Supplementary Materials

The open framework compound \( \text{Ni}_{15}\text{Te}_{12}\text{O}_{34}\text{Cl}_{10} \) - synthesis, crystal structure and magnetic properties

Dong Zhang, Mats Johnsson, Sven Lidin, and Reinhard K. Kremer

Table S1  Atomic coordinates and Equivalent Isotropic Displacement Parameters (Å\(^2\)) for \( \text{Ni}_{15}\text{Te}_{12}\text{O}_{34}\text{Cl}_{10} \).

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Note. \( U(\text{eq}) \) is defined as one third of the trace of the orthogonalized \( U_{ij} \) tensor.
### Table S2
Selected Bond Lengths (Å) and Results from Bond Valence Sum (BVS) calculations for Ni_{15}Te_{12}O_{34}Cl_{10}.

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| O(1) | Te(1)-O(1) | 1.875(4) | 1.4171 |
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| O(2) | Te(1)-O(2) | 1.939(4) | 1.1082 |
|      | Te(4)-O(2) #3 | 2.497(4) | 0.2453 |
|      | Ni(3)-O(2) #7 | 2.175(5) | 0.2446 |
|      | Ni(7)-O(2) #3 | 2.060(5) | 0.3338 |
|      |             | 1.93     |        |

| O(3) | Te(1)-O(3) | 1.891(5) | 1.2617 |
|      | Ni(1)-O(3) | 2.046(5) | 0.3466 |
|      | Ni(2)-O(3) #4 | 2.128(5) | 0.2777 |
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| O(4) | Te(2)-O(4) | 1.927(4) | 1.1447 |
|      | Ni(1)-O(4) | 2.074(4) | 0.3214 |
|      | Ni(5)-O(4) #8 | 2.007(5) | 0.3852 |
|      |             | 1.85     |        |

| O(5) | Te(2)-O(5) | 1.872(4) | 1.3281 |
|      | Ni(1)-O(5) | 2.080(4) | 0.3162 |
|      | Ni(7)-O(5) #3 | 2.024(5) | 0.3679 |
|      |             | 2.01     |        |

| O(6) | Te(3)-O(6) | 1.911(5) | 1.1953 |
|      | Ni(1)-O(6) | 2.100(4) | 0.2996 |
|      | Ni(1)-O(6) #4 | 2.194(4) | 0.2324 |
|      | Ni(2)-O(6) | 2.148(5) | 0.2631 |
|      |             | 1.99     |        |

| O(7) | Te(3)-O(7) | 1.901(4) | 1.2280 |
|      | Ni(3)-O(7) | 2.135(5) | 0.2725 |
|      | Ni(7)-O(7) #3 | 2.106(4) | 0.2948 |
|      | Ni(7)-O(7) #6 | 2.375(5) | 0.1425 |
|      |             | 1.94     |        |

| O(10) | Te(4)-O(10) | 1.959(4) | 1.050 |
|       | Ni(3)-O(10) #6 | 2.015(4) | 0.3769 |

| O(11) | Te(4)-O(11) | 1.889(4) | 1.2685 |
|       | Ni(6)-O(11) | 1.980(4) | 0.4143 |
|       | Ni(7)-O(11) | 1.981(4) | 0.4132 |
|       |             | 2.09     |        |

| O(12) | Te(5)-O(12) | 1.875(4) | 1.3174 |
|       | Ni(3)-O(12) #5 | 2.000(4) | 0.3925 |
|       | Ni(7)-O(12) | 2.013(4) | 0.3790 |
|       |             | 2.09     |        |

| O(13) | Te(5)-O(13) | 1.872(5) | 1.3281 |
|       | Ni(8)-O(13) #9 | 2.022(5) | 0.3699 |
|       |             | 1.70     |        |

| O(14) | Te(5)-O(14) | 1.881(4) | 1.2962 |
|       | Ni(6)-O(14) | 2.031(4) | 0.3610 |
|       | Ni(8)-O(14) | 2.000(5) | 0.3925 |
|       |             | 2.05     |        |

| O(15) | Te(6)-O(15) | 1.889(5) | 1.2685 |
|       | Ni(5)-O(15) | 2.085(5) | 0.3120 |
|       | Ni(8)-O(15) | 2.002(5) | 0.3904 |
|       |             | 1.97     |        |

