Electronic Supplementary Information (ESI)

Transition metal complexes of a versatile polyalkoxy oxazolidine-based ligand derived from *in-situ* cyclization

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b. Universitaet Marburg, Fachbereich Chemie, Hans-Meerwein-Str. 4, 35032 Marburg, Germany
c. Laboratoire National des Champs Magnétiques Intenses, CNRS UPR 3228, 25 Rue des Martyrs, 38042, Grenoble, France
Figure S1. (a) Extensive intermolecular hydrogen bonding between a molecule (1) and six neighboring molecules (2-7) are shown. (b) side-view and (c) top view of the hydrogen bonded two-dimensional network formed are shown.

Figure S2. (a) The packing diagram of compound 5 showing intermolecular π-π interaction along c axis forming a chain-like structure, with hydrogen bonding interaction between the neighboring chains (elongated red bonds). (b) The three-dimensional supramolecular interaction results into a porous structure with 5.9% solvent accessible pore volume for a probe of 1.2 Å radius.

Figure S3. The hydrogen bonding interactions between the neighboring units through the terminal azide units and the N-H group of the oxazolidine ring.

Figure S4. Overlay of the infrared spectra for the isostructural compounds 1 - 4

Figure S5. Infrared spectrum of Compound 5.

Figure S6. Infrared spectrum of Compound 6.

Figure S7. Overlay of the infrared spectra for compounds 1 – 6.

Figure S8. Infrared spectrum of isolated L2H3 is shown.

Figure S9. Thermogravimetric analysis (TGA) of Compound 1 is presented.

Figure S10. Thermogravimetric analysis (TGA) of Compound 2 is presented.

Figure S11. Thermogravimetric analysis (TGA) of Compound 3 is presented.

Figure S12. Thermogravimetric analysis (TGA) of Compound 4 is presented.

Figure S13. Thermogravimetric analysis (TGA) of Compound 5 is presented.

Figure S14. Thermogravimetric analysis (TGA) of Compound 5 is presented.

Figure S15. 1H NMR spectra of L2H3 in CH3OD.

Figure S16. 1H NMR spectra of Compound 4 in DMSO-d6.

Figure S17. ESI-MS of the isolated ligand H3L2 is shown.

Figure S18. ESI-MS of Compound 1 is shown.

Figure S19. ESI-MS of Compound 2 is shown.

Figure S20. ESI-MS of Compound 3 is shown.

Figure S21. ESI-MS of Compound 4 is shown.

Figure S22. ESI-MS of Compound 5 is shown.

Figure S23. ESI-MS of Compound 6 is shown.

Figure S24. Arrhenius plot for Compound 6.

Figure S25. Zones of inhibition of the ligand L2H3 and the complexes 1-6, against S. aureus (a) and E.coli (b).

Single-crystal X-ray analysis of Compound 1

Table S1. Bond lengths [Å] and angles [°] for Compound 1.

Single-crystal X-ray analysis of Compound 2

Table S2. Bond lengths [Å] and angles [°] for Compound 2.

Single-crystal X-ray analysis of Compound 3

Table S3. Bond lengths [Å] and angles [°] for Compound 3.

Single-crystal X-ray analysis of Compound 4

Table S4. Bond lengths [Å] and angles [°] for Compound 4.

Single-crystal X-ray analysis of Compound 5

Table S5. Bond lengths [Å] and angles [°] for Compound 5.

Single-crystal X-ray analysis of Compound 6

Table S6. Bond lengths [Å] and angles [°] for Compound 6.
Figure S1. (a) Extensive intermolecular hydrogen bonding between a molecule (1) and six neighboring molecules (2-7) are shown. (b) side-view and (c) top view of the hydrogen bonded two-dimensional network formed are shown. Colour code for the atoms: Blue (N), grey (H), dark-grey (C), red (O), and purple (Mn).
Figure S2. (a) The packing diagram of compound 5 showing intermolecular π-π interaction along c axis forming a chain-like structure, with hydrogen bonding interaction between the neighboring chains (elongated red bonds). (b) The three-dimensional supramolecular interaction results into a porous structure with 5.9 % solvent accessible pore volume for a probe of 1.2 Å radius. *Colour code for the atoms: Blue (N), gray (C), red (O), orange (Fe).*
**Figure S3.** The hydrogen bonding interactions between the neighboring units through the terminal azide units and the N-H group of the oxazolidine ring.

