Structural modifications and thermal stability of Cd\textsuperscript{2+} -exchanged stellerite, a zeolite with STI framework-type

G. Cametti,∗,† A. C. Scheinost,‡,¶ and S. V. Churakov†,§

†Institute of Geological Sciences, University of Bern, Baltzerstrasse 1+3, 3012 Bern, Switzerland
‡The Rossendorf Beamline at the European Synchrotron Radiation Facility (ESRF), Avenue des Martyrs 71, 38043 Grenoble, France
¶Institute of Resource Ecology, Bautzner Landstrasse 400, 01328 Dresden
§Paul Scherrer Institut, Forschungstrasse 111, 5232 Villingen PSI, Switzerland

E-mail: georgia.cametti@krist.unibe.ch

Contents

List of Figures 2

List of Tables 2

1 Refinement Strategy 3

2 Supplementary Figures 4

3 Supplementary Tables 9
List of Figures

S1  SEM-EDS spectrum of Cd-stellerite sample used for SCXRD experiments.  4
S2  (a) SEM picture of Cd-stellerite sample used for XAFS experiments. The occurrence of small shiny particles (interpreted as Cd(OH$_2$)) on Cd-stellerite fragments is highlighted with green circles. (b) Magnified view of one white particle and associated EDS spectrum demonstrating that the particle is Cd-rich. .......................... 5
S3  Experimental (blue circles) and calculated (red line) $k^3$-weighted $\chi(k)$ function obtained from EXAFS and MD simulations. .......................... 6
S4  Coordination number of Cd-Ow (oxygen of H$_2$O) contacts (a) and corresponding $k^3$-weighted $\chi(k)$ function (red line) (b) of the optimized structure of Cd-STI with 6 H$_2$O per Cd$^{2+}$ ion. Experimental data from EXAFS (blue circles) are also reported. .......................... 6
S5  Reconstructed precession images of $h0l$ and $0kl$ layers of Cd-stellerite structure at 275, 300, 325, and 375°C. .......................... 7
S6  Radial distribution function (RDF) of Ca-Ow (oxygen of H$_2$O) obtained from MD trajectories. Corresponding curve of Cd-Ow is reported for comparison. .......................... 8

List of Tables

S1  Atom coordinates, equivalent displacement parameters, and occupancy of Cd-STI at 100°C. .......................... 10
S2  Atom coordinates, equivalent displacement parameters, and occupancy of Cd-STI at 125°C. .......................... 11
S3  Atom coordinates, equivalent displacement parameters, and occupancy of Cd-STI at 225°C. .......................... 12
1 Refinement Strategy

The position of the extraframework cations was determined by difference Fourier maps. At room temperature, the displacement parameters of the W3, W5, and W10 sites were fixed due to strong disorder and correlations among the refined parameters. With the increase of temperature the assignment of the electron-density peaks to either Cd or H$_2$O was not straightforward due to the enhancement of disorder of Cd atoms over several low-occupied sites. In particular from 100 to 175°C, the structure was partially hydrated and the breaking of T-O-T connections further complicated the refinements. In general, the atomic species were assigned by taking into account the bond distances between the extraframework (EF) occupants and the O atoms of the framework. With the increase of temperature this was anyhow controversial. Thus, we consider, as an additional discriminating factor, the value of the atomic displacement parameters: EF sites which showed very high U values were refined with O scattering factors, the other (with typical U value lower than 0.06 Å$^2$) were attributed to Cd. The sites (e.g. Cd5, Cd7A in the data set obtained at 125°C) with higher U values compared to those occupied by the same atomic species should be interpreted as a mixture of O and Cd.
2 Supplementary Figures

**Figure S1:** SEM-EDS spectrum of Cd-stellerite sample used for SCXRD experiments.
Figure S2: (a) SEM picture of Cd-stellerite sample used for XAFS experiments. The occurrence of small shiny particles (interpreted as Cd(OH$_2$)) on Cd-stellerite fragments is highlighted with green circles. (b) Magnified view of one white particle and associated EDS spectrum demonstrating that the particle is Cd-rich.
Figure S3: Experimental (blue circles) and calculated (red line) $k^3$-weighted $\chi(k)$ function obtained from EXAFS and MD simulations.

