Supporting Information

Organically Templated Niobium Germanate: Ionothermal Synthesis of $(C_8H_{24}N_4)[NbOGe_6O_{13}(OH)_2F]$

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Figure S1. The observed X-ray powder pattern (**a**) and simulated powder pattern based on the results from single-crystal X-ray diffraction (**b**) of the compound $(C_8H_{24}N_4)[NbOGe_6O_{13}(OH)_2F]$ (denote as **1**).

Figure S2. The infrared spectrum of **1** (KBr pellet method).

Figure S3. The thermogravimetric analysis of **1** in flowing N_2 gas at a heating rate of 5 $^oC\ min^{-1}$.

Figure S4. The response of second harmonic generation of **1** (blue curve) and that of KDP (red curve).

Figure S5. The structure of **1** viewed along the [011] direction to show 10-ring channels. The organic ammonium cations and the H atoms of the OH groups are not shown for clarity.

Table S1. Selected N···O distances showing hydrogen bonding interactions in **1**

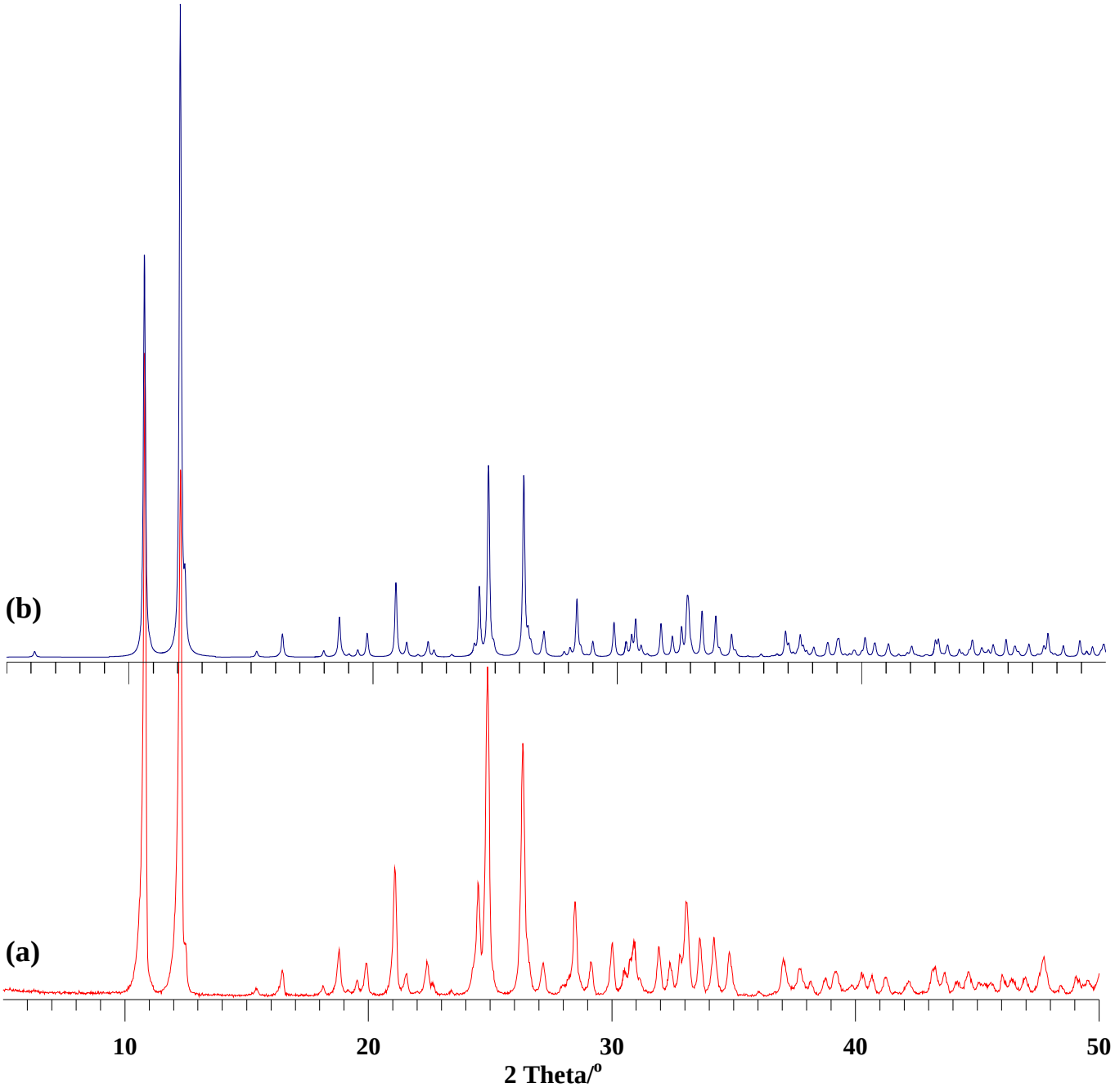

Figure S1

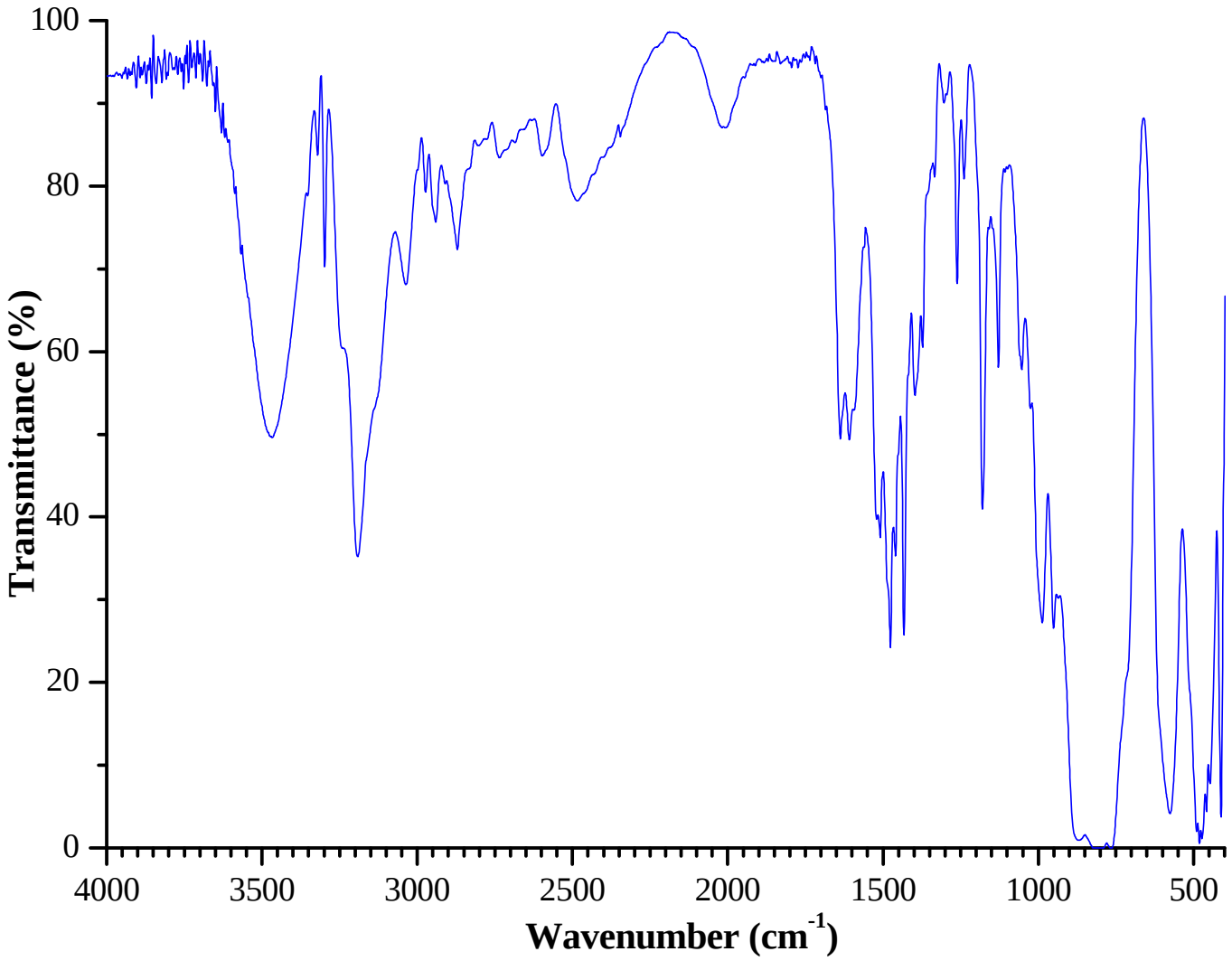

Figure S2

The FTIR spectrum of **1** was measured from a powder sample pelletized with KBr on a Jasco FTIR-4200 series spectrophotometer over the range 4000–400 cm^{-1} at the resolution of 4 cm^{-1}.