**Figure S4.** Overlay of the infrared spectra for the isostructural compounds 1 - 4.
**Figure S5.** Infrared spectrum of Compound 5.

**Figure S6.** Infrared spectrum of Compound 6.
Figure S7. Overlay of the infrared spectra for compounds 1 – 6.

Figure S8. Infrared spectrum of isolated L₂H₃ is shown.
Figure S9. Thermogravimetric analysis (TGA) of Compound 1 is presented.

Figure S10. Thermogravimetric analysis (TGA) of Compound 2 is presented.
Figure S11. Thermogravimetric analysis (TGA) of Compound 3 is presented.

Figure S12. Thermogravimetric analysis (TGA) of Compound 4 is presented.
Figure S13. Thermogravimetric analysis (TGA) of Compound 5 is presented.

Figure S14. Thermogravimetric analysis (TGA) of Compound 5 is presented.
**Figure S15.** $^1$H NMR spectra of $L_2H_3$ in CH$_3$OD.

**Figure S16.** $^1$H NMR spectra of Compound 4 in DMSO-$d_6$. 
**Figure S17.** ESI-MS of the isolated ligand $\text{H}_3\text{L}_2$ is shown. The peak at $277^{(m/z)}$ corresponds to $[\text{H}_3\text{L}_2 + \text{H}^+]^+$. 
**Figure S18.** ESI-MS of Compound 1 is shown. The peak at \(400(m/z)\) corresponds to the \([1+H]^+\) fragment and the peak at \(364(m/z)\) corresponds to the \([1-\text{Cl}]^+\) fragment.
**Figure S19.** ESI-MS of Compound 2 is shown. The peak at 404\( (m/z) \) corresponds to the \([2+H]^+\) fragment and the peak at 368\( (m/z) \) corresponds to the \([2-Cl]^+\) fragment.
Figure S20. ESI-MS of Compound 3 is shown. The peak at $369(m/z)$ corresponds to the $[3-\text{Cl}]^+$ fragment.
Figure S21. ESI-MS of Compound 4 is shown. The peak at 339 (m/z) corresponds to the [4 - Cl]⁺ fragment.
Figure S22. ESI-MS of Compound 5 is shown. The peak at 841(\textsuperscript{m/z}) corresponds to the [Fe\textsubscript{4}O(HL\textsubscript{2})\textsubscript{2}(H\textsubscript{3}L\textsubscript{3})\textsubscript{2}]\textsuperscript{2+} fragment.
Figure S23. ESI-MS of Compound 6 is shown. The compound seems unstable at the ESI conditions like many polynuclear complexes, and only shows a minor peak at 793 (m/z) which might arise from [6 - OH]+.
Figure S24. Arrhenius plot for Compound 6.
Figure S25. Zones of inhibition of the ligand $\text{L}_2\text{H}_3$ and the complexes 1-6, against $S.\text{aureus}$ (a) and $E.\text{coli}$ (b).
Single-crystal X-ray analysis of Compound 1:

Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoK\(_\alpha\) radiation, a graded multilayer mirror monochromator (\(\lambda = 0.71073\) Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multisanned reflexions (SADABS (Bruker AXS Inc., 2016)). Cell constants were refined using 9973 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on \(F^2\) using SHELXL-2018/1 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the ‘riding model’ with isotropic temperature factors at 1.2 times (for CH\(_3\) groups 1.5 times) that of the preceding carbon atom. CH\(_3\) groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

**Table S1. Bond lengths [Å] and angles [°] for Compound 1.**

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**Single-crystal X-ray analysis of compound 2:**

Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoK$_\text{α}$ radiation, a graded multilayer mirror monochromator ($\lambda = 0.71073$ Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multiscanned reflexions (SADABS (Bruker AXS Inc., 2016)). Cell constants were refined using 9972 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on $F^2$ using SHELXL-2018/1 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the ‘riding model’ with isotropic temperature factors at 1.2 times (for CH$_3$ groups 1.5 times) that of the preceding carbon atom. CH$_3$ groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