Figure S4: Coordination number of Cd-Ow (oxygen of H$_2$O) contacts (a) and corresponding $k^3$-weighted $\chi(k)$ function (red line) (b) of the optimized structure of CdSTI with 6 H$_2$O per Cd$^{2+}$ ion. Experimental data from EXAFS (blue circles) are also reported.
Figure S5: Reconstructed precession images of $h0l$ and $0kl$ layers of Cd-stellerite structure at 275, 300, 325, and 375°C.
Figure S6: Radial distribution function (RDF) of Ca-Ow (oxygen of H2O) obtained from MD trajectories. Corresponding curve of Cd-Ow is reported for comparison.
3 Supplementary Tables
Table S1: Atom coordinates, equivalent displacement parameters, and occupancy of Cd-STI at 100°C.

<table>
<thead>
<tr>
<th>Site</th>
<th>Scattering factor</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
<th>$U^{eq}$ ($\text{Å}^2$)</th>
<th>Occ.</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>Si</td>
<td>-1.13805(6)</td>
<td>-1.28030(5)</td>
<td>0.12109(5)</td>
<td>0.0224(2)</td>
<td>1</td>
</tr>
<tr>
<td>T1P</td>
<td>Si</td>
<td>-1.13625(6)</td>
<td>-1.33716(5)</td>
<td>0.36804(5)</td>
<td>0.0204(2)</td>
<td>0.951(2)</td>
</tr>
<tr>
<td>T1PD</td>
<td>Si</td>
<td>-1.1430(11)</td>
<td>-1.4083(10)</td>
<td>0.3925(10)</td>
<td>0.0204(2)</td>
<td>0.049(2)</td>
</tr>
<tr>
<td>T3</td>
<td>Si</td>
<td>-1.05088(6)</td>
<td>-1.41053(5)</td>
<td>0.21713(5)</td>
<td>0.02109(19)</td>
<td>1</td>
</tr>
<tr>
<td>T4</td>
<td>Si</td>
<td>-0.85985(6)</td>
<td>-1.31613(5)</td>
<td>0.22586(5)</td>
<td>0.0222(2)</td>
<td>1</td>
</tr>
<tr>
<td>T5</td>
<td>Si</td>
<td>-1</td>
<td>-1.29694(8)</td>
<td>0.5</td>
<td>0.0231(3)</td>
<td>1</td>
</tr>
<tr>
<td>O3P</td>
<td>O</td>
<td>-0.87208(19)</td>
<td>-1.25160(17)</td>
<td>0.15929(18)</td>
<td>0.0424(7)</td>
<td>1</td>
</tr>
<tr>
<td>O7</td>
<td>O</td>
<td>-1.25</td>
<td>-1.2798(3)</td>
<td>0.0893(3)</td>
<td>0.0484(11)</td>
<td>1</td>
</tr>
<tr>
<td>O1P</td>
<td>O</td>
<td>-1.0661(2)</td>
<td>-1.35156(17)</td>
<td>0.44468(16)</td>
