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A Neutron Diffraction and Quantum-Chemical Study of $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$

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Dedicated to Professor Werner Uhl on the Occasion of His 65th Birthday

Abstract: $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$ was obtained by careful decomposition of $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2 \cdot 4\text{ND}_3$ at room temperature. It crystallizes in the monoclinic space group $I2/m$ with $a = 8.5905(5)$, $b = 6.8506(4)$, $c = 9.7530(6)$ Å, $\beta = 94.618(6)^\circ$, $V = 572.10(6)$ Å³, $Z = 2$, at $T = 3$ K. Its crystal structure has been elucidated using powder neutron diffraction and confirmed by quantum chemical calculations. The Mn(II) cation is coordinated octahedron-like by ND_3 ligands. The azide anion is linear with $178.7(10)^\circ$ and shows N–N distances of 1.178(11) and 1.180(12) Å.

Introduction

We recently described a new route to metal azides which is based on the reaction of AgN_3 with various main-group, transition, as well as rare-earth metals.^[1,2] One example was the reaction of manganese metal and we reported the formation of $[\text{Mn}(\text{NH}_3)_6](\text{N}_3)_2 \cdot 4\text{NH}_3$ from the reaction at -36°C , its conversion to $\text{Mn}(\text{N}_3)_2(\text{NH}_3)_2$ at room temperature and its transformation into the binary azide $\text{Mn}(\text{N}_3)_2$.^[3] In order to elucidate the hydrogen bonding, the preparation of the deuterated compounds has been attempted as well. In this course we have accidentally obtained and identified another intermediate of the decomposition reaction of the tetraammoniate as $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$, which seems to be stable at room temperature, too. Here, we report on the crystal structure elucidation of this compound using powder neutron diffraction facilitated by quantum chemical calculations.

Results and Discussion

The formation of the title compound can be envisaged by the following equations 1 - 2.

The precise conditions under which the reaction according to equation 2 occurs is currently still under investigation. $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$ is obtained in the form of a white powder and its crystal structure has been investigated using neutron powder diffraction at 3 K. The structure has been solved using the Superflip algorithm^[4] in the Jana2006 software,^[5] and refined using the Rietveld method. Crystallographic details are available from Table 1 and Figure 1 shows the observed and calculated neutron powder pattern. The coherent neutron scattering lengths are 6.671 fm for D, 9.36 fm for N and -3.73 fm for Mn. The deuterium atoms could be refined using anisotropic, the N atoms isotropic and the Mn atom with fixed displacement parameters, see Table 2. The refinement in space group $I2/m$ led to very satisfactory results (Figure 1, Table 1), but the monoclinic primitive space groups could not completely be excluded because two very small shoulders in the reflections near $30^\circ 2\theta$ violate the extinction condition. If refined in primitive space groups, the models have a similar high quality, however a search for additional symmetry within the Platon software^[6] directly suggests centering to be present. So, we assume that these shoulders belong to an impurity. Quantum chemical calculations with the CRYSTAL17 program package^[7,8] have been carried out in order to assure the correctness of the space group assignment, however were of little help in these cases, see below. Usually the usage of a wrong space group in these calculations shows a compound to be either not a true local minimum or the lattice parameters strongly diverge from the experimentally determined ones. As the refinements in all these space groups yielded similar results, the one of highest symmetry was chosen.

Figure 1. Neutron powder pattern of the title compound obtained at 3 K. Ticks below the pattern indicate calculated reflection positions, the line below shows the difference plot of the Rietveld refinement. The grey-shaded area was excluded from the refinement.

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Table 1. Crystallographic details for the title compound as well as the lattice parameters obtained by Quantum chemical calculations at DFT-PBE0-D3/TZVP level of theory.

