

Ambiguities in Assigning Single-crystal NMR Data to Individual Atoms in the Crystal Structure: a Case Study of Hambergite, $\text{Be}_2\text{BO}_3\text{OH}$, by ^9Be and ^{11}B NMR Spectroscopy, XRD Measurements, and DFT Calculations

J. Steinadler, G. Krach, K. Witthaut, T. Stürzer, R. Hochleitner, W. Schnick, T. Bräuniger
Magn. Reson. Chem. **2026**

Resolving a Nearly Two-Centuries-Old Mystery: On the Structural Chemistry and Physicochemical Properties of Compounds Associated with the Term Ammelide

T.J. Koller, K. Witthaut, S.M.J. Endraß, M. Rösch, G. Krach, N. Lammer, T.M. Klapötke, W. Schnick
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Long Used but Hardly Known: Synthesis and Crystal Structure of Tritium Breeding $\text{Li}_2\text{Be}_2\text{O}_3$

G. Krach, J. Steinadler, R. Calaminus, B.V. Lotsch, W. Schnick
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Unique Mixed Valence Behaviour of Tantalum and Electronic Structure of the Novel $\text{P}_{1-x}\text{Ta}_{8+x}\text{N}_{13}$ ($x \approx 0.1 - 0.15$) Using Density Functional Theory and Soft X-ray Spectroscopy

C.R. Ceniza, M.M. Pointner, T.D. Boyko, W. Schnick, A. Moewes
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Rediscovery of the Forgotten Middle Child: A Comprehensive Study on the Coordination Chemistry of Melam

T.J. Koller, L.G. Balzat, J. Blahusch, A. Pichler, B.V. Lotsch, W. Schnick
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High-Pressure Synthesis of Ultra-Incompressible Beryllium Tungsten Nitride Pernitride $\text{BeW}_{10}\text{N}_{14}(\text{N}_2)$

G. Krach, L. Brüning, S. Ambach, E. Bykova, N. Giordano, B. Winkler, M. Bykov, W. Schnick
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Adamantane-Type Nitridophosphate Phosphors $\text{AE}_x\text{Li}_{10-2x}\text{P}_4\text{N}_{10}:\text{Eu}^{2+}$ via Medium-Pressure Ion-Exchange Reactions

R.M. Pritzl, A.T. Buda, K. Witthaut, P.J. Schmidt, W. Schnick
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Nitride Zeolites from Ammonothermal Synthesis

F.M. Engelsberger, W. Schnick
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Scalable Bulk Synthesis of Phase-Pure $\gamma\text{-Sn}_3\text{N}_4$ as a Model for an Argon-Flow-Mediated Metathesis Reaction

M. Zipkat, A. Koldemir, T. Block, C. Ceniza, T.D. Boyko, S. Kläger, R.M. Pritzl, A. Moewes, R. Pöttgen, S.S. Rudel, W. Schnick
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Highly Condensed Eu^{2+} -doped Nitrodoberyllsilicates, $M\text{BeSi}_2\text{N}_4:\text{Eu}^{2+}$ ($M = \text{Ca}, \text{Sr}$): Electronic Structure and Band Gap Studies

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$\text{Ba}_2\text{BP}_7\text{N}_{14}$ — A Quaternary Alkaline Earth Nitridoborophosphate with a Mixed 3D Network Structure

A.T. Buda, R.M. Pritzl, M.M. Pointner, J. Steinadler, W. Schnick
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Pyrrolation of Melem: A Facile Gateway into the Field of Monomeric s-Heptazine Chemistry

T.J. Koller, K. Witthaut, F. Wolf, J.N. Singer, J. Blahusch, C. Li, V. Valsamidou, D. Johrendt, W. Schnick
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Defect Imide Double Antiperovskites $AE_5AsPn(NH)_2$ ($AE = Ca, Sr$; $Pn = Sb, Bi$) as Potential Solar Cell Absorber Materials

T.G. Chau, D. Han, F. Wolf, S.S. Rudel, Y. Yao, H. Oberhofer, T. Bein, H. Ebert, W. Schnick
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Combination of Ambient and High-Temperature Beryllium Nitride Motifs in $W_2Be_4N_5$ and $W_4Be_8N_9$

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Lone Pair and Unique N-bridging of Novel Titanium Nitridophosphate