<td>0.0399(6)</td>
<td>1</td>
</tr>
<tr>
<td>O1</td>
<td>O</td>
<td>-1.0690(2)</td>
<td>-1.2603(2)</td>
<td>0.04866(18)</td>
<td>0.0536(9)</td>
<td>1</td>
</tr>
<tr>
<td>O10</td>
<td>O</td>
<td>-0.75</td>
<td>-1.3528(2)</td>
<td>0.2206(2)</td>
<td>0.0341(8)</td>
<td>1</td>
</tr>
<tr>
<td>O3</td>
<td>O</td>
<td>-0.8793(3)</td>
<td>-1.2794(2)</td>
<td>0.3093(2)</td>
<td>0.0569(9)</td>
<td>1</td>
</tr>
<tr>
<td>O9</td>
<td>O</td>
<td>-1.0577(3)</td>
<td>-1.5</td>
<td>0.1919(2)</td>
<td>0.0361(8)</td>
<td>1</td>
</tr>
<tr>
<td>O8</td>
<td>O</td>
<td>-0.93536(19)</td>
<td>-1.38542(18)</td>
<td>0.21158(18)</td>
<td>0.0438(7)</td>
<td>1</td>
</tr>
<tr>
<td>O4P</td>
<td>O</td>
<td>-1.0967(2)</td>
<td>-1.39660(19)</td>
<td>0.30277(17)</td>
<td>0.0488(8)</td>
<td>1</td>
</tr>
<tr>
<td>O4</td>
<td>O</td>
<td>-1.1140(2)</td>
<td>-1.36658(18)</td>
<td>0.1497(2)</td>
<td>0.0538(8)</td>
<td>1</td>
</tr>
<tr>
<td>O7P</td>
<td>O</td>
<td>-1.25</td>
<td>-1.3587(2)</td>
<td>0.3902(2)</td>
<td>0.0321(7)</td>
<td>1</td>
</tr>
<tr>
<td>Cd1</td>
<td>Cd</td>
<td>-1.04514(13)</td>
<td>-1.5</td>
<td>0.4052(2)</td>
<td>0.0391(8)</td>
<td>0.225(3)</td>
</tr>
<tr>
<td>Cd1A</td>
<td>Cd</td>
<td>-1.0453(16)</td>
<td>-1.5</td>
<td>0.487(2)</td>
<td>0.148(11)</td>
<td>0.072(5)</td>
</tr>
<tr>
<td>Cd1B</td>
<td>Cd</td>
<td>-0.984(3)</td>
<td>-1.5</td>
<td>0.454(2)</td>
<td>0.053(15)</td>
<td>0.015(3)</td>
</tr>
<tr>
<td>Cd1C</td>
<td>Cd</td>
<td>-1.0481(15)</td>
<td>-1.5</td>
<td>0.445(2)</td>
<td>0.026(9)</td>
<td>0.018(4)</td>
</tr>
<tr>
<td>Cd2</td>
<td>Cd</td>
<td>-1.1132(8)</td>
<td>-1.5</td>
<td>0.0659(4)</td>
<td>0.031(2)</td>
<td>0.095(8)</td>
</tr>
<tr>
<td>Cd2A</td>
<td>Cd</td>
<td>-1.0929(16)</td>
<td>-1.5212(7)</td>
<td>0.0582(5)</td>
<td>0.025(3)</td>
<td>0.043(7)</td>
</tr>
<tr>
<td>Cd2B</td>
<td>Cd</td>
<td>-1.1191(10)</td>
<td>-1.5279(6)</td>
<td>0.0569(3)</td>
<td>0.033(2)</td>
<td>0.067(6)</td>
</tr>
<tr>
<td>Cd3</td>
<td>Cd</td>
<td>-1.25</td>
