunter, O. S. Shafaat, S. I. Khan, J. R. Winkler, H. B. Gray, A. N. Alexandrova, H. D. Maynard and A. M. Spokoyny, *J. Am. Chem. Soc.*, 2016, **138**, 6952; (*b*) R. M. Dziedzic, L. M. A. Saleh, J. C. Axtell, J. L. Martin, S. L. Stevens, A. T. Royappa, A. L. Rheingold and A. M. Spokoyny, *J. Am. Chem. Soc.*, 2016, **138**, 9081; (*c*) J. C. Axtell, K. O. Kirlikovali, P. I. Djurovich, D. Jung, V. T. Nguyen, B. Munekiyo, A. T. Royappa, A. L. Rheingold and A. M. Spokoyny, *J. Am. Chem. Soc.*, 2016, **138**, 15758; (*d*) S. Rodríguez-Hermida, M. Y. Tsang, C. Vignatti, K. C. Stylianou, V. Guillerm, J. Pérez-Carvajal, F. Teixidor, C. Viñas, D. Choquesillo-Lazarte, C. Verdugo-Escamilla, I. Peral, J. Juanhuix, A. Verdaguer, I. Imaz, D. Maspoch and J. Giner Planas, *Angew. Chem., Int. Ed.*, 2016, **55**, 16049; (*e*) M. Hailmann, N. Wolf, R. Renner, T. C. Schäfer, B. Hupp, A. Steffen and M. Finze, *Angew. Chem., Int. Ed.*, 2016, **55**, 10507; (*f*) Y. O. Wong, M. D. Smith and D. V. Peryshkov, *Chem. Commun.*, 2016, **52**, 12710; (*g*) M. J. Asay, S. P. Fisher, S. E. Lee, F. S. Tham, D. Borchardt and V. Lavallo, *Chem. Commun.*, 2015, **51**, 5359; (*h*) M. Y. Tsang, C. Viñas, F. Teixidor, J. G. Planas, N. Conde, R. SanMartin, M. T. Herrero, E. Domínguez, A. Lledós, P. Vidossich and D. Choquesillo-Lazarte, *Inorg. Chem.*, 2014, **53**, 9284; (*i*) A. R. Popescu, F. Teixidor and C. Viñas, *Coord. Chem. Rev.*, 2014, **269**, 54; (*j*) J. Poater, M. Solà, C. Viñas and F. Teixidor, *Angew. Chem., Int. Ed.*, 2014, **53**, 12191; (*k*) D. Zhao, J. Zhang and Z. Xie, *Angew. Chem., Int. Ed.*, 2014, **53**, 8488; (*l*) D. Zhao, J. Zhang and Z. Xie, *Angew. Chem., Int. Ed.*, 2014, **53**, 12902; (*m*) C. Douvris and J. Michl, *Chem. Rev.*, 2013, **113**, PR179; (*n*) A. M. Spokoyny, *Pure Appl. Chem.*, 2013, **85**, 903; (*o*) D. Olid, R. Nunez, C. Vinas and F. Teixidor, *Chem. Soc. Rev.*, 2013, **42**, 3318; (*p*) P. Farras, E. J. Juarez-Perez, M. Lepsik, R. Luque, R. Nunez and F. Teixidor, *Chem. Soc. Rev.*, 2012, **41**, 3445; (*q*) A. Pepiol, F. Teixidor, R. Sillanpää, M. Lupu and C. Viñas, *Angew. Chem., Int. Ed.*, 2011, **50**, 12491; (*r*) A. Himmelspach, M. Finze and S. Raub, *Angew. Chem., Int. Ed.*, 2011, **50**, 2628; (*s*) Y. Li, P. J. Carroll and L. G. Sneddon, *Inorg. Chem.*, 2008, **47**, 9193.
9 R. T. Boeré, C. Bolli, M. Finze, A. Himmelspach, C. Knapp and T. L. Roemmele, *Chem. – Eur. J.*, 2013, **19**, 1784.
10 (*a*) W. H. Knoth, *J. Am. Chem. Soc.*, 1967, **89**, 1274; (*b*) B. Brellochs, J. Bačkovský, B. Štíbr, T. Jelínek, J. Holub, M. Bakardiev, D. Hnyk, M. Hofmann, I. Císařová and B. Wrackmeyer, *Eur. J. Inorg. Chem.*, 2004, 3605; (*c*) B. Ringstrand, D. Bateman, R. K. Shoemaker and Z. Janousek, *Collect. Czech. Chem. Commun.*, 2009, **74**, 419.
11 R. J. Wiersema and M. F. Hawthorne, *Inorg. Chem.*, 1973, **12**, 785.

Electronic Supplementary Material (ESI) for ChemComm.

Below the 12-vertex: 10-Vertex Carborane Anions as Non-corrosive, Halide Free, Electrolytes for Rechargeable Mg Batteries.

Scott. G. McArthur[a], Rahul Jay[b], Linxiao Geng[b], Juchen Guo[*bc] and Vincent Lavallo[*a]

[a.]Department of Chemistry, University of California Riverside, Riverside, CA 92521, USA. E-mail: vincent.lavallo@ucr.edu

[b.]Department of Chemical and Environmental Engineering, University of California Riverside, Riverside, CA 92521, USA. E-mail: jguo@engr.ucr.edu

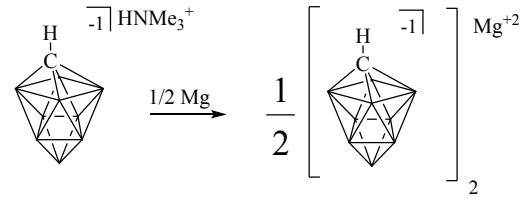
[c.]Materials Science and Engineering Program, University of California Riverside, Riverside, CA 92521, USA.

Table of Contents

General Considerations

Unless otherwise stated all manipulations were carried out using standard Schlenk or glovebox techniques (O_2, H_2O < 1ppm) under a dinitrogen or argon atmosphere. Solvents tetrahydrofuran (THF), 1,2-Dimethoxyethane (DME), and tetraethylene glycol dimethyl ether (tetraglyme or G4) were dried on K, Na or CaH_2, and distilled under argon before use. NMR spectra were recorded on Bruker Avance 300 MHz, Varian Inova 300 MHz, Varian Inova 400 MHz, or Varian Inova 500 MHz spectrometers. NMR chemical shifts are reported in parts per million (ppm). ^{1}H NMR and ^{13}C NMR chemical shifts were referenced to residual solvent. ^{11}B NMR chemical shifts were externally referenced to BF_3OEt_2.

Synthesis of 2[Mg^{+2}]



2[$HNMe_3^{1+}$] **2[Mg^{2+}]**

2[$HNMe_3^{+1}$] (2.0 g, 10.3 mmol) was added to a suspension of Mg powder (4.0 g, 165 mmol) in a minimal amount of THF (5mL) and the resulting suspension was stirred for 1 hr. After 1 hr, additional THF (30mL) was added and the suspension was left to stir for 24 hours. The THF solution was then filtered through a medium porosity fritted funnel. The collected precipitate of white powder and excess magnesium was washed with DME, dissolving the white powder of the collected precipitate. Unreacted magnesium powder was collected and reused. The DME solvent was removed under high vacuum, resulting in compound **2**[Mg^{+2}] as a white powder in 91% yield (4.1g 9.37 mmol). Once dried, compound **2**[Mg^{+2}] is only soluble in DME at cold temperatures -30°C (**Note:** Mg^{2+} counter cation is coordinated to three DME molecules). This reaction is monitored by using ^{1}H NMR by the disappearance of trimethyl ammonium counter cation peak at δ = 3.19 ppm in acetone- d_6. A crystal suitable for x-ray diffraction study was obtained by removing a concentrated sample of **2**[Mg^{+2}] in DME from the freezer at -30°C and

allowing the sample to warm to room temperature. ^{1}H NMR (300 MHz, acetone-d_6, 25°C): δ = 3.46 (s, H), 3.28 (s, H), 2.50-0.75 (bm, 11 H, B-H) ppm; ^{11}B {^{1}H} NMR (96 MHz, acetone- d_6, 25 °C): δ = 37.1, -11.9, -17.4 ppm.

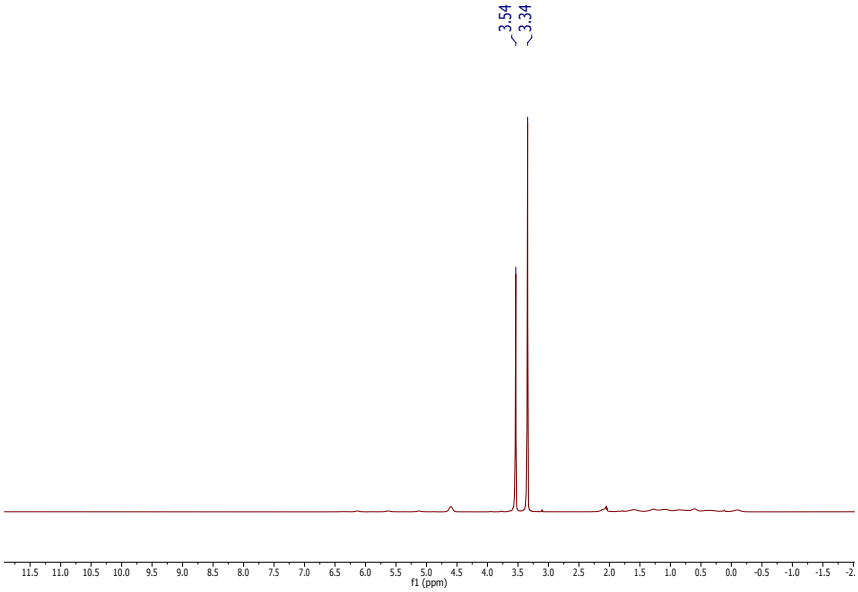


Figure S1. ^{1}H NMR of **2**[Mg^{+2}] in acetone-d_6 (**Note:** peaks at 3.54 and 3.34 ppm are DME).

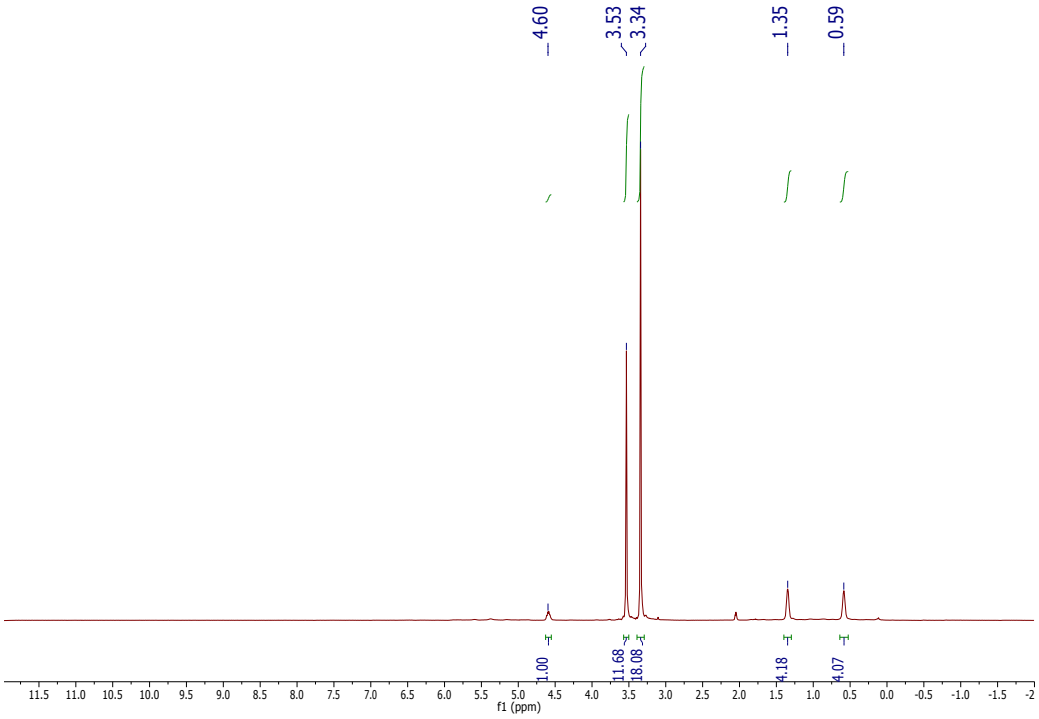


Figure S2. $^{1}H\{^{11}B\}$ NMR of **2[Mg^{2+}]** in acetone-d_6. Intergration of antipodal B-H of the carborane (4.60 ppm) and integration of DME signals (3.53 and 3.34 ppm) is used to determine the number of coordinated DME molecules.

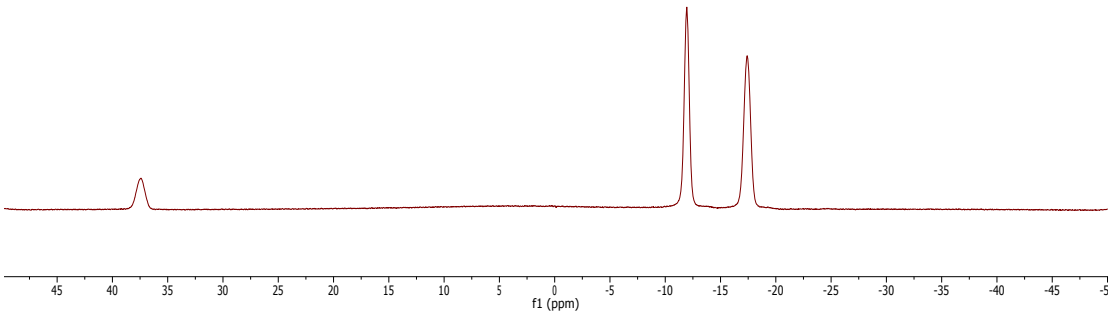


Figure S3. $^{11}B\{^{1}H\}$ NMR of compound **2[Mg^{+2}]** in acetone.