Parameter	[Mn(ND ₃) ₆](N ₃) ₂ neutron diffraction at 3 K	[Mn(ND ₃) ₆](N ₃) ₂ calculated at 0 K in <i>I</i> 2/ <i>m</i>	Mn(ND ₃) ₆ (N ₃) ₂ calculated at 0 K in <i>P</i> 2/ <i>m</i> ^[a]	Mn(ND ₃) ₆ (N ₃) ₂ calculated at 0 K in <i>P</i> <i>m</i> ^[a]
Empirical formula	D ₁₈ N ₁₂ Mn			
Color and appearance	Colorless powder			
<i>M</i> / g·mol ⁻¹	259.3			
Crystal system	Monoclinic			
Space group	<i>I</i> 2/ <i>m</i> (No. 12)			
<i>a</i> / Å	8.5905(5)	8.350	8.351	8.351
<i>b</i> / Å	6.8506(4)	6.846	6.846	6.846
<i>c</i> / Å	9.7530(6)	9.541	9.543	9.544
β / °	94.618(6)	94.95	94.95	94.96
<i>V</i> / Å ³	572.10(6)	543.4	543.6	543.6
<i>Z</i>	2			
ρ_{calc} / g·cm ⁻³	1.51			
μ / mm ⁻¹	0.011			
λ / Å	1.5484			
<i>T</i> / K	3			
<i>R</i> _p , <i>wR</i> _p	0.0274, 0.0364			
<i>R</i> (<i>F</i>) (all data), <i>wR</i> (<i>F</i> ²) (all data)	0.0134, 0.0235			
<i>S</i> (all data)	6.30			
Profile and background function	Pseudo-Voigt, Legendre polynomial with 7 terms			
No. of data points, parameters, constraints, restraints	3020, 74, 0, 0			

2 θ range measured (min; max; increment)

2 θ range refined (min; max)

$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ / e·Å⁻³

[Mn(ND₃)₆](N₃)₂ crystallizes in the monoclinic space group *I*2/*m* with *a* = 8.5905(5), *b* = 6.8506(4), *c* = 9.7530(6) Å, β = 94.618(6)°, *V* = 572.10(6) Å³, *Z* = 2 at 3 K. The manganese(II) cation occupies the special 2*c* (2/*m*) Wyckoff position and is coordinated by two perdeutero ammine ligands with N atoms N1 and N2, which reside on the general Wyckoff position 8*j* (1) and the special 4*i* (*m*) position. This leads to an octahedron-like coordination sphere of ND₃ molecules around the Mn atom with Mn–N1 distances of 2.276(6) Å and Mn–N2 distances of 2.313(9) Å. These distances agree within 3 σ . The N–Mn–N bond angles within the octahedron are close to ideal 90° and 180°. All N–D distances are also equal within this criterion and lie in the range of 1.003(11) to 1.023(12) Å. These values are in good agreement with reported Mn–N distances for ammine complexes of manganese halides and an azide in the literature. The reported Mn–N distances in the structures of [Mn(NH₃)₆]Cl₂ and [Mn(NH₃)₆]Br₂ are 2.239(15) and 2.313(18) Å (room temperature), respectively, and were obtained from X-ray powder diffraction.^[9] X-ray diffraction on single crystals at room temperature of [Mn(NH₃)₆]Cl₂ showed a distance of 2.270(3) between the metal cation and the nitrogen atoms of the ammine ligands.^[10,11] The Mn–N distances in [Mn(NH₃)₆](N₃)₂·4NH₃ were reported in between 2.2668(7) and 2.3131(7) Å at 100 K.^[3] The compound does not crystallize isotypic to known hexaammine complexes of the halides, which may be due to the different hydrogen bond acceptor characteristics of the azide anion in comparison to a halide anion. The azide anion shows N–N distances of 1.178(11) and 1.180(12) Å, its bond angle is linear with 178.7(10)°. Azide anions of compounds that also contain ammine complexes as cations show N–N distances from 1.1708(10) to 1.184(3) Å.^[3] The N–N distances agree with reported values for other azide anion containing compounds as well.^[12] In the cases of azide anions bound as a ligand to metal atoms, a significant elongation or shortening can be observed.^[13,14] Compared to N–N-distances of azide anions of compounds where no hydrogen bonding is present, no significant differences are observed.^[15] An influence of the hydrogen bonds on the N–N–N bond angle could not be detected. Overall, it seems that in these classes of compounds hydrogen bonding does have no observable influence on the structure of the azide anions. Figure 2 shows the cation and the anion of the compound.

Figure 2. The $[\text{Mn}(\text{ND}_3)_6]^{2+}$ cation and the azide anion of the title compound. Fixed displacement parameter for the Mn atom, isotropic displacement parameters for the N atoms and anisotropic displacement parameters at 70 % probability for D atoms at 3 K.

The azide anion is an acceptor of hydrogen bonds via its terminal N4 and N5 atoms. Details of the hydrogen bonds are available from Table 3. In total the N_3^- anion acts as an acceptor of seven hydrogen bonds, three via the N5 atom, and four via the N4 atom. This way it interconnects in four complex cations which are surrounding it in a tetrahedron-like manner. The $[\text{Mn}(\text{ND}_3)_6]^{2+}$ cation is surrounded by eight symmetry-equivalent azide anions and a complex, three-dimensional infinite hydrogen bonding network is built up. A section of the crystal structure of the compound is shown in Figure 3. Hydrogen bonds are not shown for clarity reasons.