<td>-1.2451(12)</td>
<td>0.4531(7)</td>
<td>0.055(5)</td>
<td>0.050(4)</td>
</tr>
<tr>
<td>Cd3A</td>
<td>Cd</td>
<td>-1.25</td>
<td>-1.210(2)</td>
<td>0.4505(13)</td>
<td>0.058(9)</td>
<td>0.027(4)</td>
</tr>
<tr>
<td>Cd4</td>
<td>Cd</td>
<td>-0.9402(12)</td>
<td>-1.3534(10)</td>
<td>0.0576(10)</td>
<td>0.021(5)</td>
<td>0.0125(12)</td>
</tr>
<tr>
<td>Cd5</td>
<td>Cd</td>
<td>-0.9260(12)</td>
<td>-1.5851(10)</td>
<td>0.3828(9)</td>
<td>0.041(5)</td>
<td>0.0189(15)</td>
</tr>
<tr>
<td>Cd6</td>
<td>Cd</td>
<td>-0.8958(8)</td>
<td>-1.5</td>
<td>0.1250(6)</td>
<td>0.077(4)</td>
<td>0.072(3)</td>
</tr>
<tr>
<td>Cd7</td>
<td>Cd</td>
<td>-0.75</td>
<td>-1.5</td>
<td>0.033(2)</td>
<td>0.047(15)</td>
<td>0.021(5)</td>
</tr>
<tr>
<td>Cd7A</td>
<td>Cd</td>
<td>-0.810(4)</td>
<td>-1.5</td>
<td>0.031(2)</td>
<td>0.081(17)</td>
<td>0.020(4)</td>
</tr>
<tr>
<td>W1</td>
<td>O</td>
<td>-1.2011(12)</td>
<td>-1.5</td>
<td>0.4556(10)</td>
<td>0.076(6)</td>
<td>0.377(18)</td>
</tr>
<tr>
<td>W2</td>
<td>O</td>
<td>-0.895(3)</td>
<td>-1.5</td>
<td>0.372(3)</td>
<td>0.29(3)</td>
<td>0.50(4)</td>
</tr>
<tr>
<td>W3</td>
<td>O</td>
<td>-0.8235(14)</td>
<td>-1.5</td>
<td>0.2275(10)</td>
<td>0.074(7)</td>
<td>0.35(2)</td>
</tr>
<tr>
<td>W4A</td>
<td>O</td>
<td>-0.9465(17)</td>
<td>-1.4220(12)</td>
<td>0.0186(12)</td>
<td>0.160(12)</td>
<td>0.42(2)</td>
</tr>
<tr>
<td>W4B</td>
<td>O</td>
<td>-0.847(3)</td>
<td>-1.4073(19)</td>
<td>0.0414(18)</td>
<td>0.26(2)</td>
<td>0.46(3)</td>
</tr>
<tr>
<td>W5</td>
<td>O</td>
<td>-1.25</td>
<td>-1.5802(19)</td>
<td>0.0711(19)</td>
<td>0.043(10)</td>
<td>0.132(16)</td>
</tr>
<tr>
<td>W6</td>
<td>O</td>
<td>-0.75</td>
<td>-1.5</td>
<td>0.1484(18)</td>
<td>0.130(15)</td>
<td>0.48(4)</td>
</tr>
<tr>
<td>W7</td>
<td>O</td>
<td>-1.25</td>
<td>-1.5</td>
<td>0.0834(8)</td>
<td>0.116(7)</td>
<td>0.92(4)</td>
</tr>
</tbody>
</table>
Table S2: Atom coordinates, equivalent displacement parameters, and occupancy of Cd-STI at 125°C.