P. Ufondu, Sakshi, T.D. Boyko, M.M. Pointner, W. Schnick, A. Moewes
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A Combined Experimental and Computational Study on the Broadening Mechanism of the Luminescence in Narrow-Band Eu^{2+} -doped Phosphors

R. Shafei, P.J. Strobel, P.J. Schmidt, D. Maganas, W. Schnick, F. Neese
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Investigation of the Binary Nitrides YN , LaN and LuN by Solid-State NMR Spectroscopy

J. Steinadler, G. Krach, W. Schnick, T. Bräuniger
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Ammonothermal Synthesis of Luminescent Imidonitridophosphate $Ba_4P_4N_8(NH)_2:Eu^{2+}$

F.M. Engelsberger, R.M. Pritzl, J. Steinadler, K. Witthaut, T. Bräuniger, P.J. Schmidt, W. Schnick
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$P_{1-x}Ta_{8+x}N_{13}$ ($x = 0.1-0.15$): A Phosphorus Tantalum Nitride Featuring Mixed-Valent Tantalum and P/Ta Disorder Visualized by Scanning Transmission Electron Microscopy

M.M. Pointner, C. Ceniza, L. Nusser, K. Witthaut, F. Wolf, M. Weidemann, L. Eisenburger, A. Moewes, O. Oeckler, W. Schnick
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$CaLi_2PN_3$ – A Quaternary Chain-Type Nitridophosphate by Medium-Pressure Synthesis

R.M. Pritzl, N. Fahle, K. Witthaut, S. Wendl, W. Schnick
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Synthesis and Comprehensive Studies of $Be-IV-N_2$ ($IV = Si, Ge$):

Solving the Mystery of Wurtzite-type $Pmc2_1$ Structures

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Trigonal Planar $[PN_3]^{4-}$ Anion in the Nitridophosphate Oxide $Ba_3[PN_3]O$

R.M. Pritzl, K. Witthaut, M. Dialer, A.T. Buda, V. Milman, L. Bayarjargal, B. Winkler, W. Schnick
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On Tautomerism and Amphoterism: An In-Depth Structural and Physicochemical Characterization of Ammeline and Some of Its Salts

T.J. Koller, S.M.J. Endraß, M. Rösch, K. Witthaut, T.M. Klapötke, W. Schnick
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Mixed Tin Valence in the Tin(II/IV)-Nitridophosphate $\text{Sn}_3\text{P}_8\text{N}_{16}$

S.J. Ambach, A. Koldemir, K. Witthaut, S. Kreiner, T. Bräuniger, R. Pöttgen, W. Schnick
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High-pressure Synthesis of Ultra-incompressible, Hard and Superconducting Tungsten Nitrides

A. Liang, I. Osmond, G. Krach, L.-T. Shi, L. Brüning, U. Ranieri, J. Spender, F. Tasnadi,
B. Massani, C.R. Stevens, R.S. McWilliams, E. Lawrence Bright, N. Giordano, S. Gallego-Parra,
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M. Bykov, F. Trybel, D. Laniel
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Order and Disorder in Mixed (Si, P)–N Networks $\text{Sr}_2\text{SiP}_2\text{N}_6:\text{Eu}^{2+}$ and $\text{Sr}_5\text{Si}_2\text{P}_6\text{N}_{16}:\text{Eu}^{2+}$

M. Dialer, M.M. Pointner, S.L. Wandelt, P. Strobel, P.J. Schmidt, L. Bayarjargal, B. Winkler, W. Schnick
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Highly Condensed and Super-Incompressible Be_2PN_3

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Ammonothermal Synthesis and Solid-State MAS NMR Study of the Imidonitridosilicate $\text{Rb}_3\text{Si}_6\text{N}_5(\text{NH})_6$

F.M. Engelsberger, T.G. Chau, T. Bräuniger, W. Schnick
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Green-Emitting Oxonitridoberyllosilicate $\text{Ba}[\text{BeSiON}_2]:\text{Eu}^{2+}$ for Wide Gamut Displays

T. Giffthaler, P. Strobel, V. Weiler, A. Haffner, A. Neuer, J. Steinadler, T. Bräuniger, S.D. Kloß,
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Building Nitridic Networks with Phosphorus and Germanium – from $\text{Ge}^{\text{II}}\text{P}_2\text{N}_4$ to $\text{Ge}^{\text{IV}}\text{PN}_3$

