

Supporting Information for:

A new type germanium-vanadate cluster, $[\text{Ge}_5\text{V}_6\text{O}_{21}(\text{heda})_6]$ (Hheda = *N*-(2-hydroxyethyl)ethylenediamine)

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1. Figures

Fig. S1. IR spectrum of compound **1**.

Fig. S2. XRD patterns for the experimental and calculated results of compound **1**.

Fig. S3. EPR result of compound **1**.

Fig. S4. TG curve for compound **1**.

Fig. S5. The XRD patterns of the dehydrated sample of compound **1** along with the original one.

2. Table S1 Selected bond lengths(Å) and angles (°).

1. Figures

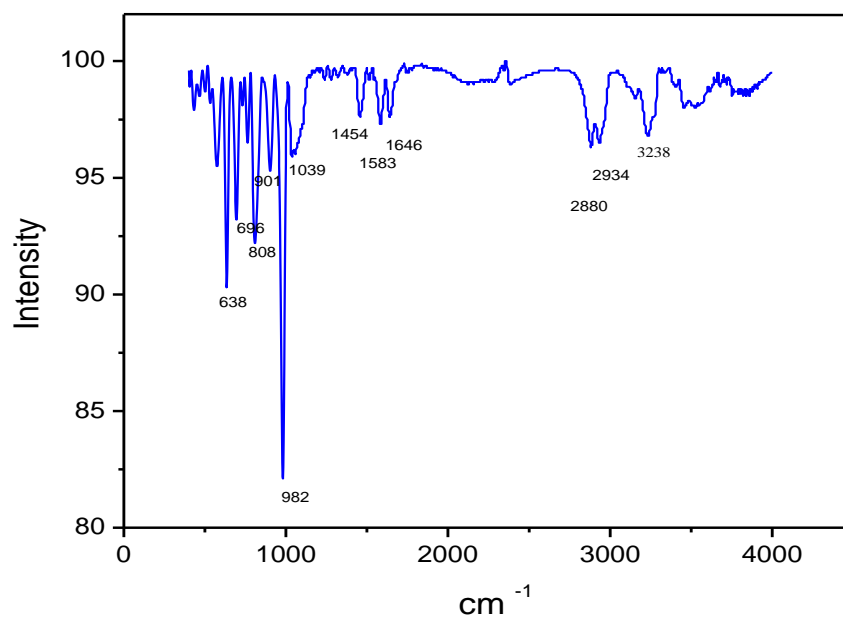


Fig. S1. IR spectrum of compound 1..

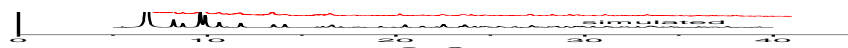


Fig. S2. XRD patterns for the experimental and calculated results of compound 1 to ensure their phase purity.

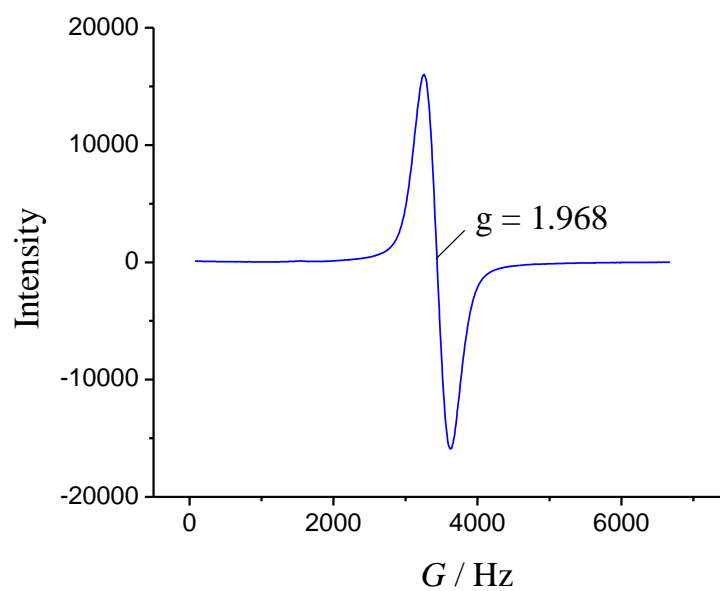


Fig. S3. EPR result of compound **1**.