<table>
<thead>
<tr>
<th>Site</th>
<th>Scattering factor</th>
<th>$x$</th>
<th>$y$</th>
<th>$z$</th>
<th>$U_{eq}$ (Å²)</th>
<th>Occ.</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1PD Si</td>
<td>-1.1423(4)</td>
<td>-1.4095(3)</td>
<td>0.3881(3)</td>
<td>0.0278(3)</td>
<td>0.186(2)</td>
<td></td>
</tr>
<tr>
<td>T3 Si</td>
<td>-1.0520(8)</td>
<td>-1.41085(6)</td>
<td>0.21096(7)</td>
<td>0.0288(3)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>T4 Si</td>
<td>-0.85968(8)</td>
<td>-1.31780(8)</td>
<td>0.22248(8)</td>
<td>0.0251(3)</td>
<td>0.814(2)</td>
<td></td>
</tr>
<tr>
<td>T4D Si</td>
<td>-0.839(3)</td>
<td>-1.372(2)</td>
<td>0.271(2)</td>
<td>0.119(8)</td>
<td>0.0928(12)</td>
<td></td>
</tr>
<tr>
<td>T4DA Si</td>
<td>-0.863(3)</td>
<td>-1.313(2)</td>
<td>0.138(2)</td>
<td>0.119(8)</td>
<td>0.0928(12)</td>
<td></td>
</tr>
<tr>
<td>T5 Si</td>
<td>-1</td>
<td>-1.30673(10)</td>
<td>0.5</td>
<td>0.0301(4)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O3P O</td>
<td>-0.8735(3)</td>
<td>-1.2494(3)</td>
<td>0.1587(3)</td>
<td>0.0506(11)</td>
<td>0.814(2)</td>
<td></td>
</tr>
<tr>
<td>O7 O</td>
<td>-1.25</td>
<td>-1.2755(4)</td>
<td>0.0850(4)</td>
<td>0.0596(15)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O1P O</td>
<td>-1.0644(3)</td>
<td>-1.3598(2)</td>
<td>0.4426(2)</td>
<td>0.0586(11)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O1 O</td>
<td>-1.0700(4)</td>
<td>-1.2503(3)</td>
<td>0.0474(3)</td>
<td>0.0804(16)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O10 O</td>
<td>-0.75</td>
<td>-1.3546(3)</td>
<td>0.2159(3)</td>
<td>0.0516(13)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O3 O</td>
<td>-0.8773(3)</td>
<td>-1.2818(3)</td>
<td>0.3070(3)</td>
<td>0.0702(13)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O9 O</td>
<td>-1.0608(4)</td>
<td>-1.5</td>
<td>0.1831(3)</td>
<td>0.0455(11)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O8 O</td>
<td>-0.9369(3)</td>
<td>-1.3862(3)</td>
<td>0.2077(3)</td>
<td>0.0625(12)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O4P O</td>
<td>-1.1003(3)</td>
<td>-1.3980(2)</td>
<td>0.2969(2)</td>
<td>0.0595(11)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O4 O</td>
<td>-1.1116(4)</td>
<td>-1.3627(2)</td>
<td>0.1444(3)</td>
<td>0.0667(12)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>O7P O</td>
<td>-1.25</td>
<td>-1.3626(3)</td>
<td>0.3916(3)</td>
<td>0.0459(11)</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>OD1 O</td>
<td>-1.163(3)</td>
<td>-1.5</td>
<td>0.420(3)</td>
<td>0.169(15)</td>