**Table S2** Bond lengths [Å] and angles [°] for Compound 2.

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C11-N2-H3  107.3(15)  N2-C11-H11  109.3
C13-N2-H3  108.6(16)  C10-C11-H11  109.3
Co1-N2-H3  112.9(16)  O4-C12-C13  107.03(15)
N1-C2-C7  121.83(16)  O4-C12-H12A  110.3
N1-C2-C3  114.94(15)  C13-C12-H12A  110.3
C7-C2-C3  123.22(16)  O4-C12-H12B  110.3
O1-C3-C4  125.59(16)  C13-C12-H12B  110.3
O1-C3-C2  117.97(15)  H12A-C12-H12B  108.6
C4-C3-C2  116.43(16)  N2-C13-C14  109.37(15)
C3-C4-C5  120.71(17)  N2-C13-C15  109.06(15)
C3-C4-H4  119.6  C14-C13-C15  111.27(15)
C5-C4-H4  119.6  N2-C13-C12  103.37(14)
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C6-C5-H5  118.7  C15-C13-C12  113.55(16)
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C5-C6-C7  119.18(17)  O3-C14-H14A  109.5
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C7-C6-H6  120.4  O3-C14-H14B  109.5
C2-C7-C6  117.82(16)  C13-C14-H14B  109.5
C2-C7-C8  116.28(16)  H14A-C14-H14B  108.1
C6-C7-C8  125.89(17)  O5-C15-C13  111.02(17)
C9-C8-C7  120.82(16)  O5-C15-H15A  109.4
C9-C8-H8  119.6  C13-C15-H15A  109.4
C7-C8-H8  119.6  O5-C15-H15B  109.4
C8-C9-C10  118.61(16)  C13-C15-H15B  109.4
C8-C9-H9  120.7  H15A-C15-H15B  108.0
C10-C9-H9  120.7  O2-C16-H16A  109.5
N1-C10-C9  121.51(16)  O2-C16-H16B  109.5
N1-C10-C11  114.17(14)  H16A-C16-H16B  109.5
C9-C10-C11  124.32(15)  O2-C16-H16C  109.5
O4-C11-N2  107.82(13)  H16A-C16-H16C  109.5
O4-C11-C10  111.02(15)  H16B-C16-H16C  109.5

Symmetry transformations used to generate equivalent atoms:
Single-crystal X-ray analysis of Compound 3:

Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoK$_\alpha$ radiation, a graded multilayer mirror monochromator ($\lambda = 0.71073$ Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multiscanned refllexions ( SADABS (Bruker AXS Inc., 2016)). Cell constants were refined using 9901 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on $F^2$ using SHELXL-2018/1 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the 'riding model' with isotropic temperature factors at 1.2 times (for CH$_3$ groups 1.5 times) that of the preceding carbon atom. CH$_3$ groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

Table S3. Bond lengths [Å] and angles [°] for Compound 3.

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Single-crystal X-ray analysis of Compound 4:

Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoK$_\text{α}$ radiation, a graded multilayer mirror monochromator ($\lambda = 0.71073$ Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multiscanned reflexions (SADABS (Bruker AXS Inc., 2016)). Cell constants were refined using 8865 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on $F^2$ using SHELXL-2018/1 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the ‘riding model’ with isotropic temperature factors at 1.2 times (for CH$_3$ groups 1.5 times) that of the preceding carbon atom. CH$_3$ groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

Table S4. Bond lengths [Å] and angles [°] for Compound 4:

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N1-Zn1-O1  79.68(6)  C9-C8-C7  120.76(18)
O3-Zn1-C1  117.56(5)  C9-C8-H8  119.6
N1-Zn1-C1  128.08(5)  C7-C8-H8  119.6
O1-Zn1-C11  103.76(4)  C8-C9-C10  118.99(18)
O3-Zn1-N2  78.93(6)  C8-C9-H9  120.5
N1-Zn1-N2  75.01(6)  C10-C9-H9  120.5
O1-Zn1-N2  153.17(6)  N1-C10-C9  120.94(18)
C11-Zn1-N2  98.82(5)  N1-C10-C11  115.70(17)
C3-O1-Zn1  112.70(11)  C9-C10-C11  123.35(17)
C14-O3-Zn1  112.78(12)  O4-C11-N2  107.20(15)
C14-O3-H3A  114.2(18)  O4-C11-C10  107.94(15)
Zn1-O3-H3A  129.6(18)  N2-C11-C10  111.31(15)
C11-O4-C12  107.05(14)  O4-C11-H11  110.1
C15-O5-H5A  109(2)  N2-C11-H11  110.1
C10-N1-C2  121.24(17)  C10-C11-H11  110.1
C10-N1-Zn1  124.69(13)  O4-C12-C13  104.28(15)
C2-N1-Zn1  114.06(12)  O4-C12-H12A  110.9
C11-N2-C13  107.39(15)  C13-C12-H12A  110.9
C11-N2-Zn1  113.12(12)  O4-C12-H12B  110.9
C13-N2-Zn1  107.73(11)  C13-C12-H12B  110.9
C11-N2-H2A  107.5(18)  H12A-C12-H12B  108.9
C13-N2-H2A  108.2(17)  N2-C13-C12  102.24(15)
Zn1-N2-H2A  112.7(17)  N2-C13-C14  108.92(15)
N1-C2-C7  121.80(17)  C12-C13-C14  110.66(16)
N1-C2-C3  115.47(17)  N2-C13-C15  110.60(16)
C7-C2-C3  122.71(17)  C12-C13-C15  114.60(16)
O1-C3-C4  125.69(18)  C14-C13-C15  109.52(16)
O1-C3-C2  117.52(17)  O3-C14-C13  108.62(16)
C4-C3-C2  116.79(18)  O3-C14-H14A  110.0
C3-C4-C5  120.75(19)  C13-C14-H14A  110.0
C3-C4-H4  119.6  O3-C14-H14B  110.0
C5-C4-H4  119.6  C13-C14-H14B  110.0
C6-C5-C4  122.67(19)  H14A-C14-H14B  108.3
C6-C5-H5  118.7  O5-C15-C13  113.13(17)
C4-C5-H5  118.7  O5-C15-H15A  109.0
C5-C6-C7  118.79(19)  C13-C15-H15A  109.0
C5-C6-H6  120.6  O5-C15-H15B  109.0
C7-C6-H6  120.6  C13-C15-H15B  109.0
C2-C7-C8  116.23(18)  H15A-C15-H15B  107.8
Single-crystal X-ray analysis of Compound 5:

Data was collected with an Bruker APEX2 diffractometer equipped with CuKα radiation, a graphite monochromator (λ = 1.54184 Å) and a APEX2 detector using an oil-coated shock-cooled crystal at 173(2) K. Absorption effects were corrected semi-empirically using multisanned reflexions (TWINABS - Bruker AXS scaling for twinned crystals - Version 2012/1). Cell constants were refined using 4782 of observed reflections of the data collection. The structure was solved by direct methods by using the program SHELXT 2014/5 (Sheldrick, 2014) and refined by full matrix least squares procedures on F² using SHELXL-2018/3 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the ‘riding model’ with isotropic temperature factors at 1.2 times (for CH₃ groups 1.5 times) that of the preceding carbon atom. CH₃ groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically. Disorder was refined using restraints for both the geometry and thermal parameters. Heavily disordered solvent was treated by using the PLATON/SQUEEZE (Spek, 2015) procedure.

Table S5. Bond lengths [Å] and angles [°] for Compound 5.