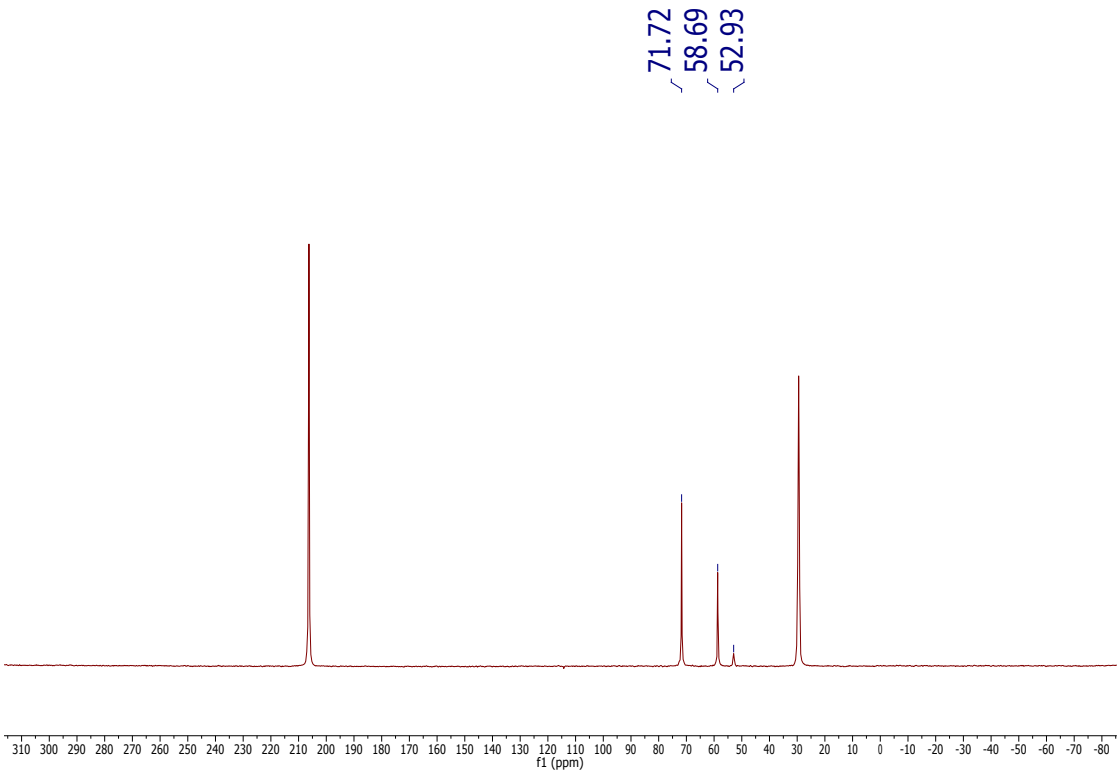


Figure S4. $^{13}C\{^{1}H\}$ NMR of **2[Mg^{2+}]** in acetone.

X-Ray Structure Determination

A colorless prism fragment (0.495 x 0.247 x 0.202 mm3) was used for the single crystal x-ray diffraction study of [C4H10O2]3Mg2+.2[CH10B9]- (sample vL170SM_0m). The crystal was coated with paratone oil and mounted on to a cryo-loop glass fiber. X-ray intensity data were collected at 100(2) K on a Bruker APEX2 (ref. 1) platform-CCD x-ray diffractometer system (fine focus Mo-radiation, λ = 0.71073 Å, 50KV/30mA power). The CCD detector was placed at a distance of 5.0600 cm from the crystal.

A total of 3600 frames were collected for a sphere of reflections (with scan width of 0.3o in ω, starting ω and 2θ angles of –30o, and φ angles of 0o, 90o, 120o, 180o, 240o, and 270o for every 600 frames, 10 sec/frame exposure time). The frames were integrated using the Bruker SAINT software package (ref. 2) and using a narrow-frame integration algorithm. Based on a orthorhombic crystal system, the integrated frames yielded a total of 75989 reflections at a maximum 2θ angle of 61.996 (0.69 Å resolution), of which 10124 were independent reflections (Rint = 0.0484, Rsig = 0.0306, redundancy = 7.5, completeness = 100%) and 9094 (89.8%) reflections were greater than 2σ(I). The unit cell parameters were, a = 20.7310(10) Å, b = 10.6782(5) Å, c = 14.3738(7) Å, α = β = γ = 90o, V = 3181.9(3) Å3, Z = 4, calculated density Dc = 1.114 g/cm3. Absorption corrections were applied (absorption coefficient μ = 0.084 mm-1; max/min transmission = 0.983/0.959) to the raw intensity data using the SADABS program (ref. 3).

The Bruker SHELXTL software package (ref. 4) was used for phase determination and structure refinement. The distribution of intensities (E2-1 = 0.762) and systematic absent

reflections indicated two possible space groups, Pna2(1) and Pnma. The space group Pna2(1) (#33) was later determined to be correct. Direct methods of phase determination followed by two Fourier cycles of refinement led to an electron density map from which most of the non-hydrogen atoms were identified in the asymmetric unit of the unit cell. With subsequent isotropic refinement, all of the non-hydrogen atoms were identified. There was one cation of [C4H10O2]3Mg2+ and two anions of [CH10B9]- present in the asymmetric unit of the unit cell.

Atomic coordinates, isotropic and anisotropic displacement parameters of all the non-hydrogen atoms were refined by means of a full matrix least-squares procedure on F2. The H-atoms were included in the refinement in calculated positions riding on the atoms to which they were attached, except the H-atoms of the two CH-group of the carboranes were refined unrestrained. The refinement converged at R1 = 0.0353, wR2 = 0.0811, with intensity I>2σ (I). Absolute structure parameter cannot be reliably determined because no heavy atom is present in the structure. The largest peak/hole in the final difference map was 0.223/-0.157 e/Å3.

Table S1. Crystal data and structure refinement for vL170SM_0m.

Identification code	vL170SM_0m
Empirical formula	C14 H50 B18 Mg O6
Formula weight	533.43
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P n a 21
Unit cell dimensions	a = 20.7310(10) Å α= 90°.
	b = 10.6782(5) Å β= 90°.
	c = 14.3738(7) Å γ = 90°.
Volume	3181.9(3) Å^3
Z	4
Density (calculated)	1.114 Mg/m^3
Absorption coefficient	0.084 mm^{-1}
F(000)	1136
Crystal size	0.495 x 0.247 x 0.202 mm^3
Theta range for data collection	1.965 to 30.998°.
Index ranges	-30<=h<=30, -15<=k<=15, -20<=l<=20
Reflections collected	75989
Independent reflections	10124 [R(int) = 0.0484]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10124 / 1 / 364
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.0811
R indices (all data)	R1 = 0.0425, wR2 = 0.0852
Absolute structure parameter	?
Extinction coefficient	n/a
Largest diff. peak and hole	0.223 and -0.157 e.Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for vL170SM_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mg(1)	3229(1)	265(1)	1854(1)	15(1)
C(1)	3045(1)	2297(2)	245(1)	24(1)
O(1)	3386(1)	1836(1)	1049(1)	19(1)
C(2)	3700(1)	2822(2)	1569(1)	21(1)
C(3)	4237(1)	2219(2)	2109(1)	21(1)
O(2)	3967(1)	1138(1)	2571(1)	20(1)
C(4)	4383(1)	667(2)	3296(1)	24(1)
C(5)	3035(1)	-1708(2)	3474(1)	25(1)
O(3)	3333(1)	-1371(1)	2607(1)	19(1)
C(6)	3458(1)	-2444(2)	2022(1)	22(1)
C(7)	3947(1)	-2042(2)	1313(1)	23(1)
O(4)	3722(1)	-878(1)	917(1)	21(1)
C(8)	4046(1)	-570(2)	62(1)	28(1)
C(9)	2215(1)	-794(2)	374(1)	25(1)
O(5)	2351(1)	-216(1)	1257(1)	19(1)
C(10)	1794(1)	415(2)	1637(1)	23(1)
C(11)	1911(1)	627(2)	2653(1)	24(1)
O(6)	2567(1)	1053(1)	2766(1)	18(1)
C(12)	2647(1)	1759(2)	3610(1)	28(1)
C(1A)	898(1)	6609(2)	1744(1)	20(1)
B(2A)	695(1)	5183(2)	1572(1)	22(1)
B(3A)	1303(1)	6036(2)	893(1)	22(1)
B(4A)	1651(1)	6650(2)	1972(1)	18(1)
B(5A)	1044(1)	5802(2)	2656(1)	19(1)
B(6A)	1183(1)	4197(2)	2310(1)	20(1)
B(7A)	1366(1)	4361(2)	1060(1)	24(1)
B(8A)	2049(1)	5399(2)	1344(1)	21(1)
B(9A)	1865(1)	5240(2)	2592(1)	20(1)
B(10A)	1934(1)	3992(2)	1870(2)	24(1)
C(1B)	4900(1)	5639(2)	5308(2)	35(1)
B(2B)	5168(1)	6744(2)	4669(1)	20(1)
B(3B)	5497(1)	5147(2)	4701(2)	35(1)
B(4B)	4677(1)	4507(2)	4657(2)	36(1)
B(5B)	4348(1)	6097(2)	4618(1)	23(1)
B(6B)	4728(1)	6742(2)	3598(1)	18(1)
B(7B)	5537(1)	6071(2)	3648(2)	25(1)
B(8B)	5192(1)	4490(2)	3635(2)	37(1)
B(9B)	4376(1)	5156(2)	3580(2)	26(1)
B(10B)	4978(1)	5619(2)	2856(2)	33(1)

Table S3. Bond lengths [Å] and angles [°] for vL170SM_0m.

Mg(1)-O(1)	2.0645(12)
Mg(1)-O(3)	2.0657(12)
Mg(1)-O(2)	2.0660(12)
Mg(1)-O(6)	2.0755(12)
Mg(1)-O(5)	2.0772(11)
Mg(1)-O(4)	2.0854(13)
C(1)-O(1)	1.4409(19)
C(1)-H(1C)	0.9800
C(1)-H(1D)	0.9800
C(1)-H(1E)	0.9800

O(1)-C(2)	1.4461(19)
C(2)-C(3)	1.502(2)
C(2)-H(2C)	0.9900
C(2)-H(2D)	0.9900
C(3)-O(2)	1.4449(19)
C(3)-H(3C)	0.9900
C(3)-H(3D)	0.9900
O(2)-C(4)	1.444(2)
C(4)-H(4C)	0.9800
C(4)-H(4D)	0.9800
C(4)-H(4E)	0.9800
C(5)-O(3)	1.437(2)
C(5)-H(5C)	0.9800
C(5)-H(5D)	0.9800
C(5)-H(5E)	0.9800
O(3)-C(6)	1.444(2)
C(6)-C(7)	1.501(2)
C(6)-H(6C)	0.9900
C(6)-H(6D)	0.9900
C(7)-O(4)	1.444(2)
C(7)-H(7C)	0.9900
C(7)-H(7D)	0.9900
O(4)-C(8)	1.439(2)
C(8)-H(8C)	0.9800
C(8)-H(8D)	0.9800
C(8)-H(8E)	0.9800
C(9)-O(5)	1.438(2)
C(9)-H(9C)	0.9800
C(9)-H(9D)	0.9800
C(9)-H(9E)	0.9800
O(5)-C(10)	1.444(2)
C(10)-C(11)	1.499(2)
C(10)-H(10C)	0.9900
C(10)-H(10D)	0.9900
C(11)-O(6)	1.4412(19)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
O(6)-C(12)	1.439(2)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(1A)-B(4A)	1.596(2)
C(1A)-B(5A)	1.597(2)
C(1A)-B(2A)	1.599(2)
C(1A)-B(3A)	1.604(3)
C(1A)-H(1A)	0.96(2)
B(2A)-B(7A)	1.802(3)
B(2A)-B(6A)	1.806(3)
B(2A)-B(3A)	1.835(3)
B(2A)-B(5A)	1.840(3)
B(2A)-H(2A)	1.1200
B(3A)-B(8A)	1.809(3)
B(3A)-B(7A)	1.810(3)
B(3A)-B(4A)	1.832(3)
B(3A)-H(3A)	1.1200
B(4A)-B(9A)	1.805(3)

B(4A)-B(8A)	1.811(3)
B(4A)-B(5A)	1.836(2)
B(4A)-H(4A)	1.1200
B(5A)-B(9A)	1.808(2)
B(5A)-B(6A)	1.808(2)
B(5A)-H(5A)	1.1200
B(6A)-B(10A)	1.694(3)
B(6A)-B(9A)	1.844(3)
B(6A)-B(7A)	1.845(3)
B(6A)-H(6A)	1.1200
B(7A)-B(10A)	1.701(3)
B(7A)-B(8A)	1.842(3)
B(7A)-H(7A)	1.1200
B(8A)-B(10A)	1.698(3)
B(8A)-B(9A)	1.842(3)
B(8A)-H(8A)	1.1200
B(9A)-B(10A)	1.695(3)
B(9A)-H(9A)	1.1200
B(10A)-H(10A)	1.1200
C(1B)-B(5B)	1.592(3)
C(1B)-B(2B)	1.596(3)
C(1B)-B(4B)	1.597(3)
C(1B)-B(3B)	1.602(4)
C(1B)-H(1B)	0.99(3)
B(2B)-B(6B)	1.788(3)
B(2B)-B(7B)	1.805(3)
B(2B)-B(5B)	1.837(3)
B(2B)-B(3B)	1.837(3)
B(2B)-H(2B)	1.1200
B(3B)-B(8B)	1.800(4)
B(3B)-B(7B)	1.809(3)
B(3B)-B(4B)	1.832(3)
B(3B)-H(3B)	1.1200
B(4B)-B(9B)	1.807(3)
B(4B)-B(8B)	1.815(4)
B(4B)-B(5B)	1.831(3)
B(4B)-H(4B)	1.1200
B(5B)-B(9B)	1.799(3)
B(5B)-B(6B)	1.801(3)
B(5B)-H(5B)	1.1200
B(6B)-B(10B)	1.687(3)
B(6B)-B(7B)	1.826(3)
B(6B)-B(9B)	1.844(3)
B(6B)-H(6B)	1.1200
B(7B)-B(10B)	1.695(3)
B(7B)-B(8B)	1.835(3)
B(7B)-H(7B)	1.1200
B(8B)-B(10B)	1.704(4)
B(8B)-B(9B)	1.835(3)
B(8B)-H(8B)	1.1200
B(9B)-B(10B)	1.699(3)
B(9B)-H(9B)	1.1200
B(10B)-H(10B)	1.1200