<td>0.371(5)</td>
<td></td>
</tr>
<tr>
<td>Cd1 Cd</td>
<td>-1.1169(3)</td>
<td>-1.5210(2)</td>
<td>0.0538(3)</td>
<td>0.0563(16)</td>
<td>0.0931(16)</td>
<td></td>
</tr>
<tr>
<td>Cd2 Cd</td>
<td>-1.25</td>
<td>-1.2572(9)</td>
<td>0.4512(3)</td>
<td>0.033(3)</td>
<td>0.091(8)</td>
<td></td>
</tr>
<tr>
<td>Cd2A Cd</td>
<td>-1.2709(8)</td>
<td>-1.2351(9)</td>
<td>0.4513(4)</td>
<td>0.027(3)</td>
<td>0.048(5)</td>
<td></td>
</tr>
<tr>
<td>Cd2B Cd</td>
<td>-1.25</td>
<td>-1.2060(18)</td>
<td>0.4509(8)</td>
<td>0.046(6)</td>
<td>0.041(5)</td>
<td></td>
</tr>
<tr>
<td>Cd3 Cd</td>
<td>-1.25</td>
<td>-1.5</td>
<td>0.2960(17)</td>
<td>0.034(8)</td>
<td>0.036(6)</td>
<td></td>
</tr>
<tr>
<td>Cd3A Cd</td>
<td>-1.25</td>
<td>-1.5</td>
<td>0.332(4)</td>
<td>0.064(15)</td>
<td>0.027(6)</td>
<td></td>
</tr>
<tr>
<td>Cd4 Cd</td>
<td>-1.1014(15)</td>
<td>-1.5</td>
<td>-0.1121(13)</td>
<td>0.057(6)</td>
<td>0.045(4)</td>
<td></td>
</tr>
<tr>
<td>Cd4A Cd</td>
<td>-1.132(2)</td>
<td>-1.5</td>
<td>-0.141(2)</td>
<td>0.046(10)</td>
<td>0.023(4)</td>
<td></td>
</tr>
<tr>
<td>Cd5 Cd</td>
<td>-1.1789(18)</td>
<td>-1.5</td>
<td>-0.2215(13)</td>
<td>0.109(10)</td>
<td>0.054(4)</td>
<td></td>
</tr>
<tr>
<td>Cd5A Cd</td>
<td>-1.25</td>
<td>-1.5</td>
<td>-0.156(4)</td>
<td>0.1</td>
<td>0.028(3)</td>
<td></td>
</tr>
<tr>
<td>Cd6 Cd</td>
<td>-1.0518(9)</td>
<td>-1.5</td>
<td>0.4083(7)</td>
<td>0.032(3)</td>
<td>0.080(7)</td>
<td></td>
</tr>
<tr>
<td>Cd6A Cd</td>
<td>-1.0299(16)</td>
<td>-1.5</td>
<td>0.3912(13)</td>
<td>0.033(4)</td>
<td>0.047(7)</td>
<td></td>
</tr>
<tr>
<td>Cd7 Cd</td>
<td>-1.0508(14)</td>
<td>-1.3560(11)</td>
<td>-0.0496(11)</td>
<td>0.061(6)</td>
<td>0.027(2)</td>
<td></td>
</tr>
<tr>
<td>Cd7A Cd</td>
<td>-1.3729(15)</td>
<td>0</td>
<td>0.081(10)</td>
<td>0.036(3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cd8 Cd</td>
<td>-1.210(2)</td>
<td>-1.5</td>
<td>0.4627(19)</td>
<td>0.1</td>
<td>0.038(3)</td>
<td></td>
</tr>
<tr>
<td>Cd9 Cd</td>
<td>-1.25</td>
<td>-1.359(2)</td>
<td>0.529(2)</td>
<td>0.035(13)</td>
<td>0.012(2)</td>
<td></td>
</tr>
<tr>
<td>CW2 Cd</td>
<td>-1.25</td>
<td>-1.5847(11)</td>
<td>0.0593(11)</td>
<td>0.076(7)</td>
<td>0.045(3)</td>
<td></td>
</tr>
<tr>
<td>W1 O</td>
<td>-1.25</td>
<td>-1.5</td>
<td>0.074(2)</td>
<td>0.22(2)</td>
<td>0.77(6)</td>
<td></td>
</tr>
<tr>
<td>W3 O</td>
<td>-1.0455(14)</td>
<td>-1.5</td>
<td>0.4859(12)</td>
<td>0.149(10)</td>
<td>0.67(3)</td>
<td></td>
</tr>
</tbody>
</table>
Table S3: Atom coordinates, equivalent displacement parameters, and occupancy of Cd-STI at 225°C.