S.J. Ambach, G. Krach, E. Bykova, K. Witthaut, N. Giordano, M. Bykov, W. Schnick
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Tunable Narrow-Band Cyan-Emission of Eu^{2+} -doped Nitridomagnesophosphates

$\text{Ba}_{3-x}\text{Sr}_x[\text{Mg}_2\text{P}_{10}\text{N}_{20}]:\text{Eu}^{2+}$ ($x = 0-3$)
R.M. Pritzl, M.M. Pointner, K. Witthaut, P. Strobel, P.J. Schmidt, W. Schnick
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Super-Tunable LaSi_3N_5 Structure Type: Insights into the Structure and Luminescence of $\text{SrSi}_2\text{PN}_5:\text{Eu}^{2+}$

M. Dialer, R.M. Pritzl, S.L. Wandelt, D. Khalyavin, P.J. Schmidt, W. Schnick
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Multicationic Tetrahedra Networks: Alkaline-Earth-Centered Polyhedra and Non-Condensed AlN_6 -Octahedra in the Imido-nitridophosphates $\text{AE}_2\text{AlP}_6\text{N}_{15}(\text{NH})$ ($\text{AE} = \text{Ca}, \text{Sr}, \text{Ba}$)

M.M. Pointner, R.M. Pritzl, J.M. Albrecht, L. Blahusch, J.P. Wright, E. Lawrence Bright, C. Giacobbe,
O. Oeckler, W. Schnick
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Investigating the Electronic Properties of Novel Titanium Oxonitridophosphate $\text{Ti}_5\text{P}_{12}\text{N}_{24}\text{O}_2$, through Structural Distortions at the Titanium Sites

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Reduction of Germanium Oxides - The Mixed-Valence Germanates $\text{A}_2\text{Ge}_4\text{O}_7$ ($\text{A} = \text{Na}, \text{K}$)

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Cr_{5.7}Si_{2.3}P₈N₂₄ – A Chromium(+IV) Nitridosilicate Phosphate with Amphibole-Type Structure

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The Critical Role of Anharmonic Lattice Dynamics for Macroscopic Properties of the Visible Light Absorbing Nitride Semiconductor CuTaN₂

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Simple Molecules under High-Pressure and High-Temperature Conditions: Synthesis and Characterization of α - and β -C(NH)₂ with Fully sp³-Hybridized Carbon

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Nitride Synthesis Under High-pressure High-temperature Conditions: Unprecedented *in-situ* Insight into the Reaction Mechanism

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A Theoretical Spectroscopy Study of the Photoluminescent Properties of Narrow Band Eu²⁺-doped Phosphors Containing Multiple Candidate Doping Centers. Prediction of an Unprecedented Narrow Band Red Phosphor

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(Dis)Order and Luminescence in Silicon-Rich (Si,P)–N Network Sr₅Si₇P₂N₁₆:Eu²⁺

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Ba₁₂[BN₂]_{6.67}H₄ – A Disordered Anti-Skutterudite Filled with Nitridoborate Anions

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Synthesis of Ultra-Incompressible and Recoverable Carbon Nitrides Featuring CN₄ Tetrahedra

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Please Mind the Gap: Highly Condensed P–N Networks in LiP₄N₇ and Li_{3-x}P₆N_{11-x}(NH)_x

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D. Han, B. Zhu, Z. Cai, K.B. Spooner, S.S. Rudel, W. Schnick, T. Bein, D.O. Scanlon, H. Ebert
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Combining Nitridoborates, Nitrides and Hydrides – Synthesis and Characterization of the Multianionic $\text{Sr}_6\text{N}[\text{BN}_2]_2\text{H}_3$

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Finding Order in Disorder: The Highly Disordered Lithium Oxonitridophosphate

Double Salt $\text{Li}_{8+x}\text{P}_3\text{O}_{10-x}\text{N}_{1+x}$ ($x = 1.4(5)$)

S. Schneider, S. Kreiner, L.G. Balzat, B.V. Lotsch, W. Schnick
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Tetra-Face-Capped Octahedra in a Tetrahedra Network – Structure Determination and Scanning Transmission Electron Microscopy of $\text{SrAl}_5\text{P}_4\text{N}_{10}\text{O}_2\text{F}_3$