O(1)-Mg(1)-O(3)	164.69(5)
O(1)-Mg(1)-O(2)	78.25(5)

O(3)-Mg(1)-O(2) 92.49(5)
O(1)-Mg(1)-O(6) 97.39(5)
O(3)-Mg(1)-O(6) 94.67(5)
O(2)-Mg(1)-O(6) 89.56(5)
O(1)-Mg(1)-O(5) 96.15(5)
O(3)-Mg(1)-O(5) 95.65(5)
O(2)-Mg(1)-O(5) 165.11(5)
O(6)-Mg(1)-O(5) 77.39(5)
O(1)-Mg(1)-O(4) 92.08(5)
O(3)-Mg(1)-O(4) 78.00(5)
O(2)-Mg(1)-O(4) 102.91(5)
O(6)-Mg(1)-O(4) 165.69(5)
O(5)-Mg(1)-O(4) 90.98(5)
O(1)-C(1)-H(1C) 109.5
O(1)-C(1)-H(1D) 109.5
H(1C)-C(1)-H(1D) 109.5
O(1)-C(1)-H(1E) 109.5
H(1C)-C(1)-H(1E) 109.5
H(1D)-C(1)-H(1E) 109.5
C(1)-O(1)-C(2) 112.78(12)
C(1)-O(1)-Mg(1) 130.56(10)
C(2)-O(1)-Mg(1) 111.85(9)
O(1)-C(2)-C(3) 106.82(13)
O(1)-C(2)-H(2C) 110.4
C(3)-C(2)-H(2C) 110.4
O(1)-C(2)-H(2D) 110.4
C(3)-C(2)-H(2D) 110.4
H(2C)-C(2)-H(2D) 108.6
O(2)-C(3)-C(2) 106.96(12)
O(2)-C(3)-H(3C) 110.3
C(2)-C(3)-H(3C) 110.3
O(2)-C(3)-H(3D) 110.3
C(2)-C(3)-H(3D) 110.3
H(3C)-C(3)-H(3D) 108.6
C(4)-O(2)-C(3) 112.16(12)
C(4)-O(2)-Mg(1) 130.22(10)
C(3)-O(2)-Mg(1) 114.76(9)
O(2)-C(4)-H(4C) 109.5
O(2)-C(4)-H(4D) 109.5
H(4C)-C(4)-H(4D) 109.5
O(2)-C(4)-H(4E) 109.5
H(4C)-C(4)-H(4E) 109.5
H(4D)-C(4)-H(4E) 109.5
O(3)-C(5)-H(5C) 109.5
O(3)-C(5)-H(5D) 109.5
H(5C)-C(5)-H(5D) 109.5
O(3)-C(5)-H(5E) 109.5
H(5C)-C(5)-H(5E) 109.5
H(5D)-C(5)-H(5E) 109.5
C(5)-O(3)-C(6) 112.54(12)
C(5)-O(3)-Mg(1) 128.41(10)
C(6)-O(3)-Mg(1) 112.67(9)
O(3)-C(6)-C(7) 106.85(13)
O(3)-C(6)-H(6C) 110.4
C(7)-C(6)-H(6C) 110.4
O(3)-C(6)-H(6D) 110.4

C(7)-C(6)-H(6D) 110.4
H(6C)-C(6)-H(6D) 108.6
O(4)-C(7)-C(6) 107.19(13)
O(4)-C(7)-H(7C) 110.3
C(6)-C(7)-H(7C) 110.3
O(4)-C(7)-H(7D) 110.3
C(6)-C(7)-H(7D) 110.3
H(7C)-C(7)-H(7D) 108.5
C(8)-O(4)-C(7) 112.43(13)
C(8)-O(4)-Mg(1) 130.31(11)
C(7)-O(4)-Mg(1) 114.06(10)
O(4)-C(8)-H(8C) 109.5
O(4)-C(8)-H(8D) 109.5
H(8C)-C(8)-H(8D) 109.5
O(4)-C(8)-H(8E) 109.5
H(8C)-C(8)-H(8E) 109.5
H(8D)-C(8)-H(8E) 109.5
O(5)-C(9)-H(9C) 109.5
O(5)-C(9)-H(9D) 109.5
H(9C)-C(9)-H(9D) 109.5
O(5)-C(9)-H(9E) 109.5
H(9C)-C(9)-H(9E) 109.5
H(9D)-C(9)-H(9E) 109.5
C(9)-O(5)-C(10) 112.14(12)
C(9)-O(5)-Mg(1) 130.01(10)
C(10)-O(5)-Mg(1) 115.34(9)
O(5)-C(10)-C(11) 108.07(13)
O(5)-C(10)-H(10C) 110.1
C(11)-C(10)-H(10C) 110.1
O(5)-C(10)-H(10D) 110.1
C(11)-C(10)-H(10D) 110.1
H(10C)-C(10)-H(10D) 108.4
O(6)-C(11)-C(10) 108.01(13)
O(6)-C(11)-H(11A) 110.1
C(10)-C(11)-H(11A) 110.1
O(6)-C(11)-H(11B) 110.1
C(10)-C(11)-H(11B) 110.1
H(11A)-C(11)-H(11B) 108.4
C(12)-O(6)-C(11) 111.66(13)
C(12)-O(6)-Mg(1) 131.91(10)
C(11)-O(6)-Mg(1) 115.16(10)
O(6)-C(12)-H(12A) 109.5
O(6)-C(12)-H(12B) 109.5
H(12A)-C(12)-H(12B) 109.5
O(6)-C(12)-H(12C) 109.5
H(12A)-C(12)-H(12C) 109.5
H(12B)-C(12)-H(12C) 109.5
B(4A)-C(1A)-B(5A) 70.20(11)
B(4A)-C(1A)-B(2A) 108.37(13)
B(5A)-C(1A)-B(2A) 70.30(11)
B(4A)-C(1A)-B(3A) 69.82(11)
B(5A)-C(1A)-B(3A) 108.68(13)
B(2A)-C(1A)-B(3A) 69.90(12)
B(4A)-C(1A)-H(1A) 122.6(12)
B(5A)-C(1A)-H(1A) 125.3(13)
B(2A)-C(1A)-H(1A) 129.1(12)

B(3A)-C(1A)-H(1A)	125.9(13)
C(1A)-B(2A)-B(7A)	108.92(13)
C(1A)-B(2A)-B(6A)	108.49(13)
B(7A)-B(2A)-B(6A)	61.52(11)
C(1A)-B(2A)-B(3A)	55.19(10)
B(7A)-B(2A)-B(3A)	59.67(11)
B(6A)-B(2A)-B(3A)	102.55(12)
C(1A)-B(2A)-B(5A)	54.81(10)
B(7A)-B(2A)-B(5A)	102.55(12)
B(6A)-B(2A)-B(5A)	59.44(10)
B(3A)-B(2A)-B(5A)	90.12(11)
C(1A)-B(2A)-H(2A)	121.9
B(7A)-B(2A)-H(2A)	120.4
B(6A)-B(2A)-H(2A)	120.6
B(3A)-B(2A)-H(2A)	130.7
B(5A)-B(2A)-H(2A)	130.9
C(1A)-B(3A)-B(8A)	108.54(13)
C(1A)-B(3A)-B(7A)	108.31(13)
B(8A)-B(3A)-B(7A)	61.21(11)
C(1A)-B(3A)-B(4A)	54.87(10)
B(8A)-B(3A)-B(4A)	59.67(10)
B(7A)-B(3A)-B(4A)	102.31(13)
C(1A)-B(3A)-B(2A)	54.91(10)
B(8A)-B(3A)-B(2A)	102.11(13)
B(7A)-B(3A)-B(2A)	59.27(10)
B(4A)-B(3A)-B(2A)	89.92(12)
C(1A)-B(3A)-H(3A)	122.0
B(8A)-B(3A)-H(3A)	120.7
B(7A)-B(3A)-H(3A)	120.8
B(4A)-B(3A)-H(3A)	130.8
B(2A)-B(3A)-H(3A)	131.0
C(1A)-B(4A)-B(9A)	108.58(12)
C(1A)-B(4A)-B(8A)	108.80(13)
B(9A)-B(4A)-B(8A)	61.23(10)
C(1A)-B(4A)-B(3A)	55.31(10)
B(9A)-B(4A)-B(3A)	102.46(12)
B(8A)-B(4A)-B(3A)	59.54(10)
C(1A)-B(4A)-B(5A)	54.93(10)
B(9A)-B(4A)-B(5A)	59.52(10)
B(8A)-B(4A)-B(5A)	102.40(12)
B(3A)-B(4A)-B(5A)	90.35(11)
C(1A)-B(4A)-H(4A)	121.8
B(9A)-B(4A)-H(4A)	120.7
B(8A)-B(4A)-H(4A)	120.6
B(3A)-B(4A)-H(4A)	130.6
B(5A)-B(4A)-H(4A)	130.8
C(1A)-B(5A)-B(9A)	108.41(13)
C(1A)-B(5A)-B(6A)	108.47(14)
B(9A)-B(5A)-B(6A)	61.35(10)
C(1A)-B(5A)-B(4A)	54.87(10)
B(9A)-B(5A)-B(4A)	59.39(10)
B(6A)-B(5A)-B(4A)	102.19(12)
C(1A)-B(5A)-B(2A)	54.89(10)
B(9A)-B(5A)-B(2A)	101.98(12)
B(6A)-B(5A)-B(2A)	59.33(11)
B(4A)-B(5A)-B(2A)	89.62(11)

C(1A)-B(5A)-H(5A)	122.0
B(9A)-B(5A)-H(5A)	120.8
B(6A)-B(5A)-H(5A)	120.7
B(4A)-B(5A)-H(5A)	131.0
B(2A)-B(5A)-H(5A)	131.1
B(10A)-B(6A)-B(2A)	111.70(14)
B(10A)-B(6A)-B(5A)	111.82(13)
B(2A)-B(6A)-B(5A)	61.23(10)
B(10A)-B(6A)-B(9A)	57.04(10)
B(2A)-B(6A)-B(9A)	101.89(12)
B(5A)-B(6A)-B(9A)	59.32(10)
B(10A)-B(6A)-B(7A)	57.24(11)
B(2A)-B(6A)-B(7A)	59.15(11)
B(5A)-B(6A)-B(7A)	102.14(12)
B(9A)-B(6A)-B(7A)	89.91(12)
B(10A)-B(6A)-H(6A)	118.6
B(2A)-B(6A)-H(6A)	120.4
B(5A)-B(6A)-H(6A)	120.2
B(9A)-B(6A)-H(6A)	131.3
B(7A)-B(6A)-H(6A)	131.1
B(10A)-B(7A)-B(2A)	111.56(14)
B(10A)-B(7A)-B(3A)	111.69(13)
B(2A)-B(7A)-B(3A)	61.06(11)
B(10A)-B(7A)-B(8A)	57.11(11)
B(2A)-B(7A)-B(8A)	102.07(12)
B(3A)-B(7A)-B(8A)	59.36(10)
B(10A)-B(7A)-B(6A)	56.90(11)
B(2A)-B(7A)-B(6A)	59.33(10)
B(3A)-B(7A)-B(6A)	101.99(13)
B(8A)-B(7A)-B(6A)	89.98(12)
B(10A)-B(7A)-H(7A)	118.8
B(2A)-B(7A)-H(7A)	120.3
B(3A)-B(7A)-H(7A)	120.3
B(8A)-B(7A)-H(7A)	131.1
B(6A)-B(7A)-H(7A)	131.2
B(10A)-B(8A)-B(3A)	111.86(13)
B(10A)-B(8A)-B(4A)	111.52(13)
B(3A)-B(8A)-B(4A)	60.80(10)
B(10A)-B(8A)-B(9A)	57.04(11)
B(3A)-B(8A)-B(9A)	101.93(12)
B(4A)-B(8A)-B(9A)	59.23(10)
B(10A)-B(8A)-B(7A)	57.24(11)
B(3A)-B(8A)-B(7A)	59.42(11)
B(4A)-B(8A)-B(7A)	101.84(12)
B(9A)-B(8A)-B(7A)	90.09(12)
B(10A)-B(8A)-H(8A)	118.7
B(3A)-B(8A)-H(8A)	120.3
B(4A)-B(8A)-H(8A)	120.6
B(9A)-B(8A)-H(8A)	131.2
B(7A)-B(8A)-H(8A)	131.0
B(10A)-B(9A)-B(4A)	111.98(13)
B(10A)-B(9A)-B(5A)	111.79(13)
B(4A)-B(9A)-B(5A)	61.09(10)
B(10A)-B(9A)-B(8A)	57.22(11)
B(4A)-B(9A)-B(8A)	59.54(10)
B(5A)-B(9A)-B(8A)	102.32(12)