<table>
<thead>
<tr>
<th>Site</th>
<th>Scattering factor</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>$U_{eq}$ (Å²)</th>
<th>Occ.</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>Si</td>
<td>-1.1418(3)</td>
<td>-1.2693(3)</td>
<td>0.1171(3)</td>
<td>0.0775(14)</td>
<td>0.682(5)</td>
</tr>
<tr>
<td>T1D</td>
<td>Si</td>
<td>-1.1458(7)</td>
<td>-1.3112(6)</td>
<td>0.0479(6)</td>
<td>0.0775(14)</td>
<td>0.318(5)</td>
</tr>
<tr>
<td>T1P</td>
<td>Si</td>
<td>-1.1371(3)</td>
<td>-1.3520(3)</td>
<td>0.3633(3)</td>
<td>0.0666(13)</td>
<td>0.597(4)</td>
</tr>
<tr>
<td>T1PD</td>
<td>Si</td>
<td>-1.1408(5)</td>
<td>-1.4091(5)</td>
<td>0.3763(4)</td>
<td>0.0666(13)</td>
<td>0.403(4)</td>
</tr>
<tr>
<td>T3</td>
<td>Si</td>
<td>-1.0509(2)</td>
<td>-1.41005(17)</td>
<td>0.19886(18)</td>
<td>0.0744(11)</td>
<td>1</td>
</tr>
<tr>
<td>T4</td>
<td>Si</td>
<td>-0.8554(3)</td>
<td>-1.3167(3)</td>
<td>0.2162(4)</td>
<td>0.0833(17)</td>
<td>0.597(4)</td>
</tr>
<tr>
<td>T4D</td>
<td>Si</td>
<td>-0.844(2)</td>
<td>-1.372(2)</td>
<td>0.263(2)</td>
<td>0.078(9)</td>
<td>0.09</td>
</tr>
<tr>
<td>T4DA</td>
<td>Si</td>
<td>-0.8505(13)</td>
<td>-1.3308(14)</td>
<td>0.1405(14)</td>
<td>0.0833(17)</td>
<td>0.159(2)</td>
</tr>
<tr>
<td>T4DB</td>
<td>Si</td>
<td>-0.8382(14)</td>
<td>-1.4064(13)</td>
<td>0.1354(13)</td>
<td>0.0833(17)</td>
<td>0.159(2)</td>
</tr>
<tr>
<td>T5</td>
<td>Si</td>
<td>-1</td>
<td>-1.3203(3)</td>
<td>0.5</td>
<td>0.0758(14)</td>
<td>1</td>
</tr>
<tr>
<td>O3P</td>
<td>O</td>
<td>-0.8707(9)</td>
<td>-1.2416(7)</td>
<td>0.1564(8)</td>
<td>0.095(4)</td>
<td>0.597(4)</td>
</tr>
<tr>
<td>O7</td>
<td>O</td>
<td>-1.25</td>
<td>-1.2758(9)</td>
<td>0.0676(9)</td>
<td>0.131(5)</td>
<td>1</td>
</tr>
<tr>
<td>O1P</td>
<td>O</td>
<td>-1.0634(7)</td>
<td>-1.3750(6)</td>
<td>0.4408(6)</td>
<td>0.120(3)</td>
<td>1</td>
</tr>
<tr>
<td>O1</td>
<td>O</td>
<td>-1.0739(8)</td>
<td>-1.2348(7)</td>
<td>0.0463(7)</td>
<td>0.158(4)</td>
<td>1</td>
</tr>
<tr>
<td>O10</td>
<td>O</td>
<td>-0.75</td>
<td>-1.3586(10)</td>
<td>0.1920(10)</td>
<td>0.141(5)</td>
<td>1</td>
</tr>
<tr>
<td>O3</td>
<td>O</td>
<td>-0.8645(14)</td>
<td>-1.2857(9)</td>
<td>0.3022(8)</td>
<td>0.149(6)</td>
<td>0.682(5)</td>
</tr>
<tr>
<td>O9</td>
<td>O</td>
<td>-1.0579(10)</td>
<td>-1.5</td>
<td>0.1676(8)</td>