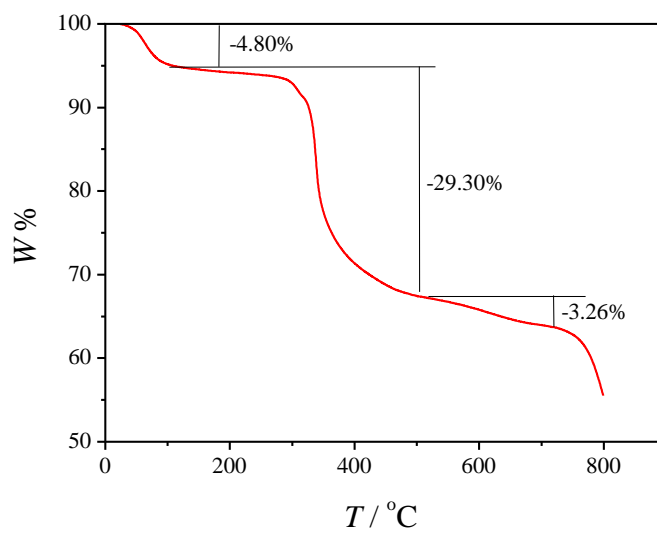


Fig. S4. TG curve for compound **1**.

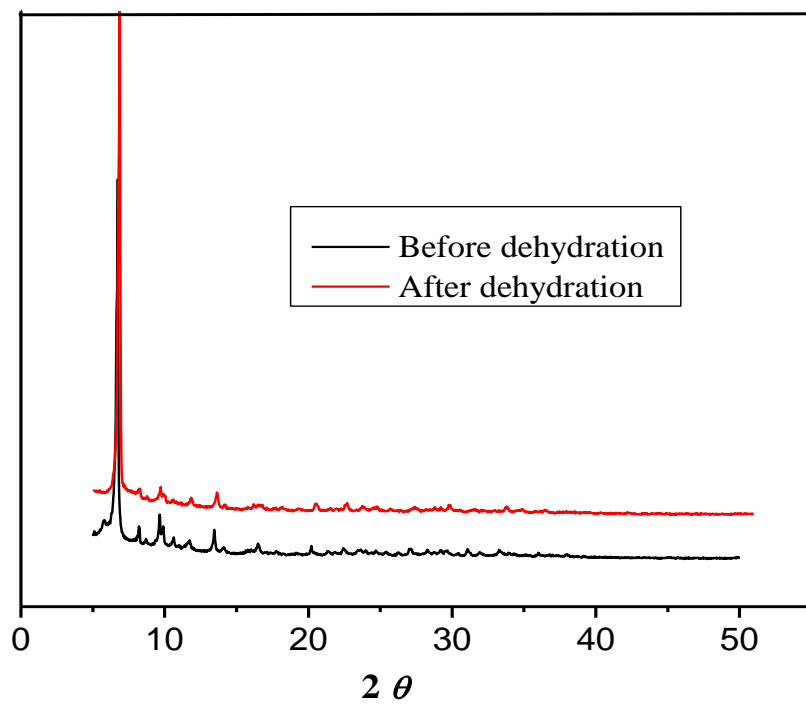


Fig. S5. The XRD patterns of the dehydrated sample of compound **1** along with the original one.

2. Table

Table S1 Selected bond lengths(Å) and angles (°).