B(10A)-B(9A)-B(6A)	57.01(10)
B(4A)-B(9A)-B(6A)	101.97(12)
B(5A)-B(9A)-B(6A)	59.33(10)
B(8A)-B(9A)-B(6A)	90.02(12)
B(10A)-B(9A)-H(9A)	118.6
B(4A)-B(9A)-H(9A)	120.2
B(5A)-B(9A)-H(9A)	120.2
B(8A)-B(9A)-H(9A)	130.9
B(6A)-B(9A)-H(9A)	131.3
B(6A)-B(10A)-B(9A)	65.95(11)
B(6A)-B(10A)-B(8A)	100.44(13)
B(9A)-B(10A)-B(8A)	65.75(11)
B(6A)-B(10A)-B(7A)	65.85(12)
B(9A)-B(10A)-B(7A)	100.32(13)
B(8A)-B(10A)-B(7A)	65.65(12)
B(6A)-B(10A)-H(10A)	129.7
B(9A)-B(10A)-H(10A)	129.8
B(8A)-B(10A)-H(10A)	129.9
B(7A)-B(10A)-H(10A)	129.9
B(5B)-C(1B)-B(2B)	70.37(12)
B(5B)-C(1B)-B(4B)	70.08(14)
B(2B)-C(1B)-B(4B)	108.84(17)
B(5B)-C(1B)-B(3B)	108.44(17)
B(2B)-C(1B)-B(3B)	70.13(14)
B(4B)-C(1B)-B(3B)	69.88(15)
B(5B)-C(1B)-H(1B)	125.4(15)
B(2B)-C(1B)-H(1B)	126.7(14)
B(4B)-C(1B)-H(1B)	124.4(14)
B(3B)-C(1B)-H(1B)	126.1(15)
C(1B)-B(2B)-B(6B)	108.48(14)
C(1B)-B(2B)-B(7B)	108.74(15)
B(6B)-B(2B)-B(7B)	61.07(11)
C(1B)-B(2B)-B(5B)	54.71(11)
B(6B)-B(2B)-B(5B)	59.56(10)
B(7B)-B(2B)-B(5B)	102.15(13)
C(1B)-B(2B)-B(3B)	55.09(14)
B(6B)-B(2B)-B(3B)	102.10(13)
B(7B)-B(2B)-B(3B)	59.56(13)
B(5B)-B(2B)-B(3B)	89.70(12)
C(1B)-B(2B)-H(2B)	121.9
B(6B)-B(2B)-H(2B)	120.8
B(7B)-B(2B)-H(2B)	120.6
B(5B)-B(2B)-H(2B)	131.1
B(3B)-B(2B)-H(2B)	130.9
C(1B)-B(3B)-B(8B)	108.67(16)
C(1B)-B(3B)-B(7B)	108.24(15)
B(8B)-B(3B)-B(7B)	61.09(14)
C(1B)-B(3B)-B(4B)	54.92(14)
B(8B)-B(3B)-B(4B)	59.96(14)
B(7B)-B(3B)-B(4B)	102.58(15)
C(1B)-B(3B)-B(2B)	54.77(12)
B(8B)-B(3B)-B(2B)	102.13(14)
B(7B)-B(3B)-B(2B)	59.32(11)
B(4B)-B(3B)-B(2B)	90.09(13)
C(1B)-B(3B)-H(3B)	122.1
B(8B)-B(3B)-H(3B)	120.6

B(7B)-B(3B)-H(3B)	120.8
B(4B)-B(3B)-H(3B)	130.5
B(2B)-B(3B)-H(3B)	131.0
C(1B)-B(4B)-B(9B)	108.14(14)
C(1B)-B(4B)-B(8B)	108.20(16)
B(9B)-B(4B)-B(8B)	60.89(13)
C(1B)-B(4B)-B(5B)	54.83(12)
B(9B)-B(4B)-B(5B)	59.27(11)
B(8B)-B(4B)-B(5B)	101.75(15)
C(1B)-B(4B)-B(3B)	55.20(14)
B(9B)-B(4B)-B(3B)	101.92(15)
B(8B)-B(4B)-B(3B)	59.16(14)
B(5B)-B(4B)-B(3B)	90.06(13)
C(1B)-B(4B)-H(4B)	122.0
B(9B)-B(4B)-H(4B)	121.0
B(8B)-B(4B)-H(4B)	121.1
B(5B)-B(4B)-H(4B)	131.0
B(3B)-B(4B)-H(4B)	130.8
C(1B)-B(5B)-B(9B)	108.76(16)
C(1B)-B(5B)-B(6B)	108.07(15)
B(9B)-B(5B)-B(6B)	61.62(11)
C(1B)-B(5B)-B(4B)	55.09(13)
B(9B)-B(5B)-B(4B)	59.71(13)
B(6B)-B(5B)-B(4B)	102.51(14)
C(1B)-B(5B)-B(2B)	54.92(11)
B(9B)-B(5B)-B(2B)	102.29(13)
B(6B)-B(5B)-B(2B)	58.89(10)
B(4B)-B(5B)-B(2B)	90.15(13)
C(1B)-B(5B)-H(5B)	122.0
B(9B)-B(5B)-H(5B)	120.4
B(6B)-B(5B)-H(5B)	120.9
B(4B)-B(5B)-H(5B)	130.6
B(2B)-B(5B)-H(5B)	131.1
B(10B)-B(6B)-B(2B)	112.86(15)
B(10B)-B(6B)-B(5B)	112.17(14)
B(2B)-B(6B)-B(5B)	61.55(11)
B(10B)-B(6B)-B(7B)	57.53(11)
B(2B)-B(6B)-B(7B)	59.90(11)
B(5B)-B(6B)-B(7B)	102.72(13)
B(10B)-B(6B)-B(9B)	57.31(12)
B(2B)-B(6B)-B(9B)	102.40(13)
B(5B)-B(6B)-B(9B)	59.13(11)
B(7B)-B(6B)-B(9B)	90.19(11)
B(10B)-B(6B)-H(6B)	118.1
B(2B)-B(6B)-H(6B)	119.6
B(5B)-B(6B)-H(6B)	120.0
B(7B)-B(6B)-H(6B)	130.8
B(9B)-B(6B)-H(6B)	131.3
B(10B)-B(7B)-B(2B)	111.69(14)
B(10B)-B(7B)-B(3B)	112.02(15)
B(2B)-B(7B)-B(3B)	61.11(12)
B(10B)-B(7B)-B(6B)	57.13(11)
B(2B)-B(7B)-B(6B)	59.03(10)
B(3B)-B(7B)-B(6B)	101.76(14)
B(10B)-B(7B)-B(8B)	57.58(14)
B(2B)-B(7B)-B(8B)	102.07(15)

B(3B)-B(7B)-B(8B)	59.22(14)
B(6B)-B(7B)-B(8B)	90.10(12)
B(10B)-B(7B)-H(7B)	118.4
B(2B)-B(7B)-H(7B)	120.4
B(3B)-B(7B)-H(7B)	120.3
B(6B)-B(7B)-H(7B)	131.3
B(8B)-B(7B)-H(7B)	130.9
B(10B)-B(8B)-B(3B)	112.01(14)
B(10B)-B(8B)-B(4B)	111.86(15)
B(3B)-B(8B)-B(4B)	60.88(14)
B(10B)-B(8B)-B(7B)	57.10(12)
B(3B)-B(8B)-B(7B)	59.69(12)
B(4B)-B(8B)-B(7B)	102.23(15)
B(10B)-B(8B)-B(9B)	57.22(13)
B(3B)-B(8B)-B(9B)	102.04(16)
B(4B)-B(8B)-B(9B)	59.33(13)
B(7B)-B(8B)-B(9B)	90.18(13)
B(10B)-B(8B)-H(8B)	118.5
B(3B)-B(8B)-H(8B)	120.2
B(4B)-B(8B)-H(8B)	120.3
B(7B)-B(8B)-H(8B)	130.9
B(9B)-B(8B)-H(8B)	131.1
B(10B)-B(9B)-B(5B)	111.73(14)
B(10B)-B(9B)-B(4B)	112.54(16)
B(5B)-B(9B)-B(4B)	61.02(13)
B(10B)-B(9B)-B(8B)	57.50(14)
B(5B)-B(9B)-B(8B)	102.20(15)
B(4B)-B(9B)-B(8B)	59.79(14)
B(10B)-B(9B)-B(6B)	56.71(11)
B(5B)-B(9B)-B(6B)	59.25(10)
B(4B)-B(9B)-B(6B)	101.77(13)
B(8B)-B(9B)-B(6B)	89.52(12)
B(10B)-B(9B)-H(9B)	118.4
B(5B)-B(9B)-H(9B)	120.3
B(4B)-B(9B)-H(9B)	120.0
B(8B)-B(9B)-H(9B)	131.0
B(6B)-B(9B)-H(9B)	131.7
B(6B)-B(10B)-B(7B)	65.33(12)
B(6B)-B(10B)-B(9B)	65.98(12)
B(7B)-B(10B)-B(9B)	99.96(16)
B(6B)-B(10B)-B(8B)	99.60(16)
B(7B)-B(10B)-B(8B)	65.32(14)
B(9B)-B(10B)-B(8B)	65.27(14)
B(6B)-B(10B)-H(10B)	130.0
B(7B)-B(10B)-H(10B)	130.2
B(9B)-B(10B)-H(10B)	129.9
B(8B)-B(10B)-H(10B)	130.4

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for vL170SM_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mg(1)	14(1)	17(1)	13(1)	0(1)	-1(1)	-1(1)

C(1)	26(1)	25(1)	20(1)	6(1)	-1(1)	-1(1)
O(1)	22(1)	18(1)	17(1)	1(1)	-2(1)	-4(1)
C(2)	20(1)	18(1)	25(1)	-3(1)	2(1)	-4(1)
C(3)	16(1)	21(1)	26(1)	-3(1)	1(1)	-5(1)
O(2)	15(1)	25(1)	19(1)	0(1)	-3(1)	-4(1)
C(4)	17(1)	36(1)	19(1)	-3(1)	-5(1)	1(1)
C(5)	24(1)	32(1)	20(1)	9(1)	0(1)	-1(1)
O(3)	20(1)	20(1)	18(1)	3(1)	0(1)	0(1)
C(6)	23(1)	18(1)	26(1)	-1(1)	-6(1)	0(1)
C(7)	22(1)	22(1)	25(1)	-3(1)	-2(1)	5(1)
O(4)	23(1)	22(1)	17(1)	0(1)	2(1)	3(1)
C(8)	30(1)	37(1)	18(1)	-3(1)	6(1)	1(1)
C(9)	27(1)	28(1)	21(1)	-3(1)	-9(1)	-6(1)
O(5)	16(1)	21(1)	20(1)	-2(1)	-6(1)	-2(1)
C(10)	15(1)	26(1)	27(1)	0(1)	-6(1)	1(1)
C(11)	14(1)	30(1)	26(1)	1(1)	2(1)	-2(1)
O(6)	14(1)	24(1)	17(1)	-2(1)	0(1)	0(1)
C(12)	26(1)	40(1)	18(1)	-9(1)	1(1)	3(1)
C(1A)	16(1)	21(1)	24(1)	5(1)	-1(1)	1(1)
B(2A)	17(1)	26(1)	22(1)	3(1)	-2(1)	-6(1)
B(3A)	23(1)	25(1)	18(1)	3(1)	-2(1)	-6(1)
B(4A)	17(1)	18(1)	19(1)	1(1)	0(1)	-2(1)
B(5A)	18(1)	21(1)	18(1)	1(1)	3(1)	1(1)
B(6A)	20(1)	18(1)	23(1)	2(1)	2(1)	-2(1)
B(7A)	27(1)	22(1)	23(1)	-4(1)	3(1)	-7(1)
B(8A)	17(1)	22(1)	22(1)	-2(1)	4(1)	-2(1)
B(9A)	18(1)	21(1)	20(1)	2(1)	-2(1)	0(1)
B(10A)	21(1)	20(1)	32(1)	0(1)	5(1)	2(1)
C(1B)	45(1)	33(1)	28(1)	15(1)	-9(1)	-10(1)
B(2B)	24(1)	18(1)	18(1)	2(1)	-5(1)	-3(1)
B(3B)	27(1)	18(1)	62(2)	10(1)	-19(1)	-3(1)
B(4B)	29(1)	19(1)	59(2)	15(1)	-10(1)	-6(1)
B(5B)	25(1)	21(1)	23(1)	3(1)	4(1)	-4(1)
B(6B)	17(1)	20(1)	16(1)	-2(1)	0(1)	-1(1)
B(7B)	18(1)	19(1)	38(1)	-6(1)	2(1)	1(1)
B(8B)	21(1)	20(1)	70(2)	-15(1)	-3(1)	1(1)
B(9B)	19(1)	20(1)	38(1)	-10(1)	-4(1)	-1(1)
B(10B)	31(1)	38(1)	30(1)	-18(1)	4(1)	-3(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for vL170SM_0m.

	x	y	z	U(eq)
H(1C)	3350	2703	-179	35
H(1D)	2718	2905	442	35
H(1E)	2835	1597	-75	35
H(2C)	3390	3228	1998	25
H(2D)	3874	3465	1142	25
H(3C)	4589	1961	1685	26
H(3D)	4415	2813	2572	26
H(4C)	4463	1330	3753	36
H(4D)	4794	398	3024	36
H(4E)	4176	-46	3603	36

H(5C)	3319	-2280	3816	38
H(5D)	2622	-2123	3353	38
H(5E)	2961	-952	3846	38
H(6C)	3057	-2722	1712	27
H(6D)	3629	-3147	2398	27
H(7C)	4373	-1921	1610	27
H(7D)	3990	-2686	821	27
H(8C)	3957	-1219	-403	42
H(8D)	4512	-522	173	42
H(8E)	3890	240	-166	42
H(9C)	1901	-1471	462	38
H(9D)	2614	-1136	112	38
H(9E)	2036	-167	-52	38
H(10C)	1404	-104	1547	27
H(10D)	1728	1226	1317	27
H(11A)	1608	1264	2896	28
H(11B)	1844	-161	3003	28
H(12A)	2371	2503	3592	42
H(12B)	3099	2018	3671	42
H(12C)	2527	1237	4144	42
H(1A)	636(10)	7348(19)	1723(15)	24
H(2A)	188	4912	1394	26
H(3A)	1282	6448	177	26
H(4A)	1909	7552	2115	22
H(5A)	817	6024	3343	23
H(6A)	958	3411	2711	24
H(7A)	1288	3707	462	29
H(8A)	2515	5572	972	25
H(9A)	2186	5289	3217	23
H(10A)	2262	3161	1913	29
H(1B)	4871(12)	5640(20)	5990(20)	42
H(2B)	5354	7641	4972	24
H(3B)	5946	4766	5030	42
H(4B)	4473	3619	4949	43
H(5B)	3877	6476	4877	27
H(6B)	4552	7649	3300	21
H(7B)	6012	6431	3390	30
H(8B)	5390	3585	3365	45
H(9B)	3921	4783	3266	31
H(10B)	4999	5620	2077	39

Table 6. Torsion angles [°] for vL170SM_0m.

