In the crystal structure of the title compound, \([\text{Na}_2(\text{H}_2\text{O})_5]\)_{(\text{C}_{19}\text{H}_{15}\text{BN})_2}, the Na atom is octahedrally coordinated by three water molecules and three N atoms of triphenylcyanoborate anions. The basic structural unit is composed of two octahedra sharing a common face, and this unit is connected by a common edge with the next unit, forming an infinite chain along the crystallographic c axis.

**Comment**

The triphenylcyanoborate anion (as a sodium salt, ‘caesignost’) has been used as a gravimetric reagent for the determination of caesium, thallium and large organic cations (Havir, 1961; Bauman, 1968). The goal of this study was the investigation of the crystal structure of the hydrated sodium salt of triphenylcyanoborate, (I), using X-ray structure analysis and vibrational spectroscopy.

The environment of the sodium ion is a distorted octahedron, with three water molecules (O1, O2, O3) and one N atom of a cyano group in the equatorial plane, while two cyano groups are axially positioned (Fig. 1 and Table 1). Two such octahedra share a common face defined by water molecule O2 (located on a twofold axis) and atoms N1 and N1B, forming a basic structural unit that is repeated by an inversion operation through a common edge (of two N atoms) generating an infinite chain along the c axis (Figs. 2 and 3). The resulting structure is additionally stabilized by O—H⋯O and O—H⋯C(aromatic) hydrogen bonds (Table 2).

The high level of hydration of the sodium salt explains its good solubility in water, which makes it a suitable reagent for caesium precipitation from aqueous solutions.
Crystal data

\[
\begin{align*}
\text{[Na}_2\text{(H}_2\text{O})_5\text{]}\text{(C}_19\text{H}_15\text{BN})_2 \quad D_s = 1.219 \text{ Mg m}^{-3} \\
M_r = 672.32 \\
\text{Monoclinic, C2/c} \\
a = 26.200 (5) \, \text{Å} \\
b = 14.719 (3) \, \text{Å} \\
c = 9.5537 (19) \, \text{Å} \\
\beta = 96.12 (3) \degree \\
\nu = 3663.4 (13) \, \text{Å}^3 \\
Z = 4 \\
\end{align*}
\]

Mo Kα radiation

Cell parameters from 25 reflections

\( \theta = 30-35 \degree \)

\( \mu = 0.10 \text{ mm}^{-1} \)

\( T = 293 (2) \, \text{K} \)

Prism, colourless

\( 0.50 \times 0.30 \times 0.25 \, \text{mm} \)

Data collection

Rigaku AFC-75 diffractometer

\( \omega \) scans

Absorption correction: \( \psi \) scan

(TEXSAN; Molecular Structure Corporation, 1999)

\( T_{\text{min}} = 0.95, \, T_{\text{max}} = 0.98 \)

4207 measured reflections

4206 independent reflections

3143 reflections with \( I > 2\sigma(I) \)

Refinement

Refinement on \( F^2 \)

\( R[F^2 > 2\sigma(F^2)] = 0.048 \)

\( wR(F^2) = 0.140 \)

\( S = 1.02 \)

4206 reflections

253 parameters

H atoms treated by a mixture of independent and constrained refinement

\( w = 1/[\sigma^2(F_o^2) + (0.0735P)^2 + 0.6203P] \)

where \( P = (F_o^2 + 2F_c^2)/3 \)

\( \Delta \sigma_{\text{max}} < 0.001 \)

\( \Delta \rho_{\text{max}} = 0.25 \, \text{e Å}^{-3} \)

\( \Delta \rho_{\text{min}} = -0.18 \, \text{e Å}^{-3} \)

Extinction correction: SHELXL97

Extinction coefficient: 0.0052 (8)

Table 1

<table>
<thead>
<tr>
<th>Symmetry codes</th>
<th>( D_{\text{Na}} - \text{O1} )</th>
<th>( D_{\text{Na}} - \text{O3} )</th>
<th>( D_{\text{Na}} - \text{O2} )</th>
<th>( D_{\text{Na}} - \text{N1} )</th>
<th>( D_{\text{Na}} - \text{N1}^\ddagger )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i)</td>
<td>2.3118 (18)</td>
<td>103.87 (7)</td>
<td>169.03 (6)</td>
<td>2.5455 (15)</td>
<td>2.7034 (16)</td>
</tr>
<tr>
<td>(ii)</td>
<td>2.3488 (16)</td>
<td>85.43 (5)</td>
<td>89.83 (7)</td>
<td>2.3869 (17)</td>
<td>2.7097 (16)</td>
</tr>
<tr>
<td>(iii)</td>
<td>2.3869 (17)</td>
<td>161.17 (6)</td>
<td>82.52 (5)</td>
<td>81.79 (6)</td>
<td>170.53 (5)</td>
</tr>
</tbody>
</table>

Symmetry codes: (i) \(-x, y - 1, z + 1; (ii) x - x + 1, y, -z + \frac{1}{2}; (iii) x, y - 1, z + \frac{1}{2} \)

Table 2

Hydrogen-bond geometry (Å, °).

\[ \begin{array}{cccccc}
D - H \cdot \cdot \cdot A & D - H & H \cdot \cdot \cdot A & D \cdot \cdot \cdot A & D - H \cdot \cdot \cdot A \\
\hline
\text{O1} - \text{H1A} \cdot \cdot \cdot \text{O3}^\ddagger & 0.85 (2) & 2.04 (2) & 2.858 (2) & 160 (2) \\
\text{O1} - \text{H1B} \cdot \cdot \cdot \text{C16}^\ddagger & 0.83 (2) & 2.65 (3) & 3.352 (3) & 143 (2) \\
\text{O2} - \text{H2} \cdot \cdot \cdot \text{O1}^\ddagger & 0.82 (2) & 2.28 (2) & 3.001 (2) & 146 (2) \\
\text{O3} - \text{H3A} \cdot \cdot \cdot \text{C26}^\ddagger & 0.81 (2) & 2.57 (2) & 3.142 (2) & 159 (2) \\
\text{O3} - \text{H3B} \cdot \cdot \cdot \text{C31}^\ddagger & 0.82 (2) & 2.42 (2) & 3.214 (2) & 161 (2) \\
\end{array} \]

Symmetry codes: (i) \(-x, y + 1, z + 1; (ii) x - x + 1, y, -z + \frac{1}{2}; (iii) x, y - 1, z + \frac{1}{2} \)

All H atoms of phenyl groups were located in a difference map and allowed to ride on their parent C atoms, with C–H = 0.91–1.02 Å, and \( U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C) \). Water H atoms were located in a Fourier map and refined with restrained bond lengths [O–H = 0.83 (2) Å and \( U_{\text{iso}}(H) = 1.3U_{\text{eq}}(O) \)].
Data collection: MSC/AFC Diffractometer Control Software (Molecular Structure Corporation, 1991); cell refinement: MSC/AFC Diffractometer Control Software; data reduction: TEXSAN (Molecular Structure Corporation, 1999); program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and ATOMS (Dowty, 2004); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2003).

The packing diagram given in Fig. 3 was prepared by the program ATOMS (Dowty, 2004) kindly provided by Dr B Perić, Rudjer Boskovic Institute, Zagreb, Croatia.

References