Figure 3. A section of the crystal structure of $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$. All atoms shown isotropic with arbitrary radii, $[\text{Mn}(\text{ND}_3)_6]^{2+}$ shown as octahedral, D atoms omitted for clarity.

Table 2. Atom coordinates, Wyckoff positions, site symmetry, and isotropic displacement parameters.

Atom	Wyckoff position (site symmetry)	x	y	z	$U_{\text{iso}} / \text{\AA}^2$
Mn1	2c (2/m)	$-\frac{1}{2}$	0	0	0.004
N1 _{eq}	8j (1)	-0.5308(8)	0.2311(8)	-0.1677(7)	0.0059(13)
D1	8j (1)	-0.6153(11)	0.3297(15)	-0.1507(10)	0.020(3)
D2	8j (1)	-0.4313(12)	0.3093(15)	-0.1800(10)	0.020(3)
D3	8j (1)	-0.5613(11)	0.1675(16)	-0.2599(9)	0.019(3)
N2 _{ax}	4i (m)	-0.2333(11)	0	-0.0186(9)	0.0080(19)
D4	4i (m)	-0.2186(16)	0	-0.1199(14)	0.021(5)
D5	8j (1)	-0.1775(13)	0.1190(15)	0.0200(10)	0.028(4)
N3	4i (m)	-0.7939(9)	$\frac{1}{2}$	0.0421(8)	0.0053(19)
N4	4i (m)	-0.8115(9)	$\frac{1}{2}$	-0.0790(8)	0.0082(17)
N5	4i (m)	-0.7731(12)	$\frac{1}{2}$	0.1632(9)	0.011(2)

Table 3. Details on the hydrogen bonds of the title compound.

	$d(\text{N} \cdots \text{D}) / \text{\AA}$	$d(\text{D} \cdots \text{N}) / \text{\AA}$	$d(\text{N} \cdots \text{N}) / \text{\AA}$	$\angle(\text{N} \cdots \text{D} \cdots \text{H}) / ^\circ$
N1–D1 $\cdots$ N4	1.015(12)	2.210(12)	3.209(9)	167.7(9)
N1–D2 $\cdots$ N5	1.023(12)	2.184(13)	3.192(10)	167.9(9)
N1–D3 $\cdots$ N4	1.014(11)	2.169(11)	3.147(9)	161.5(9)
N2–D4 $\cdots$ N5	1.006(16)	2.130(16)	3.095(12)	160.1(13)

Using quantum-chemical calculations at the DFT-PBE0-D3/TZVP level of theory (CRYSTAL17 program package),^[7,8] we carried out full structural optimizations in the three possible space groups of $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$: $I2/m$, $P2_1/m$ and Pm . The obtained total energies and the cell parameters were almost identical (see Table 1) and did not allow to choose one of the space groups as the most favorable. The deviations of the calculated cell parameters

from the experimentally obtained ones are below 3 %, the volume differences are less than 5 %. Additionally, we calculated the vibrational frequencies of the compound in all three space groups to verify if there are any imaginary frequencies present. However, in all three cases only real frequencies were found, which means that the structures are true local minima in the selected space groups. When we checked the optimized $P2/m$ and Pm structures for additional symmetry, space group $I2/m$ was suggested indicating that all three calculated structures are identical. Therefore, we can safely assume that $I2/m$ is the real space group of $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$ under the investigated conditions.

Conclusions

To conclude, we have obtained the compound $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$ and determined its crystal structure by powder neutron diffraction at 3 K. By quantum chemical calculations for the 3D-periodic solid, and by searches for additional symmetry its space group has been chosen as $I2/m$ with $a = 8.5905(5)$, $b = 6.8506(4)$, $c = 9.7530(6)$ Å, $\beta = 94.618(6)^\circ$, $V = 572.10(6)$ Å³, $Z = 2$, at $T = 3$ K. The Mn(II) atom is coordinated octahedron-like by ND_3 ligands with essentially similar Mn–N distances. The azide anion shows N–N distances of 1.178(11) and 1.180(12) Å, its bond angle is almost linear with $178.7(10)^\circ$. Despite the azide anion being a pseudohalide anion but likely due to differences in hydrogen bonding, the title compound does not crystallize isotypic to known hexaammine manganese(II) halides.