C(1)-O(1)-C(2)-C(3)	-156.90(13)
Mg(1)-O(1)-C(2)-C(3)	44.93(14)
O(1)-C(2)-C(3)-O(2)	-48.81(16)
C(2)-C(3)-O(2)-C(4)	-164.93(13)
C(2)-C(3)-O(2)-Mg(1)	32.19(15)
C(5)-O(3)-C(6)-C(7)	-161.92(13)
Mg(1)-O(3)-C(6)-C(7)	43.62(14)
O(3)-C(6)-C(7)-O(4)	-49.19(16)
C(6)-C(7)-O(4)-C(8)	-163.99(14)
C(6)-C(7)-O(4)-Mg(1)	34.05(15)
C(9)-O(5)-C(10)-C(11)	162.47(14)
Mg(1)-O(5)-C(10)-C(11)	-33.63(15)
O(5)-C(10)-C(11)-O(6)	43.16(17)

C(10)-C(11)-O(6)-C(12)	155.88(14)
C(10)-C(11)-O(6)-Mg(1)	-35.48(16)
B(4A)-C(1A)-B(2A)-B(7A)	-32.11(18)
B(5A)-C(1A)-B(2A)-B(7A)	-92.25(14)
B(3A)-C(1A)-B(2A)-B(7A)	27.32(13)
B(4A)-C(1A)-B(2A)-B(6A)	33.24(18)
B(5A)-C(1A)-B(2A)-B(6A)	-26.89(13)
B(3A)-C(1A)-B(2A)-B(6A)	92.67(14)
B(4A)-C(1A)-B(2A)-B(3A)	-59.43(13)
B(5A)-C(1A)-B(2A)-B(3A)	-119.56(13)
B(4A)-C(1A)-B(2A)-B(5A)	60.13(13)
B(3A)-C(1A)-B(2A)-B(5A)	119.56(13)
B(4A)-C(1A)-B(3A)-B(8A)	27.48(12)
B(5A)-C(1A)-B(3A)-B(8A)	-32.18(17)
B(2A)-C(1A)-B(3A)-B(8A)	-92.00(14)
B(4A)-C(1A)-B(3A)-B(7A)	92.39(14)
B(5A)-C(1A)-B(3A)-B(7A)	32.74(17)
B(2A)-C(1A)-B(3A)-B(7A)	-27.09(13)
B(5A)-C(1A)-B(3A)-B(4A)	-59.65(13)
B(2A)-C(1A)-B(3A)-B(4A)	-119.48(13)
B(4A)-C(1A)-B(3A)-B(2A)	119.48(13)
B(5A)-C(1A)-B(3A)-B(2A)	59.82(13)
B(7A)-B(2A)-B(3A)-C(1A)	-149.81(14)
B(6A)-B(2A)-B(3A)-C(1A)	-103.94(14)
B(5A)-B(2A)-B(3A)-C(1A)	-45.30(11)
C(1A)-B(2A)-B(3A)-B(8A)	104.28(14)
B(7A)-B(2A)-B(3A)-B(8A)	-45.53(12)
B(6A)-B(2A)-B(3A)-B(8A)	0.34(15)
B(5A)-B(2A)-B(3A)-B(8A)	58.98(13)
C(1A)-B(2A)-B(3A)-B(7A)	149.81(14)
B(6A)-B(2A)-B(3A)-B(7A)	45.87(12)
B(5A)-B(2A)-B(3A)-B(7A)	104.51(12)
C(1A)-B(2A)-B(3A)-B(4A)	45.40(11)
B(7A)-B(2A)-B(3A)-B(4A)	-104.41(13)
B(6A)-B(2A)-B(3A)-B(4A)	-58.54(13)
B(5A)-B(2A)-B(3A)-B(4A)	0.10(12)
B(5A)-C(1A)-B(4A)-B(9A)	27.14(13)
B(2A)-C(1A)-B(4A)-B(9A)	-33.06(18)
B(3A)-C(1A)-B(4A)-B(9A)	-92.53(14)
B(5A)-C(1A)-B(4A)-B(8A)	92.19(13)
B(2A)-C(1A)-B(4A)-B(8A)	31.99(17)
B(3A)-C(1A)-B(4A)-B(8A)	-27.49(12)
B(5A)-C(1A)-B(4A)-B(3A)	119.67(13)
B(2A)-C(1A)-B(4A)-B(3A)	59.48(13)
B(2A)-C(1A)-B(4A)-B(5A)	-60.20(13)
B(3A)-C(1A)-B(4A)-B(5A)	-119.67(13)
B(8A)-B(3A)-B(4A)-C(1A)	-149.54(13)
B(7A)-B(3A)-B(4A)-C(1A)	-103.87(13)
B(2A)-B(3A)-B(4A)-C(1A)	-45.43(11)
C(1A)-B(3A)-B(4A)-B(9A)	104.12(13)
B(8A)-B(3A)-B(4A)-B(9A)	-45.43(11)
B(7A)-B(3A)-B(4A)-B(9A)	0.25(15)
B(2A)-B(3A)-B(4A)-B(9A)	58.69(13)
C(1A)-B(3A)-B(4A)-B(8A)	149.54(13)
B(7A)-B(3A)-B(4A)-B(8A)	45.68(12)
B(2A)-B(3A)-B(4A)-B(8A)	104.12(12)

C(1A)-B(3A)-B(4A)-B(5A)	45.33(10)
B(8A)-B(3A)-B(4A)-B(5A)	-104.22(12)
B(7A)-B(3A)-B(4A)-B(5A)	-58.54(13)
B(2A)-B(3A)-B(4A)-B(5A)	-0.10(12)
B(4A)-C(1A)-B(5A)-B(9A)	-27.07(13)
B(2A)-C(1A)-B(5A)-B(9A)	91.92(13)
B(3A)-C(1A)-B(5A)-B(9A)	32.35(17)
B(4A)-C(1A)-B(5A)-B(6A)	-92.13(13)
B(2A)-C(1A)-B(5A)-B(6A)	26.85(13)
B(3A)-C(1A)-B(5A)-B(6A)	-32.72(17)
B(2A)-C(1A)-B(5A)-B(4A)	118.99(13)
B(3A)-C(1A)-B(5A)-B(4A)	59.42(12)
B(4A)-C(1A)-B(5A)-B(2A)	-118.99(13)
B(3A)-C(1A)-B(5A)-B(2A)	-59.57(13)
B(9A)-B(4A)-B(5A)-C(1A)	-149.89(14)
B(8A)-B(4A)-B(5A)-C(1A)	-104.41(14)
B(3A)-B(4A)-B(5A)-C(1A)	-45.59(11)
C(1A)-B(4A)-B(5A)-B(9A)	149.89(14)
B(8A)-B(4A)-B(5A)-B(9A)	45.47(12)
B(3A)-B(4A)-B(5A)-B(9A)	104.29(12)
C(1A)-B(4A)-B(5A)-B(6A)	104.14(14)
B(9A)-B(4A)-B(5A)-B(6A)	-45.75(12)
B(8A)-B(4A)-B(5A)-B(6A)	-0.27(15)
B(3A)-B(4A)-B(5A)-B(6A)	58.55(13)
C(1A)-B(4A)-B(5A)-B(2A)	45.69(11)
B(9A)-B(4A)-B(5A)-B(2A)	-104.19(12)
B(8A)-B(4A)-B(5A)-B(2A)	-58.72(13)
B(3A)-B(4A)-B(5A)-B(2A)	0.10(12)
B(7A)-B(2A)-B(5A)-C(1A)	104.46(14)
B(6A)-B(2A)-B(5A)-C(1A)	150.12(14)
B(3A)-B(2A)-B(5A)-C(1A)	45.58(11)
C(1A)-B(2A)-B(5A)-B(9A)	-104.21(13)
B(7A)-B(2A)-B(5A)-B(9A)	0.25(15)
B(6A)-B(2A)-B(5A)-B(9A)	45.92(11)
B(3A)-B(2A)-B(5A)-B(9A)	-58.63(13)
C(1A)-B(2A)-B(5A)-B(6A)	-150.12(14)
B(7A)-B(2A)-B(5A)-B(6A)	-45.67(12)
B(3A)-B(2A)-B(5A)-B(6A)	-104.55(12)
C(1A)-B(2A)-B(5A)-B(4A)	-45.67(10)
B(7A)-B(2A)-B(5A)-B(4A)	58.78(13)
B(6A)-B(2A)-B(5A)-B(4A)	104.45(12)
B(3A)-B(2A)-B(5A)-B(4A)	-0.10(12)
C(1A)-B(2A)-B(6A)-B(10A)	-78.34(17)
B(7A)-B(2A)-B(6A)-B(10A)	23.64(13)
B(3A)-B(2A)-B(6A)-B(10A)	-21.17(17)
B(5A)-B(2A)-B(6A)-B(10A)	-103.76(15)
C(1A)-B(2A)-B(6A)-B(5A)	25.42(13)
B(7A)-B(2A)-B(6A)-B(5A)	127.40(12)
B(3A)-B(2A)-B(6A)-B(5A)	82.59(12)
C(1A)-B(2A)-B(6A)-B(9A)	-19.31(16)
B(7A)-B(2A)-B(6A)-B(9A)	82.67(12)
B(3A)-B(2A)-B(6A)-B(9A)	37.86(15)
B(5A)-B(2A)-B(6A)-B(9A)	-44.73(11)
C(1A)-B(2A)-B(6A)-B(7A)	-101.98(14)
B(3A)-B(2A)-B(6A)-B(7A)	-44.81(12)
B(5A)-B(2A)-B(6A)-B(7A)	-127.40(12)

C(1A)-B(5A)-B(6A)-B(10A)	78.12(17)
B(9A)-B(5A)-B(6A)-B(10A)	-23.23(14)
B(4A)-B(5A)-B(6A)-B(10A)	21.39(18)
B(2A)-B(5A)-B(6A)-B(10A)	103.57(16)
C(1A)-B(5A)-B(6A)-B(2A)	-25.44(12)
B(9A)-B(5A)-B(6A)-B(2A)	-126.80(13)
B(4A)-B(5A)-B(6A)-B(2A)	-82.18(12)
C(1A)-B(5A)-B(6A)-B(9A)	101.36(14)
B(4A)-B(5A)-B(6A)-B(9A)	44.62(11)
B(2A)-B(5A)-B(6A)-B(9A)	126.80(13)
C(1A)-B(5A)-B(6A)-B(7A)	18.79(16)
B(9A)-B(5A)-B(6A)-B(7A)	-82.57(13)
B(4A)-B(5A)-B(6A)-B(7A)	-37.94(15)
B(2A)-B(5A)-B(6A)-B(7A)	44.23(11)
C(1A)-B(2A)-B(7A)-B(10A)	77.75(17)
B(6A)-B(2A)-B(7A)-B(10A)	-23.52(13)
B(3A)-B(2A)-B(7A)-B(10A)	103.63(15)
B(5A)-B(2A)-B(7A)-B(10A)	20.97(16)
C(1A)-B(2A)-B(7A)-B(3A)	-25.88(13)
B(6A)-B(2A)-B(7A)-B(3A)	-127.15(13)
B(5A)-B(2A)-B(7A)-B(3A)	-82.66(12)
C(1A)-B(2A)-B(7A)-B(8A)	18.58(17)
B(6A)-B(2A)-B(7A)-B(8A)	-82.69(13)
B(3A)-B(2A)-B(7A)-B(8A)	44.46(12)
B(5A)-B(2A)-B(7A)-B(8A)	-38.20(15)
C(1A)-B(2A)-B(7A)-B(6A)	101.27(14)
B(3A)-B(2A)-B(7A)-B(6A)	127.15(13)
B(5A)-B(2A)-B(7A)-B(6A)	44.49(11)
C(1A)-B(3A)-B(7A)-B(10A)	-77.73(17)
B(8A)-B(3A)-B(7A)-B(10A)	23.83(13)
B(4A)-B(3A)-B(7A)-B(10A)	-20.97(17)
B(2A)-B(3A)-B(7A)-B(10A)	-103.41(15)
C(1A)-B(3A)-B(7A)-B(2A)	25.69(12)
B(8A)-B(3A)-B(7A)-B(2A)	127.24(13)
B(4A)-B(3A)-B(7A)-B(2A)	82.45(13)
C(1A)-B(3A)-B(7A)-B(8A)	-101.55(14)
B(4A)-B(3A)-B(7A)-B(8A)	-44.79(11)
B(2A)-B(3A)-B(7A)-B(8A)	-127.24(13)
C(1A)-B(3A)-B(7A)-B(6A)	-18.81(16)
B(8A)-B(3A)-B(7A)-B(6A)	82.74(13)
B(4A)-B(3A)-B(7A)-B(6A)	37.95(15)
B(2A)-B(3A)-B(7A)-B(6A)	-44.50(12)
B(2A)-B(6A)-B(7A)-B(10A)	153.70(14)
B(5A)-B(6A)-B(7A)-B(10A)	108.29(14)
B(9A)-B(6A)-B(7A)-B(10A)	49.77(11)
B(10A)-B(6A)-B(7A)-B(2A)	-153.70(14)
B(5A)-B(6A)-B(7A)-B(2A)	-45.42(11)
B(9A)-B(6A)-B(7A)-B(2A)	-103.94(12)
B(10A)-B(6A)-B(7A)-B(3A)	-108.22(14)
B(2A)-B(6A)-B(7A)-B(3A)	45.49(12)
B(5A)-B(6A)-B(7A)-B(3A)	0.07(15)
B(9A)-B(6A)-B(7A)-B(3A)	-58.45(13)
B(10A)-B(6A)-B(7A)-B(8A)	-49.62(11)
B(2A)-B(6A)-B(7A)-B(8A)	104.08(12)
B(5A)-B(6A)-B(7A)-B(8A)	58.67(13)
B(9A)-B(6A)-B(7A)-B(8A)	0.15(12)