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High-Pressure Synthesis, Crystal Structure, and Characterization of the New Non-Centrosymmetric Terbium Borate $\text{Tb}_3\text{B}_{10}\text{O}_{17}(\text{OH})_5$

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A Novel Nitridoborate Hydride $\text{Sr}_{13}(\text{BN}_2)_6\text{H}_8$ Elucidated from X-Ray and Neutron Diffraction Data

S.L. Wandelt, A. Mutschke, D. Khalyavin, J. Steinadler, W. Schnick
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From Framework to Layers Driven by Pressure – The Monophyllo-Oxonitridophosphate $\beta\text{-MgSrP}_3\text{N}_5\text{O}_2$ and Comparison to its α -Polymorph

R.M. Pritzl, N. Prinz, P. Strobel, P.J. Schmidt, D. Johrendt, W. Schnick
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Oxonitridoberyllsilicate Phosphors

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Lumileds LLC, Ludwig-Maximilians-Universität München

Combining MN_6 Octahedra and PN_5 Trigonal Bipyramids in the Mica-like Nitridophosphates MP_6N_{11} ($M = \text{Al}, \text{In}$)

S.J. Ambach, M. Pointner, S. Falkai, C. Paulmann, O. Oeckler, W. Schnick
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The Importance of Lone Pairs to Structure and Bonding of the Novel Germanium Nitridophosphate GeP_2N_4

T. de Boer, C. Somers, T. Boyko, S. Ambach, L. Eisenburger, W. Schnick, A. Moewes
J. Mater. Chem. A **2023**, 11, 6198

Comprehensive Investigation of Anion Species in Crystalline Li^+ -ion Conductor $\text{Li}_{27-x}[\text{P}_4\text{O}_{7+x}\text{N}_{9-x}]\text{O}_3$ ($x \approx 1.9(3)$)

S. Schneider, E.-M. Wendinger, V. Baran, A.-K. Hatz, B.V. Lotsch, M. Nentwig, O. Oeckler, T. Bräuniger, W. Schnick
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Structure Determination of Crystalline LiPON Model Structure $\text{Li}_{5+x}\text{P}_2\text{O}_{6-x}\text{N}_{1+x}$ with $x \approx 0.9$

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Sodalite-type $\text{Ga}_{16/3}[\text{P}_{12}\text{N}_{24}]\text{O}_2$: Synthesis, Electron Crystallography and Powder X-ray Diffraction

D. Günther, L. Eisenburger, W. Schnick, O. Oeckler
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Revealing Phosphorus Nitrides up to the Megabar Regime: Synthesis of α' - P_3N_5 , δ - P_3N_5 and PN_2

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Strontium Nitridoborate Hydride $\text{Sr}_2\text{BN}_2\text{H}$, Verified by Single-Crystal X-ray and Neutron Powder Diffraction

S.L. Wandelt, A. Karnas, A. Mutschke, N. Kunkel, C. Ritter, W. Schnick
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T. de Boer, T.D. Boyko, C. Braun, W. Schnick, A. Moewes
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Energy Levels of Eu^{2+} States in the Next-Generation LED-Phosphor $\text{SrLi}_2\text{Al}_2\text{O}_2\text{N}_2:\text{Eu}^{2+}$

M. Ruhul Amin, P. Strobel, W. Schnick, P.J. Schmidt, A. Moewes
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Synthesis and Luminescence Properties of Amber Emitting $\text{La}_7\text{Sr}[\text{Si}_{10}\text{N}_{19}\text{O}_3]:\text{Eu}^{2+}$ and Syntheses of the Substitutional Variants $\text{RE}_{8-x}\text{AE}_x[\text{Si}_{10}\text{N}_{20-x}\text{O}_{2+x}]:\text{Eu}^{2+}$ with $\text{RE} = \text{La, Ce}$; $\text{AE} = \text{Ca, Sr, Ba}$; $0 \leq x \leq 2$

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Electronic and Optical Properties of Eu^{2+} -activated Narrow-Band Phosphors for Phosphor-Converted Light-Emitting Diode Applications: Insights from a Theoretical Spectroscopy Perspective

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Band Gap and Electronic Structure of Defects in the Ternary Nitride BP_3N_6 : Experiment and Theory

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Self-doping Behavior and Cation Disorder in MgSnN_2

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