<p>| O(16) | Te(6)-O(16) | 1.862(5) | 1.3645 |
|       | Ni(1)-O(16) #1 | 2.053(5) | 0.3401 |
|       | Ni(2)-O(16) #1 | 2.059(5) | 0.3347 |
|       |             | 2.04     |        |</p>
<table>
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<th></th>
<th>Te-X-X</th>
<th>r0</th>
<th>r</th>
<th>( \Sigma_{\text{BVS}} )</th>
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<td>1.2754</td>
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<tr>
<td>Ni(4)-O(8)</td>
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<td>Ni(6)-O(8) #6</td>
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<td>Te(6)-O(17)</td>
<td>1.897(4)</td>
<td>1.2414</td>
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<td>O(9) Te(4)-O(9)</td>
<td>1.950(4)</td>
<td>1.0757</td>
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<td>Ni(6)-O(9)</td>
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<td>Cl(4) Ni(5)-Cl(4)</td>
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<td>0.4110</td>
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<tr>
<td>Ni(3)-Cl(1)</td>
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<td>Ni(6)-Cl(5)</td>
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<td>Ni(3)-Cl(2)</td>
<td>2.5210(18)</td>
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<td>Ni(5)-Cl(2)</td>
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<tr>
<td>Ni(2)-Cl(3)</td>
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<td>Ni(6)-Cl(3)</td>
<td>2.577(2)</td>
<td>0.0825</td>
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</table>

**Note.** Symmetry transformations used to generate equivalent atoms:

#1 1+x, y, z  
#2 2-x, 2-y, -z  
#3 x, y-1, z  
#4 -x+2, 1-y, -z  
#5 x, y+1, z  
#6 -x+1, 1-y, -z  
#7 1-x, 2-y, -z  
#8 x-1, y, z  
#9 1-x, -y, 1-z  
#10 -x, 1-y, 1-z

Bond valence sum (BVS) calculations according to Brown and Altermatt [A].

The \( r_0 \) values used are Te-O: 1.977, Te-Cl: 2.37, Ni-O: 1.654, Ni-Cl: 2.02 [B]
Table S3  Selected Bond Angles (º) for Ni$_{15}$Te$_{12}$O$_{34}$Cl$_{10}$.

<table>
<thead>
<tr>
<th>Bond Angle</th>
<th>Value (º)</th>
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<tbody>
<tr>
<td>O(1)-Te(1)-O(3)</td>
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<tr>
<td>O(1)-Te(1)-O(2)</td>
<td>92.1(2)</td>
</tr>
<tr>
<td>O(3)-Te(1)-O(2)</td>
<td>101.12</td>
</tr>
<tr>
<td>O(1)-Te(1)-Cl(3)</td>
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<tr>
<td>O(3)-Te(1)-Cl(3)</td>
<td>78.31(16)</td>
</tr>
<tr>
<td>O(2)-Te(1)-Cl(3)</td>
<td>174.28(16)</td>
</tr>
<tr>
<td>O(1)-Te(1)-Cl(2)</td>
<td>86.08(17)</td>
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<tr>
<td>O(3)-Te(1)-Cl(2)</td>
<td>176.13(16)</td>
</tr>
<tr>
<td>O(2)-Te(1)-Cl(2)</td>
<td>75.21(16)</td>
</tr>
<tr>
<td>O(5)-Te(2)-O(4)</td>
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<td>O(5)-Te(2)-O(17)</td>
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<td>O(4)-Te(2)-O(17)</td>
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<td>O(16)-Te(6)-O(17)</td>
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<td>O(15)-Te(6)-Cl(5)</td>
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</table>
Note. Symmetry transformations used to generate equivalent atoms:

<table>
<thead>
<tr>
<th>#1</th>
<th>1+x, y, z</th>
<th>#2</th>
<th>2-x, 2-y, -z</th>
<th>#3</th>
<th>x, y-1, z</th>
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<td>#9</td>
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<td>-x, 1-y, 1-z</td>
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</table>

References