C(1A)-B(3A)-B(8A)-B(10A)	77.28(17)
B(7A)-B(3A)-B(8A)-B(10A)	-23.89(14)
B(4A)-B(3A)-B(8A)-B(10A)	103.21(15)
B(2A)-B(3A)-B(8A)-B(10A)	20.53(18)
C(1A)-B(3A)-B(8A)-B(4A)	-25.93(12)
B(7A)-B(3A)-B(8A)-B(4A)	-127.10(13)
B(2A)-B(3A)-B(8A)-B(4A)	-82.69(12)
C(1A)-B(3A)-B(8A)-B(9A)	18.24(15)
B(7A)-B(3A)-B(8A)-B(9A)	-82.93(12)
B(4A)-B(3A)-B(8A)-B(9A)	44.17(11)
B(2A)-B(3A)-B(8A)-B(9A)	-38.52(14)
C(1A)-B(3A)-B(8A)-B(7A)	101.18(14)
B(4A)-B(3A)-B(8A)-B(7A)	127.10(13)
B(2A)-B(3A)-B(8A)-B(7A)	44.42(12)
C(1A)-B(4A)-B(8A)-B(10A)	-77.66(17)
B(9A)-B(4A)-B(8A)-B(10A)	23.71(13)
B(3A)-B(4A)-B(8A)-B(10A)	-103.78(15)
B(5A)-B(4A)-B(8A)-B(10A)	-20.79(17)
C(1A)-B(4A)-B(8A)-B(3A)	26.12(12)
B(9A)-B(4A)-B(8A)-B(3A)	127.49(12)
B(5A)-B(4A)-B(8A)-B(3A)	82.99(12)
C(1A)-B(4A)-B(8A)-B(9A)	-101.37(13)
B(3A)-B(4A)-B(8A)-B(9A)	-127.49(12)
B(5A)-B(4A)-B(8A)-B(9A)	-44.50(11)
C(1A)-B(4A)-B(8A)-B(7A)	-18.43(16)
B(9A)-B(4A)-B(8A)-B(7A)	82.93(13)
B(3A)-B(4A)-B(8A)-B(7A)	-44.55(12)
B(5A)-B(4A)-B(8A)-B(7A)	38.43(15)
B(2A)-B(7A)-B(8A)-B(10A)	108.02(15)
B(3A)-B(7A)-B(8A)-B(10A)	153.45(15)
B(6A)-B(7A)-B(8A)-B(10A)	49.46(12)
B(10A)-B(7A)-B(8A)-B(3A)	-153.45(15)
B(2A)-B(7A)-B(8A)-B(3A)	-45.43(12)
B(6A)-B(7A)-B(8A)-B(3A)	-103.99(13)
B(10A)-B(7A)-B(8A)-B(4A)	-108.11(14)
B(2A)-B(7A)-B(8A)-B(4A)	-0.09(16)
B(3A)-B(7A)-B(8A)-B(4A)	45.34(12)
B(6A)-B(7A)-B(8A)-B(4A)	-58.65(13)
B(10A)-B(7A)-B(8A)-B(9A)	-49.61(12)
B(2A)-B(7A)-B(8A)-B(9A)	58.41(13)
B(3A)-B(7A)-B(8A)-B(9A)	103.84(12)
B(6A)-B(7A)-B(8A)-B(9A)	-0.15(12)
C(1A)-B(4A)-B(9A)-B(10A)	77.89(17)
B(8A)-B(4A)-B(9A)-B(10A)	-23.84(13)
B(3A)-B(4A)-B(9A)-B(10A)	20.62(16)
B(5A)-B(4A)-B(9A)-B(10A)	103.56(14)
C(1A)-B(4A)-B(9A)-B(5A)	-25.67(13)
B(8A)-B(4A)-B(9A)-B(5A)	-127.41(13)
B(3A)-B(4A)-B(9A)-B(5A)	-82.94(12)
C(1A)-B(4A)-B(9A)-B(8A)	101.73(14)
B(3A)-B(4A)-B(9A)-B(8A)	44.46(11)
B(5A)-B(4A)-B(9A)-B(8A)	127.41(13)
C(1A)-B(4A)-B(9A)-B(6A)	18.87(16)
B(8A)-B(4A)-B(9A)-B(6A)	-82.86(13)
B(3A)-B(4A)-B(9A)-B(6A)	-38.40(14)
B(5A)-B(4A)-B(9A)-B(6A)	44.54(11)

C(1A)-B(5A)-B(9A)-B(10A)	-78.24(16)
B(6A)-B(5A)-B(9A)-B(10A)	23.22(13)
B(4A)-B(5A)-B(9A)-B(10A)	-103.86(15)
B(2A)-B(5A)-B(9A)-B(10A)	-21.54(16)
C(1A)-B(5A)-B(9A)-B(4A)	25.62(12)
B(6A)-B(5A)-B(9A)-B(4A)	127.08(13)
B(2A)-B(5A)-B(9A)-B(4A)	82.33(12)
C(1A)-B(5A)-B(9A)-B(8A)	-18.87(16)
B(6A)-B(5A)-B(9A)-B(8A)	82.58(12)
B(4A)-B(5A)-B(9A)-B(8A)	-44.50(11)
B(2A)-B(5A)-B(9A)-B(8A)	37.83(14)
C(1A)-B(5A)-B(9A)-B(6A)	-101.46(15)
B(4A)-B(5A)-B(9A)-B(6A)	-127.08(13)
B(2A)-B(5A)-B(9A)-B(6A)	-44.76(11)
B(3A)-B(8A)-B(9A)-B(10A)	108.45(14)
B(4A)-B(8A)-B(9A)-B(10A)	153.52(14)
B(7A)-B(8A)-B(9A)-B(10A)	49.76(11)
B(10A)-B(8A)-B(9A)-B(4A)	-153.52(14)
B(3A)-B(8A)-B(9A)-B(4A)	-45.07(11)
B(7A)-B(8A)-B(9A)-B(4A)	-103.76(12)
B(10A)-B(8A)-B(9A)-B(5A)	-108.14(14)
B(3A)-B(8A)-B(9A)-B(5A)	0.31(14)
B(4A)-B(8A)-B(9A)-B(5A)	45.38(11)
B(7A)-B(8A)-B(9A)-B(5A)	-58.38(13)
B(10A)-B(8A)-B(9A)-B(6A)	-49.61(11)
B(3A)-B(8A)-B(9A)-B(6A)	58.84(13)
B(4A)-B(8A)-B(9A)-B(6A)	103.91(11)
B(7A)-B(8A)-B(9A)-B(6A)	0.15(12)
B(2A)-B(6A)-B(9A)-B(10A)	-108.29(15)
B(5A)-B(6A)-B(9A)-B(10A)	-154.12(15)
B(7A)-B(6A)-B(9A)-B(10A)	-49.92(12)
B(10A)-B(6A)-B(9A)-B(4A)	108.57(14)
B(2A)-B(6A)-B(9A)-B(4A)	0.27(15)
B(5A)-B(6A)-B(9A)-B(4A)	-45.55(11)
B(7A)-B(6A)-B(9A)-B(4A)	58.65(13)
B(10A)-B(6A)-B(9A)-B(5A)	154.12(15)
B(2A)-B(6A)-B(9A)-B(5A)	45.83(12)
B(7A)-B(6A)-B(9A)-B(5A)	104.20(13)
B(10A)-B(6A)-B(9A)-B(8A)	49.77(12)
B(2A)-B(6A)-B(9A)-B(8A)	-58.52(13)
B(5A)-B(6A)-B(9A)-B(8A)	-104.35(12)
B(7A)-B(6A)-B(9A)-B(8A)	-0.15(12)
B(2A)-B(6A)-B(10A)-B(9A)	90.35(14)
B(5A)-B(6A)-B(10A)-B(9A)	23.85(14)
B(7A)-B(6A)-B(10A)-B(9A)	114.52(13)
B(2A)-B(6A)-B(10A)-B(8A)	33.01(18)
B(5A)-B(6A)-B(10A)-B(8A)	-33.49(19)
B(9A)-B(6A)-B(10A)-B(8A)	-57.34(12)
B(7A)-B(6A)-B(10A)-B(8A)	57.18(13)
B(2A)-B(6A)-B(10A)-B(7A)	-24.17(13)
B(5A)-B(6A)-B(10A)-B(7A)	-90.67(15)
B(9A)-B(6A)-B(10A)-B(7A)	-114.52(13)
B(4A)-B(9A)-B(10A)-B(6A)	-90.27(14)
B(5A)-B(9A)-B(10A)-B(6A)	-23.85(13)
B(8A)-B(9A)-B(10A)-B(6A)	-114.75(13)
B(4A)-B(9A)-B(10A)-B(8A)	24.48(13)

B(5A)-B(9A)-B(10A)-B(8A)	90.91(14)
B(6A)-B(9A)-B(10A)-B(8A)	114.75(13)
B(4A)-B(9A)-B(10A)-B(7A)	-32.72(16)
B(5A)-B(9A)-B(10A)-B(7A)	33.70(17)
B(8A)-B(9A)-B(10A)-B(7A)	-57.20(12)
B(6A)-B(9A)-B(10A)-B(7A)	57.55(12)
B(3A)-B(8A)-B(10A)-B(6A)	-32.82(18)
B(4A)-B(8A)-B(10A)-B(6A)	33.17(18)
B(9A)-B(8A)-B(10A)-B(6A)	57.48(13)
B(7A)-B(8A)-B(10A)-B(6A)	-57.32(13)
B(3A)-B(8A)-B(10A)-B(9A)	-90.31(14)
B(4A)-B(8A)-B(10A)-B(9A)	-24.32(13)
B(7A)-B(8A)-B(10A)-B(9A)	-114.80(13)
B(3A)-B(8A)-B(10A)-B(7A)	24.50(14)
B(4A)-B(8A)-B(10A)-B(7A)	90.49(14)
B(9A)-B(8A)-B(10A)-B(7A)	114.80(13)
B(2A)-B(7A)-B(10A)-B(6A)	24.19(13)
B(3A)-B(7A)-B(10A)-B(6A)	90.44(14)
B(8A)-B(7A)-B(10A)-B(6A)	114.89(13)
B(2A)-B(7A)-B(10A)-B(9A)	-33.43(16)
B(3A)-B(7A)-B(10A)-B(9A)	32.82(17)
B(8A)-B(7A)-B(10A)-B(9A)	57.27(12)
B(6A)-B(7A)-B(10A)-B(9A)	-57.62(12)
B(2A)-B(7A)-B(10A)-B(8A)	-90.70(14)
B(3A)-B(7A)-B(10A)-B(8A)	-24.45(13)
B(6A)-B(7A)-B(10A)-B(8A)	-114.89(13)
B(5B)-C(1B)-B(2B)-B(6B)	-27.00(15)
B(4B)-C(1B)-B(2B)-B(6B)	32.7(2)
B(3B)-C(1B)-B(2B)-B(6B)	92.08(16)
B(5B)-C(1B)-B(2B)-B(7B)	-91.84(15)
B(4B)-C(1B)-B(2B)-B(7B)	-32.1(2)
B(3B)-C(1B)-B(2B)-B(7B)	27.24(15)
B(4B)-C(1B)-B(2B)-B(5B)	59.74(16)
B(3B)-C(1B)-B(2B)-B(5B)	119.08(16)
B(5B)-C(1B)-B(2B)-B(3B)	-119.08(16)
B(4B)-C(1B)-B(2B)-B(3B)	-59.34(17)
B(5B)-C(1B)-B(3B)-B(8B)	-31.7(2)
B(2B)-C(1B)-B(3B)-B(8B)	-91.88(16)
B(4B)-C(1B)-B(3B)-B(8B)	28.00(16)
B(5B)-C(1B)-B(3B)-B(7B)	33.1(2)
B(2B)-C(1B)-B(3B)-B(7B)	-27.09(14)
B(4B)-C(1B)-B(3B)-B(7B)	92.79(16)
B(5B)-C(1B)-B(3B)-B(4B)	-59.69(15)
B(2B)-C(1B)-B(3B)-B(4B)	-119.88(15)
B(5B)-C(1B)-B(3B)-B(2B)	60.19(14)
B(4B)-C(1B)-B(3B)-B(2B)	119.88(15)
B(6B)-B(2B)-B(3B)-C(1B)	-104.22(15)
B(7B)-B(2B)-B(3B)-C(1B)	-149.81(16)
B(5B)-B(2B)-B(3B)-C(1B)	-45.51(13)
C(1B)-B(2B)-B(3B)-B(8B)	104.43(17)
B(6B)-B(2B)-B(3B)-B(8B)	0.20(18)
B(7B)-B(2B)-B(3B)-B(8B)	-45.39(15)
B(5B)-B(2B)-B(3B)-B(8B)	58.92(16)
C(1B)-B(2B)-B(3B)-B(7B)	149.81(16)
B(6B)-B(2B)-B(3B)-B(7B)	45.59(12)
B(5B)-B(2B)-B(3B)-B(7B)	104.31(13)