The band centered at 3468 cm^{-1} is the stretching vibrations of OH and N–H groups. The bands at 3294, 3190 and from 3030 to 2870 cm^{-1} correspond to the stretching vibrations of the secondary amine N–H, the protonated amine R–NH_3^+, and the CH_2 groups, respectively.[1-4] The bending vibrations of the OH, NH_3^+ groups are at 1638 and 1605 cm^{-1}.[3] The bands at 1510, 1478 and 1431 cm^{-1} are bending vibrations of N–H, C–N and CH_2 groups, respectively. The band at 1181 cm^{-1} is assigned to the C–N stretching vibration of the amine.[4] The broad, strong bands from 871 to 753 cm^{-1} can be assigned to the vibrations of Ge–O and Ge–F bonds.[2] The bands at 574 and 476 cm^{-1} are attributed to the symmetrical stretching and bending vibration of the Ge–O bonds.[3] The bands at 984 and 951 cm^{-1} are for the Nb–O vibrations.[5]

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3. Beitone, L.; Loiseau, T.; Férey, G. *Inorg. Chem.* **2002**, *41*, 3962–3966.
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5. Andersen, K. B.; Christensen, E.; Berg, R. W.; Bjerrum, N. J.; von Barner, J. H. *Inorg. Chem*. **2000**, *39*, 3449–3454.