| Bond lengths (Å) | | | | | |
|------------------|----------|------------|----------|-------------|----------|
| Ge1—O3 | 1.730(6) | Ge1—O5 | 1.727(7) | Ge1—O7 | 1.737(7) |
| Ge1—O17 | 1.752(8) | Ge2—O4 | 1.772(7) | Ge2—O8 | 1.760(6) |
| Ge2—O9 | 1.733(7) | Ge2—O23 | 1.743(8) | Ge3—O1 | 1.728(6) |
| Ge3—O4 | 1.786(8) | Ge3—O12 | 1.765(7) | Ge3—O21 | 1.733(8) |
| Ge4—O2 | 1.888(7) | Ge4—O3 | 1.831(7) | Ge4—O6 | 1.853(7) |
| Ge4—O27 | 1.867(8) | Ge4—N5 | 2.105(9) | Ge4—N6 | 2.03(1) |
| Ge5—O7 | 1.850(6) | Ge5—O10 | 1.872(7) | Ge5—O13 | 1.884(7) |
| Ge5—O28 | 1.867(8) | Ge5—N11 | 2.090(9) | Ge5—N12 | 2.050(9) |
| V1—O5 | 2.235(7) | V1—O10 | 1.937(7) | V1—O11 | 1.609(8) |
| V1—O12 | 2.029(7) | V1—O14 | 2.030(7) | V1—O25 | 2.15(1) |
| V2—O1 | 2.300(7) | V2—O2 | 1.966(7) | V2—O5 | 1.957(7) |
| V2—O14 | 1.963(8) | V2—O15 | 1.609(8) | V2—N7 | 2.17(1) |
| V3—O9 | 1.974(8) | V3—O10 | 1.946(7) | V3—O12 | 1.999(7) |
| V3—O13 | 1.954(7) | V3—O18 | 1.618(8) | V4—O1 | 1.962(7) |
| V4—O2 | 1.961(7) | V4—O6 | 1.948(7) | V4—O8 | 2.001(7) |
| V4—O19 | 1.603(7) | V5—O9 | 2.294(8) | V5—O13 | 1.983(8) |
| V5—O16 | 1.615(8) | V5—O17 | 1.955(7) | V5—O20 | 1.962(7) |
| V5—N1 | 2.19(1) | V6—O6 | 1.945(7) | V6—O8 | 2.053(7) |
| V6—O17 | 2.247(7) | V6—O20 | 1.995(7) | V6—O22 | 1.614(8) |
| V6—O24 | 2.16(1) | | | | |
| angles (°) | | | | | |
| O5—V1—O10 | 86.2(3) | O5—V1—O12 | 83.3(3) | O5—V1—O14 | 71.9(3) |
| O1—V2—N7 | 82.3(3) | O2—V2—N7 | 98.6(3) | O14—V2—N7 | 80.0(4) |
| O1—V2—O2 | 73.5(3) | O1—V2—O5 | 82.4(3) | O1—V2—O14 | 82.6(3) |
| O9—V3—O12 | 97.1(3) | O9—V3—O13 | 81.1(3) | O9—V3—O18 | 108.5(4) |
| O1—V4—O2 | 81.8(3) | O2—V4—O6 | 75.9(3) | O6—V4—O8 | 80.9(3) |
| O9—V5—O13 | 72.9(3) | O9—V5—N1 | 81.6(3) | O13—V5—N1 | 102.4(3) |
| O6—V6—O8 | 79.7(3) | O3—Ge1—O5 | 109.0(3) | O3—Ge1—O7 | 112.9(3) |
| O3—Ge1—O17 | 106.5(3) | O4—Ge2—O8 | 105.2(3) | O4—Ge2—O9 | 107.6(3) |
| O8—Ge2—O9 | 115.8(3) | O1—Ge3—O4 | 108.5(3) | O1—Ge3—O12 | 113.0(3) |
| O4—Ge3—O12 | 104.7(3) | O2—Ge4—O3 | 100.2(3) | O2—Ge4—O6 | 79.9(3) |
| O3—Ge4—O27 | 90.9(3) | O2—Ge4—N5 | 87.1(3) | O2—Ge4—N6 | 89.1(3) |
| N5—Ge4—N6 | 82.0(4) | O7—Ge5—N11 | 166.8(3) | N11—Ge5—N12 | 81.9(4) |

Table S2 X···Y distances of hydrogen bonds (Å).*

| | | | | | |
|----------------|-------|---------------|-------|------------|-------|
| N2···O29w | 2.865 | N4···O11 | 2.710 | N5···O31w | 2.863 |
| N6···O4 | 2.913 | N6···O15 (in) | 2.970 | N10···O30w | 2.946 |
| N10···O31w | 2.806 | N12···O7 | 2.990 | N12···O29w | 2.932 |
| N12···O16 (in) | 3.015 | O29w···O23 | 2.669 | O30w···O23 | 2.856 |
| O31w···O18 | 2.886 | O31w···O19 | 2.773 | | |

* Because the hydrogen atoms of the water and the amine groups can not be located, only the X···Y distances' are listed.

w: oxygen of water; in: intra-cluster