C(1B)-B(2B)-B(3B)-B(4B)	45.20(15)
B(6B)-B(2B)-B(3B)-B(4B)	-59.02(17)
B(7B)-B(2B)-B(3B)-B(4B)	-104.61(16)
B(5B)-B(2B)-B(3B)-B(4B)	-0.30(16)
B(5B)-C(1B)-B(4B)-B(9B)	27.30(16)
B(2B)-C(1B)-B(4B)-B(9B)	-32.6(2)
B(3B)-C(1B)-B(4B)-B(9B)	-92.12(18)
B(5B)-C(1B)-B(4B)-B(8B)	91.75(17)
B(2B)-C(1B)-B(4B)-B(8B)	31.8(2)
B(3B)-C(1B)-B(4B)-B(8B)	-27.67(16)
B(2B)-C(1B)-B(4B)-B(5B)	-59.91(15)
B(3B)-C(1B)-B(4B)-B(5B)	-119.42(15)
B(5B)-C(1B)-B(4B)-B(3B)	119.42(15)
B(2B)-C(1B)-B(4B)-B(3B)	59.50(16)
B(8B)-B(3B)-B(4B)-C(1B)	-149.09(17)
B(7B)-B(3B)-B(4B)-C(1B)	-103.61(16)
B(2B)-B(3B)-B(4B)-C(1B)	-45.10(13)
C(1B)-B(3B)-B(4B)-B(9B)	103.94(16)
B(8B)-B(3B)-B(4B)-B(9B)	-45.15(14)
B(7B)-B(3B)-B(4B)-B(9B)	0.33(19)
B(2B)-B(3B)-B(4B)-B(9B)	58.84(17)
C(1B)-B(3B)-B(4B)-B(8B)	149.09(17)
B(7B)-B(3B)-B(4B)-B(8B)	45.48(15)
B(2B)-B(3B)-B(4B)-B(8B)	103.99(15)
C(1B)-B(3B)-B(4B)-B(5B)	45.40(13)
B(8B)-B(3B)-B(4B)-B(5B)	-103.68(15)
B(7B)-B(3B)-B(4B)-B(5B)	-58.20(17)
B(2B)-B(3B)-B(4B)-B(5B)	0.31(16)
B(2B)-C(1B)-B(5B)-B(9B)	92.07(15)
B(4B)-C(1B)-B(5B)-B(9B)	-27.54(16)
B(3B)-C(1B)-B(5B)-B(9B)	32.03(19)
B(2B)-C(1B)-B(5B)-B(6B)	26.73(14)
B(4B)-C(1B)-B(5B)-B(6B)	-92.88(16)
B(3B)-C(1B)-B(5B)-B(6B)	-33.32(19)
B(2B)-C(1B)-B(5B)-B(4B)	119.60(17)
B(3B)-C(1B)-B(5B)-B(4B)	59.56(16)
B(4B)-C(1B)-B(5B)-B(2B)	-119.60(17)
B(3B)-C(1B)-B(5B)-B(2B)	-60.04(14)
B(9B)-B(4B)-B(5B)-C(1B)	-149.54(17)
B(8B)-B(4B)-B(5B)-C(1B)	-104.11(17)
B(3B)-B(4B)-B(5B)-C(1B)	-45.67(15)
C(1B)-B(4B)-B(5B)-B(9B)	149.54(17)
B(8B)-B(4B)-B(5B)-B(9B)	45.43(14)
B(3B)-B(4B)-B(5B)-B(9B)	103.87(17)
C(1B)-B(4B)-B(5B)-B(6B)	103.45(16)
B(9B)-B(4B)-B(5B)-B(6B)	-46.09(12)
B(8B)-B(4B)-B(5B)-B(6B)	-0.66(17)
B(3B)-B(4B)-B(5B)-B(6B)	57.78(17)
C(1B)-B(4B)-B(5B)-B(2B)	45.36(14)
B(9B)-B(4B)-B(5B)-B(2B)	-104.18(13)
B(8B)-B(4B)-B(5B)-B(2B)	-58.75(15)
B(3B)-B(4B)-B(5B)-B(2B)	-0.31(16)
B(6B)-B(2B)-B(5B)-C(1B)	150.04(17)
B(7B)-B(2B)-B(5B)-C(1B)	104.50(16)
B(3B)-B(2B)-B(5B)-C(1B)	45.78(15)
C(1B)-B(2B)-B(5B)-B(9B)	-104.44(17)

B(6B)-B(2B)-B(5B)-B(9B)	45.60(12)
B(7B)-B(2B)-B(5B)-B(9B)	0.06(15)
B(3B)-B(2B)-B(5B)-B(9B)	-58.65(15)
C(1B)-B(2B)-B(5B)-B(6B)	-150.04(17)
B(7B)-B(2B)-B(5B)-B(6B)	-45.54(11)
B(3B)-B(2B)-B(5B)-B(6B)	-104.26(14)
C(1B)-B(2B)-B(5B)-B(4B)	-45.48(15)
B(6B)-B(2B)-B(5B)-B(4B)	104.56(14)
B(7B)-B(2B)-B(5B)-B(4B)	59.02(15)
B(3B)-B(2B)-B(5B)-B(4B)	0.31(16)
C(1B)-B(2B)-B(6B)-B(10B)	-78.27(19)
B(7B)-B(2B)-B(6B)-B(10B)	23.40(14)
B(5B)-B(2B)-B(6B)-B(10B)	-103.73(15)
B(3B)-B(2B)-B(6B)-B(10B)	-21.32(18)
C(1B)-B(2B)-B(6B)-B(5B)	25.45(15)
B(7B)-B(2B)-B(6B)-B(5B)	127.13(12)
B(3B)-B(2B)-B(6B)-B(5B)	82.40(13)
C(1B)-B(2B)-B(6B)-B(7B)	-101.67(16)
B(5B)-B(2B)-B(6B)-B(7B)	-127.13(12)
B(3B)-B(2B)-B(6B)-B(7B)	-44.72(13)
C(1B)-B(2B)-B(6B)-B(9B)	-18.77(18)
B(7B)-B(2B)-B(6B)-B(9B)	82.91(12)
B(5B)-B(2B)-B(6B)-B(9B)	-44.22(11)
B(3B)-B(2B)-B(6B)-B(9B)	38.18(15)
C(1B)-B(5B)-B(6B)-B(10B)	79.40(18)
B(9B)-B(5B)-B(6B)-B(10B)	-22.63(14)
B(4B)-B(5B)-B(6B)-B(10B)	22.37(18)
B(2B)-B(5B)-B(6B)-B(10B)	104.86(15)
C(1B)-B(5B)-B(6B)-B(2B)	-25.46(14)
B(9B)-B(5B)-B(6B)-B(2B)	-127.48(13)
B(4B)-B(5B)-B(6B)-B(2B)	-82.49(14)
C(1B)-B(5B)-B(6B)-B(7B)	19.54(17)
B(9B)-B(5B)-B(6B)-B(7B)	-82.48(12)
B(4B)-B(5B)-B(6B)-B(7B)	-37.48(15)
B(2B)-B(5B)-B(6B)-B(7B)	45.00(11)
C(1B)-B(5B)-B(6B)-B(9B)	102.02(16)
B(4B)-B(5B)-B(6B)-B(9B)	44.99(12)
B(2B)-B(5B)-B(6B)-B(9B)	127.48(13)
C(1B)-B(2B)-B(7B)-B(10B)	78.16(19)
B(6B)-B(2B)-B(7B)-B(10B)	-23.08(15)
B(5B)-B(2B)-B(7B)-B(10B)	21.59(18)
B(3B)-B(2B)-B(7B)-B(10B)	103.97(17)
C(1B)-B(2B)-B(7B)-B(3B)	-25.81(14)
B(6B)-B(2B)-B(7B)-B(3B)	-127.06(13)
B(5B)-B(2B)-B(7B)-B(3B)	-82.38(13)
C(1B)-B(2B)-B(7B)-B(6B)	101.24(15)
B(5B)-B(2B)-B(7B)-B(6B)	44.68(11)
B(3B)-B(2B)-B(7B)-B(6B)	127.06(13)
C(1B)-B(2B)-B(7B)-B(8B)	18.49(18)
B(6B)-B(2B)-B(7B)-B(8B)	-82.75(14)
B(5B)-B(2B)-B(7B)-B(8B)	-38.07(16)
B(3B)-B(2B)-B(7B)-B(8B)	44.31(13)
C(1B)-B(3B)-B(7B)-B(10B)	-77.80(19)
B(8B)-B(3B)-B(7B)-B(10B)	23.92(15)
B(4B)-B(3B)-B(7B)-B(10B)	-20.9(2)
B(2B)-B(3B)-B(7B)-B(10B)	-103.42(16)

C(1B)-B(3B)-B(7B)-B(2B)	25.62(14)
B(8B)-B(3B)-B(7B)-B(2B)	127.34(14)
B(4B)-B(3B)-B(7B)-B(2B)	82.50(15)
C(1B)-B(3B)-B(7B)-B(6B)	-18.71(18)
B(8B)-B(3B)-B(7B)-B(6B)	83.00(14)
B(4B)-B(3B)-B(7B)-B(6B)	38.16(17)
B(2B)-B(3B)-B(7B)-B(6B)	-44.34(11)
C(1B)-B(3B)-B(7B)-B(8B)	-101.72(17)
B(4B)-B(3B)-B(7B)-B(8B)	-44.84(14)
B(2B)-B(3B)-B(7B)-B(8B)	-127.34(14)
B(2B)-B(6B)-B(7B)-B(10B)	154.30(16)
B(5B)-B(6B)-B(7B)-B(10B)	108.35(16)
B(9B)-B(6B)-B(7B)-B(10B)	50.03(14)
B(10B)-B(6B)-B(7B)-B(2B)	-154.30(16)
B(5B)-B(6B)-B(7B)-B(2B)	-45.94(11)
B(9B)-B(6B)-B(7B)-B(2B)	-104.26(13)
B(10B)-B(6B)-B(7B)-B(3B)	-108.76(16)
B(2B)-B(6B)-B(7B)-B(3B)	45.54(12)
B(5B)-B(6B)-B(7B)-B(3B)	-0.40(15)
B(9B)-B(6B)-B(7B)-B(3B)	-58.72(14)
B(10B)-B(6B)-B(7B)-B(8B)	-50.24(15)
B(2B)-B(6B)-B(7B)-B(8B)	104.05(15)
B(5B)-B(6B)-B(7B)-B(8B)	58.11(16)
B(9B)-B(6B)-B(7B)-B(8B)	-0.21(16)
C(1B)-B(3B)-B(8B)-B(10B)	77.2(2)
B(7B)-B(3B)-B(8B)-B(10B)	-23.78(16)
B(4B)-B(3B)-B(8B)-B(10B)	103.57(17)
B(2B)-B(3B)-B(8B)-B(10B)	20.6(2)
C(1B)-B(3B)-B(8B)-B(4B)	-26.35(15)
B(7B)-B(3B)-B(8B)-B(4B)	-127.35(14)
B(2B)-B(3B)-B(8B)-B(4B)	-82.97(15)
C(1B)-B(3B)-B(8B)-B(7B)	101.00(16)
B(4B)-B(3B)-B(8B)-B(7B)	127.35(14)
B(2B)-B(3B)-B(8B)-B(7B)	44.38(12)
C(1B)-B(3B)-B(8B)-B(9B)	17.9(2)
B(7B)-B(3B)-B(8B)-B(9B)	-83.06(15)
B(4B)-B(3B)-B(8B)-B(9B)	44.29(13)
B(2B)-B(3B)-B(8B)-B(9B)	-38.68(19)
C(1B)-B(4B)-B(8B)-B(10B)	-77.45(19)
B(9B)-B(4B)-B(8B)-B(10B)	23.63(14)
B(5B)-B(4B)-B(8B)-B(10B)	-20.88(19)
B(3B)-B(4B)-B(8B)-B(10B)	-103.81(16)
C(1B)-B(4B)-B(8B)-B(3B)	26.36(15)
B(9B)-B(4B)-B(8B)-B(3B)	127.44(13)
B(5B)-B(4B)-B(8B)-B(3B)	82.93(14)
C(1B)-B(4B)-B(8B)-B(7B)	-18.2(2)
B(9B)-B(4B)-B(8B)-B(7B)	82.83(14)
B(5B)-B(4B)-B(8B)-B(7B)	38.33(17)
B(3B)-B(4B)-B(8B)-B(7B)	-44.61(13)
C(1B)-B(4B)-B(8B)-B(9B)	-101.08(16)
B(5B)-B(4B)-B(8B)-B(9B)	-44.51(12)
B(3B)-B(4B)-B(8B)-B(9B)	-127.44(13)
B(2B)-B(7B)-B(8B)-B(10B)	108.18(15)
B(3B)-B(7B)-B(8B)-B(10B)	153.56(17)
B(6B)-B(7B)-B(8B)-B(10B)	49.90(13)
B(10B)-B(7B)-B(8B)-B(3B)	-153.56(17)