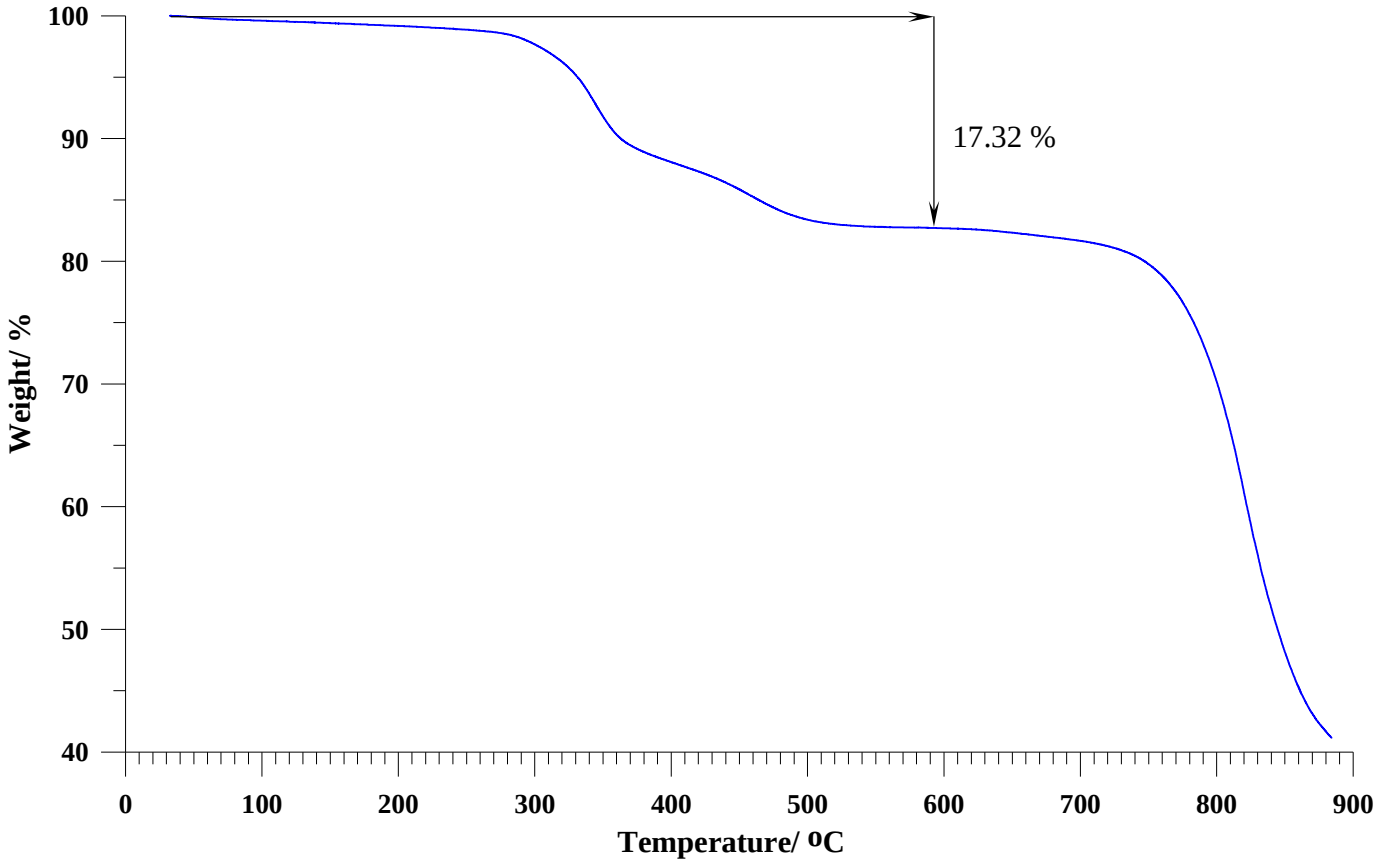

Figure S3

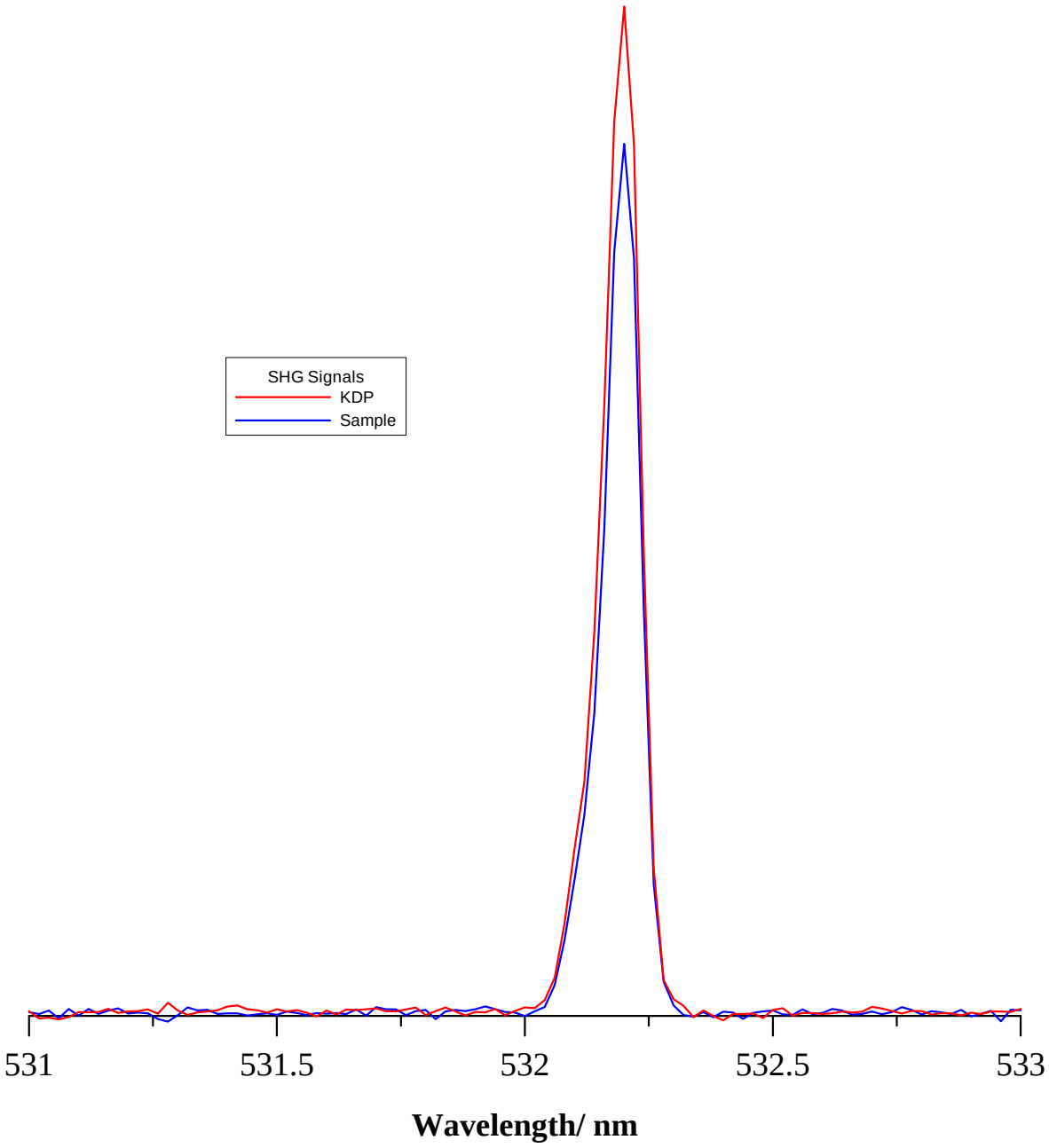

Figure S4

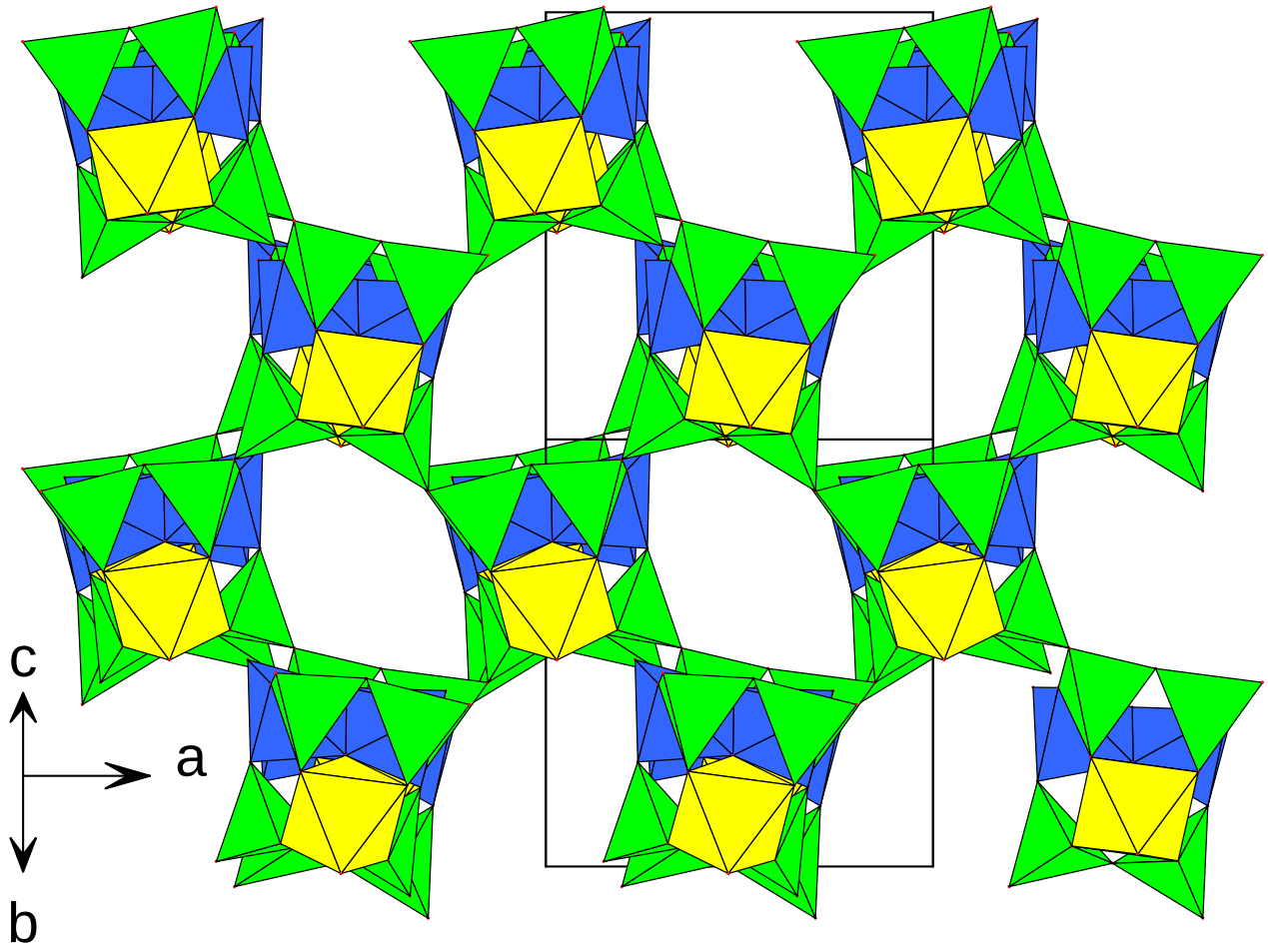

Figure S5

Table S1. Selected N···O distances showing hydrogen bonding interactions in **1**

	Distances/ Å
N(1)···O(1)	3.177(7)
N(1)···O(4)	3.301(5)
N(1)···O(5)	2.954(5)
N(1)···O(14)	2.752(5)
N(1)···O(15)	3.282(5)
N(1)···O(16)	3.334(5)
N(2)···O(3)	3.001(4)
N(2)···O(6)	3.335(4)
N(2)···O(13)	2.796(4)
N(2)···O(15A)	3.294(4)
N(3)···O(11)	3.263(6)
N(3)···O(15B)	3.113(6)
N(4)···O(7)	3.294(6)
N(4)···O(10)	3.029(5)
N(4)···O(12)	3.042(6)
N(4)···O(15C)	2.907(5)
N(4)···O(16C)	2.786(6)