<p>|          | Fe1-O1  | Fe1-O30 | Fe1-N1  | Fe1-O38 | Fe1-N22 | Fe1-O9  | Fe1-N33 | Fe2-O100 | Fe2-O309 | Fe2-O30  | Fe2-O9   | Fe2-N301 | Fe2-N401 | N1-C2   | N1-C10  | C2-C3   | C2-C11  | C3-C4   | C3-H3   | C4-C5   | C4-H4   | C5-C6   | C5-C10  | C6-C7   | C6-H6   | C7-C8   | C7-H7   | C8-C9   | C8-H10F | O9-C9   | C9-C10  | C11-O11 | C11-N33 | C11-H11A | O11-H11 | N22-C23 | N22-C31 |
|----------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
|          | 1.7912(7) | 2.129(3) | 2.138(4) | 2.153(3) | 2.164(4) | 2.182(3) | 2.431(4) | 1.889(4) | 1.998(4) | 2.023(3) | 2.052(3) | 2.056(14) | 2.155(18) | 2.296(4) | 1.325(6) | 1.348(6) | 1.408(7) | 1.498(7) | 1.357(8) | 0.9500  | 1.412(8) | 0.9500  | 1.412(8) | 1.416(7) | 1.354(9) | 0.9500  | 1.408(8) | 0.9500  | 1.375(7) | 0.9500  | 1.343(6) | 1.435(7) | 1.392(6) | 1.484(6) | 1.0000  | 0.8400  | 1.317(6) | 1.372(6) |</p>
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| O315-C103-C313 | 105.1(7) | C310-N301-Fe2 | 114.1(8) 
| O315-C103-H10E | 110.7 | N301-C302-C303 | 120.8(10) 
| C313-C103-H10E | 110.7 | N301-C302-C311 | 116.1(9) 
| O315-C103-H10F | 110.7 | C303-C302-C311 | 123.1(9) 
| C313-C103-H10F | 110.7 | C304-C303-C302 | 120.1(10) 
| H10E-C103-H10F | 108.8 | C304-C303-H303 | 119.9 
| C201-O100-Fe2 | 115.2(7) | C302-C303-H303 | 119.9 
| C101-O100-Fe2 | 118.9(5) | C303-C304-C305 | 119.7(9) 
| O100-C201-C313 | 112.1(9) | C303-C304-H304 | 120.2 
| O100-C201-H20A | 109.2 | C305-C304-H304 | 120.2 
| C313-C201-H20A | 109.2 | C310-C305-C304 | 117.2(8) 
| O100-C201-H20B | 109.2 | C310-C305-C306 | 116.5(8) 
| C313-C201-H20B | 109.2 | C304-C305-C306 | 126.2(9) 
| H20A-C201-H20B | 107.9 | C307-C306-C305 | 119.8(9) 
| C202-O201-H201 | 109.5 | C307-C306-H306 | 120.1 
| O201-C202-C313 | 110.3(13) | C305-C306-H306 | 120.1 
| O201-C202-H20C | 109.6 | C306-C307-C308 | 122.2(9) 
| C313-C202-H20C | 109.6 | C306-C307-H307 | 118.9 
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| C313-C202-H20D | 109.6 | C309-C308-C307 | 120.2(9) 
| H20C-C202-H20D | 108.1 | C309-C308-H308 | 119.9 
| C313-C203-O315 | 101.4(9) | C307-C308-H308 | 119.9 
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| O315-C311-C402 | 110.9(13) | C402-N401-C410 | 121.2(11) 
| O315-C311-N312 | 107.4(4) | C402-N401-Fe2 | 125.7(11) 
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| N312-C312-C312 | 111.1 | C404-C403-C402 | 119.2(13) 
| C302-C312-C312 | 111.1 | C404-C403-H403 | 120.4 
| O315-C311-H411 | 108.1 | C402-C403-H403 | 120.4 
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| N312-C312-H411 | 108.1 | C403-C404-H404 | 119.7 
| C313-N312-C311 | 105.9(4) | C405-C404-C405 | 119.7 
| C313-N312-Fe2 | 106.5(3) | C410-C405-C404 | 116.7(10) 
| C311-N312-Fe2 | 114.0(3) | C410-C405-C406 | 115.2(11) 
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| C311-N312-H312 | 110.1 | C407-C406-C405 | 119.6(11) 
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| N312-C313-C101 | 107.8(6) | C405-C406-H406 | 120.2 
| N312-C313-C102 | 110.2(6) | C406-C407-C408 | 124.7(12) 
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| C311-O315-C203 | 103.8(6) | N501-C502-C503 | 166.4(19) 
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Symmetry transformations used to generate equivalent atoms:

#1 -x, y+1, z+1
Single-crystal X-ray analysis of Compound 6:
Data was collected with an Bruker D8 QUEST area detector diffractometer equipped with with MoKα radiation, a graded multilayer mirror monochromator (λ = 0.71073 Å) and a PHOTON-100 CMOS detector using an oil-coated shock-cooled crystal at 100(2) K. Absorption effects were corrected semi-empirical using multisccanned reflexions (SADABS-2016/2 - Bruker AXS area detector scaling and absorption correction). Cell constants were refined using 8108 of observed reflections of the data collection. The structure was solved by direct methods by using the program XT V2014/1 (Bruker AXS Inc., 2014) and refined by full matrix least squares procedures on F² using SHELXL-2016/2 (Sheldrick, 2018). The non-hydrogen atoms have been refined anisotropically, carbon bonded hydrogen atoms were included at calculated positions and refined using the ‘riding model’ with isotropic temperature factors at 1.2 times (for CH3 groups 1.5 times) that of the preceding carbon atom. CH3 groups were allowed to rotate about the bond to their next atom to fit the electron density. Nitrogen or oxygen bonded hydrogen atoms were located and allowed to refine isotropically.

Table S6. Bond lengths [Å] and angles [°] for Compound 6.

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Symmetry transformations used to generate equivalent atoms:
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