B(2B)-B(7B)-B(8B)-B(3B)	-45.38(14)
B(6B)-B(7B)-B(8B)-B(3B)	-103.66(15)
B(10B)-B(7B)-B(8B)-B(4B)	-108.28(16)
B(2B)-B(7B)-B(8B)-B(4B)	-0.10(17)
B(3B)-B(7B)-B(8B)-B(4B)	45.28(15)
B(6B)-B(7B)-B(8B)-B(4B)	-58.37(16)
B(10B)-B(7B)-B(8B)-B(9B)	-49.69(14)
B(2B)-B(7B)-B(8B)-B(9B)	58.48(17)
B(3B)-B(7B)-B(8B)-B(9B)	103.87(17)
B(6B)-B(7B)-B(8B)-B(9B)	0.21(16)
C(1B)-B(5B)-B(9B)-B(10B)	-78.49(19)
B(6B)-B(5B)-B(9B)-B(10B)	22.39(15)
B(4B)-B(5B)-B(9B)-B(10B)	-104.53(17)
B(2B)-B(5B)-B(9B)-B(10B)	-21.66(19)
C(1B)-B(5B)-B(9B)-B(4B)	26.04(14)
B(6B)-B(5B)-B(9B)-B(4B)	126.93(13)
B(2B)-B(5B)-B(9B)-B(4B)	82.87(14)
C(1B)-B(5B)-B(9B)-B(8B)	-18.86(19)
B(6B)-B(5B)-B(9B)-B(8B)	82.03(14)
B(4B)-B(5B)-B(9B)-B(8B)	-44.90(14)
B(2B)-B(5B)-B(9B)-B(8B)	37.97(16)
C(1B)-B(5B)-B(9B)-B(6B)	-100.88(15)
B(4B)-B(5B)-B(9B)-B(6B)	-126.93(13)
B(2B)-B(5B)-B(9B)-B(6B)	-44.06(11)
C(1B)-B(4B)-B(9B)-B(10B)	77.3(2)
B(8B)-B(4B)-B(9B)-B(10B)	-23.82(14)
B(5B)-B(4B)-B(9B)-B(10B)	103.20(15)
B(3B)-B(4B)-B(9B)-B(10B)	20.3(2)
C(1B)-B(4B)-B(9B)-B(5B)	-25.86(16)
B(8B)-B(4B)-B(9B)-B(5B)	-127.02(14)
B(3B)-B(4B)-B(9B)-B(5B)	-82.86(15)
C(1B)-B(4B)-B(9B)-B(8B)	101.17(18)
B(5B)-B(4B)-B(9B)-B(8B)	127.02(14)
B(3B)-B(4B)-B(9B)-B(8B)	44.17(14)
C(1B)-B(4B)-B(9B)-B(6B)	18.7(2)
B(8B)-B(4B)-B(9B)-B(6B)	-82.46(13)
B(5B)-B(4B)-B(9B)-B(6B)	44.57(12)
B(3B)-B(4B)-B(9B)-B(6B)	-38.29(17)
B(3B)-B(8B)-B(9B)-B(10B)	108.58(16)
B(4B)-B(8B)-B(9B)-B(10B)	153.75(16)
B(7B)-B(8B)-B(9B)-B(10B)	49.60(14)
B(10B)-B(8B)-B(9B)-B(5B)	-108.14(15)
B(3B)-B(8B)-B(9B)-B(5B)	0.44(18)
B(4B)-B(8B)-B(9B)-B(5B)	45.61(13)
B(7B)-B(8B)-B(9B)-B(5B)	-58.54(17)
B(10B)-B(8B)-B(9B)-B(4B)	-153.75(16)
B(3B)-B(8B)-B(9B)-B(4B)	-45.17(14)
B(7B)-B(8B)-B(9B)-B(4B)	-104.15(16)
B(10B)-B(8B)-B(9B)-B(6B)	-49.81(12)
B(3B)-B(8B)-B(9B)-B(6B)	58.77(16)
B(4B)-B(8B)-B(9B)-B(6B)	103.94(13)
B(7B)-B(8B)-B(9B)-B(6B)	-0.21(15)
B(2B)-B(6B)-B(9B)-B(10B)	-109.36(16)
B(5B)-B(6B)-B(9B)-B(10B)	-154.95(17)
B(7B)-B(6B)-B(9B)-B(10B)	-50.21(14)
B(10B)-B(6B)-B(9B)-B(5B)	154.95(17)

B(2B)-B(6B)-B(9B)-B(5B)	45.59(12)
B(7B)-B(6B)-B(9B)-B(5B)	104.75(13)
B(10B)-B(6B)-B(9B)-B(4B)	109.37(17)
B(2B)-B(6B)-B(9B)-B(4B)	0.00(16)
B(5B)-B(6B)-B(9B)-B(4B)	-45.59(14)
B(7B)-B(6B)-B(9B)-B(4B)	59.16(15)
B(10B)-B(6B)-B(9B)-B(8B)	50.42(15)
B(2B)-B(6B)-B(9B)-B(8B)	-58.94(16)
B(5B)-B(6B)-B(9B)-B(8B)	-104.54(16)
B(7B)-B(6B)-B(9B)-B(8B)	0.21(16)
B(2B)-B(6B)-B(10B)-B(7B)	-24.03(15)
B(5B)-B(6B)-B(10B)-B(7B)	-91.29(15)
B(9B)-B(6B)-B(10B)-B(7B)	-114.40(16)
B(2B)-B(6B)-B(10B)-B(9B)	90.37(15)
B(5B)-B(6B)-B(10B)-B(9B)	23.10(15)
B(7B)-B(6B)-B(10B)-B(9B)	114.40(16)
B(2B)-B(6B)-B(10B)-B(8B)	33.04(18)
B(5B)-B(6B)-B(10B)-B(8B)	-34.22(18)
B(7B)-B(6B)-B(10B)-B(8B)	57.07(14)
B(9B)-B(6B)-B(10B)-B(8B)	-57.33(14)
B(2B)-B(7B)-B(10B)-B(6B)	23.59(15)
B(3B)-B(7B)-B(10B)-B(6B)	90.02(16)
B(8B)-B(7B)-B(10B)-B(6B)	114.39(16)
B(2B)-B(7B)-B(10B)-B(9B)	-34.03(19)
B(3B)-B(7B)-B(10B)-B(9B)	32.40(19)
B(6B)-B(7B)-B(10B)-B(9B)	-57.62(13)
B(8B)-B(7B)-B(10B)-B(9B)	56.77(15)
B(2B)-B(7B)-B(10B)-B(8B)	-90.80(17)
B(3B)-B(7B)-B(10B)-B(8B)	-24.37(16)
B(6B)-B(7B)-B(10B)-B(8B)	-114.39(16)
B(5B)-B(9B)-B(10B)-B(6B)	-23.06(15)
B(4B)-B(9B)-B(10B)-B(6B)	-89.52(16)
B(8B)-B(9B)-B(10B)-B(6B)	-113.97(15)
B(5B)-B(9B)-B(10B)-B(7B)	34.11(19)
B(4B)-B(9B)-B(10B)-B(7B)	-32.36(19)
B(8B)-B(9B)-B(10B)-B(7B)	-56.80(14)
B(6B)-B(9B)-B(10B)-B(7B)	57.17(12)
B(5B)-B(9B)-B(10B)-B(8B)	90.91(16)
B(4B)-B(9B)-B(10B)-B(8B)	24.45(15)
B(6B)-B(9B)-B(10B)-B(8B)	113.97(15)
B(3B)-B(8B)-B(10B)-B(6B)	-32.6(2)
B(4B)-B(8B)-B(10B)-B(6B)	33.63(19)
B(7B)-B(8B)-B(10B)-B(6B)	-57.08(13)
B(9B)-B(8B)-B(10B)-B(6B)	57.83(13)
B(3B)-B(8B)-B(10B)-B(7B)	24.49(16)
B(4B)-B(8B)-B(10B)-B(7B)	90.70(17)
B(9B)-B(8B)-B(10B)-B(7B)	114.91(15)
B(3B)-B(8B)-B(10B)-B(9B)	-90.41(18)
B(4B)-B(8B)-B(10B)-B(9B)	-24.20(15)
B(7B)-B(8B)-B(10B)-B(9B)	-114.91(15)

Symmetry transformations used to generate equivalent atoms:

Ionic Conductivity

Experimental: Conductivity of the electrolyte was measured using an electrochemical cell with two symmetric Pt film-electrodes. Potentiostatic EIS program from Gamry reference 1000 potentiostat was used to measure the impedance across the cell for each concentration. Conductivity was calculated by using the following equation

$$\sigma = \frac{l}{RA}$$

where σ is the conductivity, l is the distance between the electrodes, A is the cross sectional area and R is the resistance. The cell was calibrated using standard aqueous KCl solution.

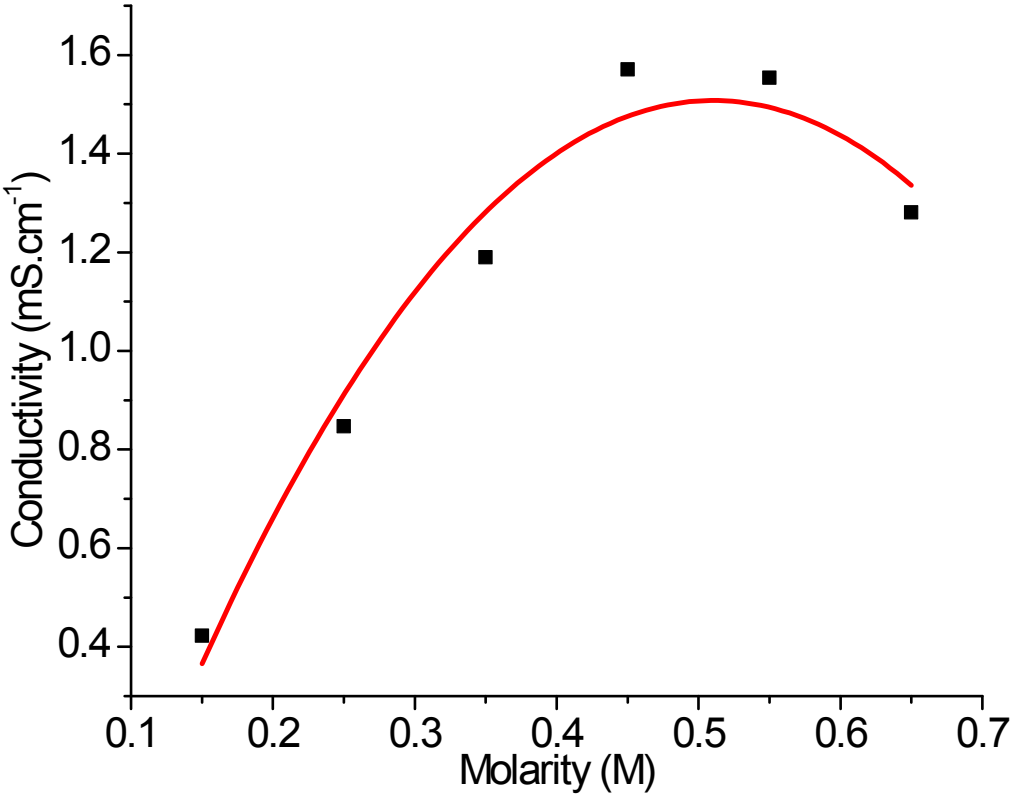


Figure S5. Ionic conductivity of 2[Mg] in G4 as function of salt concentration.

Electrochemical performance of Mg-Mo_6S_8 Cells

Experimental: Mg-ion battery performances were demonstrated with coin cells (CR2032) with Mg anode and Chevrel phase Mo_6S_8 cathode using 0.45 M **$Mg(CB_9H_9)_2$** in G4. The electrochemical performance of the Mg vs. Mo_6S_8 battery was tested in 4 cells, and the capacity data are consistent with +- 10% error. Chevrel phase Mo_6S_8 was prepared with a method previously established by Aurbach et.al[5], Mo_6S_8 electrodes were prepared by mixing 70wt% active material, 20% carbon black and 10% polyvinylidene fluoride (PVDF) in N-methyl-2-pyrrolidone (NMP). The mixed paste was then applied as a thin uniform coating on a Ni foil and then dried in a vacuum oven overnight at 50 °C. Cells were assembled in an argon filled glovebox. 6mm diameter disc of Mo_6S_8 coating on Ni

foil were punched out as the cathode and placed on the bottom base of the CR2032 coin cells, 40µl of the $Mg(CB_9H_9)_2$ in G4 was pippetted onto the cathode. A polypropelene seperator was carefully placed over the cathode and 60µl electrolyte was added (total of 100 µl) to wet the seperator surface. A polished Mg disc of 6mm in diameter was placed on the wetted seperator the cell was then filled with two spacers and a washer to fill the base, the top cap was then placed on the top and the cell was hydraulically pressed to seal the cell.

Table S6. Elemental analysis via EDX on the SS coin cell casing surface before and after cycling in Mg-Mo6S8 cell using **2[Mg^{2+}]** electrolyte.

Element	**Pristine SS surface (wt. %)**	**SS surface after 30 cycles (wt. %)**
Fe	65.1 ± 0.4	63.3 ± 0.5
Cr	16.9 ± 0.2	16.9 ± 0.2
Ni	7.3 ± 0.2	7.0 ± 0.2
C	8.6 ± 0.4	10.5 ± 0.5
Mn	0.9 ± 0.1	0.8 ± 0.1
O	0.8 ± 0.1	1.2 ± 0.2
Si	0.4 ± 0.1	0.3 ± 0.1

Figure S6. Image of coin cell

REFERENCES

1. APEX 2, version 2014.1-1, Bruker (2014), Bruker AXS Inc., Madison, Wisconsin, USA.

2. SAINT, version V8.34A, Bruker (2012), Bruker AXS Inc., Madison, Wisconsin, USA.

3. SADABS, version 2012/1, Bruker (2012), Bruker AXS Inc., Madison, Wisconsin, USA.

4. SHELXTL, version 2013/4, Bruker (2013), Bruker AXS Inc., Madison, Wisconsin, USA.

5. Levi, E., Goffer, Y., Vestfreed, Y., Lancry, E., & Aurbach, D. Chemistry of Materials 2002 *14* (6), 2767-2773.