Experimental Section

Unless otherwise stated, all work was carried out by excluding moisture and air under dried and purified argon (Praxair, > 99.999) using high-vacuum glass lines or a glove box (MBRAUN). Liquid ammonia (Air Liquide, 99.98 %) was dried and stored over sodium (VWR) in a special high-vacuum glass line. All glass vessels were flame-dried under vacuum before use. We trust that the well-educated reader is aware that azides, depending on the bonding situation, may be sensitive towards heat, friction, impact and/or electrostatic discharge; sometimes explosions were reported without obvious provocation. No incidents occurred during our investigations as the complex cations seem to sufficiently separate the azide anions from each other, and additionally the azide anions are not coordinating to the metal cations.

Silver azide, was synthesized according to the literature on air.^[15] Sodium azide (Merck, zur Synthese) and silver nitrate (VWR, 99.9 %) were used as supplied without any purification. $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2 \cdot 4\text{ND}_3$ was obtained according to the literature^[3] and slowly decomposed under inert conditions at room temperature to circa 4 g of $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$. The compound was filled into a vanadium cuvette, sealed, and investigated by powder neutron diffraction.

The powder pattern recorded in an indium sealed vanadium ampoule of 12.7 mm diameter and approximately 60 mm height at 3 K using the SPODI neutron powder diffractometer ($\lambda = 1.5484$ Å) at the neutron source FRM II / Heinz Maier-Leibnitz Zentrum.^[16] The indexing of the powder pattern was done in the WinXPOW software.^[17] The structure solution and Rietveld refinement were performed using the Jana2006 software^[5] and the SUPERFLIP algorithm.^[4] As the space group choice was ambiguous,

the initial structure solution was done in the space group type Pm . Possibly due to the very extensive peak overlaps, no proper structure model could be obtained. By careful examination of the Fourier nuclear density map, the azide nitrogen nuclei were located. The rest of the nitrogen and the deuterium nuclei were located after series of subsequent Rietveld refinement iterations followed by an examination of the Fourier difference map. The manganese nucleus was found last as a negative maximum on the Fourier difference map. When the complete model was built, it was checked for overlooked symmetry elements using the PLATON software.^[6] Based on the PLATON results, the space group was subsequently changed first to $P2/m$ and then to $I2/m$. The deuterium atoms were refined anisotropic, the nitrogen atoms were refined isotropic. The atomic displacement parameter of the manganese atom was refined to a physically unreasonable value (presumably due to the lowest absolute value of the scattering factor in comparison to nitrogen and deuterium), therefore, it was fixed.

The structural and vibrational properties of $[\text{Mn}(\text{ND}_3)_6](\text{N}_3)_2$ were investigated using the CRYSTAL17 program package within the dispersion-corrected density functional theory.^[7,8] Both the atomic positions and lattice constants were fully optimized using the PBE0 hybrid density functional method.^[18,19] Van der Waals dispersion interactions were taken into account by using Grimme's DFT-D3 method with zero-damping.^[20] Triple-zeta valence + polarization (TZVP) level basis sets were derived from the molecular Karlsruhe basis sets^[21] and applied for all atoms (see^[22] and Supporting Information for additional basis set details). Due to the unpaired electrons of Mn, all calculations were carried using spin-unrestricted formalism. Antiferromagnetic ordering of the spins at Mn atoms was used for all structures. The reciprocal space was sampled using Monkhorst-Pack-type k-point grids: 6x6x6 for $I2/m$ and 4x6x4 for the rest.^[23] For the evaluation of the Coulomb and exchange integrals (TOLINTEG), tight tolerance factors of 8, 8, 8, 8, and 16 were used. Default optimization convergence thresholds and DFT integration grids were applied in all calculations. The harmonic vibrational frequencies were obtained by using the computational schemes implemented in CRYSTAL17.^[24,25]

Further details of the crystal structures investigations may be obtained from the Fachinformationszentrum Karlsruhe, 76344 Eggenstein-Leopoldshafen, Germany (Fax: +49-7247-808-666; E-Mail: crysdata@fiz-karlsruhe.de, <http://www.fiz-karlsruhe.de/request-for-deposited-data.html>) on quoting the depository number CSD-434409.

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Keywords: manganese • azide • liquid ammonia • crystal structure • neutron diffraction

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ARTICLE

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