<td>0.113(4)</td>
<td>1</td>
</tr>
<tr>
<td>O8</td>
<td>O</td>
<td>-0.9381(7)</td>
<td>-1.3823(6)</td>
<td>0.1991(8)</td>
<td>0.141(4)</td>
<td>1</td>
</tr>
<tr>
<td>O4P</td>
<td>O</td>
<td>-1.1050(9)</td>
<td>-1.3989(5)</td>
<td>0.2844(6)</td>
<td>0.130(4)</td>
<td>1</td>
</tr>
<tr>
<td>O4</td>
<td>O</td>
<td>-1.1071(9)</td>
<td>-1.3607(6)</td>
<td>0.1306(6)</td>
<td>0.143(4)</td>
<td>1</td>
</tr>
<tr>
<td>O7P</td>
<td>O</td>
<td>-1.25</td>
<td>-1.3764(7)</td>
<td>0.3901(8)</td>
<td>0.110(4)</td>
<td>1</td>
</tr>
<tr>
<td>OD</td>
<td>O</td>
<td>-1.147(3)</td>
<td>-1.5</td>
<td>0.395(2)</td>
<td>0.137(12)</td>
<td>0.403(4)</td>
</tr>
<tr>
<td>OD1</td>
<td>O</td>
<td>-1.141(3)</td>
<td>-1.354(2)</td>
<td>-0.051(2)</td>
<td>0.146(12)</td>
<td>0.318(5)</td>
</tr>
<tr>
<td>OD2</td>
<td>O</td>
<td>-1.144(3)</td>
<td>-1.5</td>
<td>-0.126(3)</td>
<td>0.062(11)</td>
<td>0.202(2)</td>
</tr>
<tr>
<td>OD2A</td>
<td>O</td>
<td>-1.187(5)</td>
<td>-1.5</td>
<td>-0.166(4)</td>
<td>0.098(16)</td>
<td>0.202(2)</td>
</tr>
<tr>
<td>Cd1</td>
<td>Cd</td>
<td>-1.0255(17)</td>
<td>-1.5</td>
<td>0.5271(13)</td>
<td>0.131(12)</td>
<td>0.079(6)</td>
</tr>
<tr>
<td>Cd1A</td>
<td>Cd</td>
<td>-0.9949(16)</td>
<td>-1.5</td>
<td>0.3871(12)</td>
<td>0.118(10)</td>
<td>0.081(6)</td>
</tr>
<tr>
<td>Cd2</td>
<td>Cd</td>
<td>-1.129(3)</td>
<td>-1.5</td>
<td>0.0403(19)</td>
<td>0.188(19)</td>
<td>0.082(9)</td>
</tr>
<tr>
<td>Cd3</td>
<td>Cd</td>
<td>-1</td>
<td>-1.371(2)</td>
<td>0</td>
<td>0.111(19)</td>
<td>0.038(5)</td>
</tr>
<tr>
<td>Cd4</td>
<td>Cd</td>
<td>-1.25</td>
<td>-1.2581(17)</td>
<td>0.4530(9)</td>
<td>0.061(6)</td>
<td>0.098(12)</td>
</tr>
<tr>
<td>Cd4A</td>
<td>Cd</td>
<td>-1.276(2)</td>
<td>-1.231(3)</td>
<td>0.4434(15)</td>
<td>0.042(12)</td>
<td>0.026(6)</td>
</tr>
<tr>
<td>Cd6</td>
<td>Cd</td>
<td>-1.25</td>
<td>-1.524(2)</td>
<td>0.095(2)</td>
<td>0.25(3)</td>
<td>0.092(9)</td>
</tr>
<tr>
<td>Cd8</td>
<td>Cd</td>
<td>-1.25</td>
<td>-1.3678(11)</td>
<td>0.5344(11)</td>
<td>0.088(8)</td>
<td>0.069(5)</td>
</tr>
<tr>
<td>Cd9</td>
<td>Cd</td>
<td>-1.25</td>
<td>-1.5</td>
<td>0.269(3)</td>
<td>0.046(9)</td>
<td>0.069(12)</td>
</tr>
<tr>
<td>Cd9A</td>
<td>Cd</td>
<td>-1.25</td>
<td>-1.5</td>
<td>0.303(3)</td>
<td>0.037(11)</td>
<td>0.051(12)</td>
</tr>
</tbody>
</table>