# Report for {{ cif.block.name }}, Single Crystal X-ray Structure Determination

A {{crystal\_colour}} {{crystal\_shape}} shaped crystal of sample {{cif.block.name}} with formula {{ sum\_formula }} having approximate dimensions of {{crystal\_size}} mm was mounted on a Mitegen micromesh mount in a random orientation. Data were collected from a shock-cooled single crystal at {{cif.\_diffrn\_ambient\_temperature}} K on {{diffr\_type|inv\_article}} {{diffr\_type}} {{diffr\_device}} with {{diffr\_source|inv\_article}} {{diffr\_source}} using a {{monochromator}} as monochromator and {{detector|inv\_article}} {{detector}} detector. The diffractometer {% if lowtemp\_dev %}was equipped with {{lowtemp\_dev|inv\_article}} {{lowtemp\_dev}} low temperature device and {%endif%}used {{radiation}} radiation {%if wavelength%}(λ = {{wavelength}} Å){%endif%}. All data were integrated with {{integration\_progr}} and a {{abstype}} absorption correction using {{abs\_details}} was applied. [{{literature.integration|ref\_num}},{{literature.absorption|ref\_num}}] The structure was solved by {{solution\_method}} methods with {{solution\_program}} and refined by full-matrix least-squares methods against *F*2 using {{refinement\_prog}}.[{{literature.solution|ref\_num}},{{literature.refinement|ref\_num}}] All non-hydrogen atoms were refined with anisotropic displacement parameters. {%if cif.hydrogen\_atoms\_present%}Carbon and boron bound hydrogen atoms, alcohol hydroxyl H atoms, H atoms of planar (sp2 hybridized) N-H, N-H+ and NH2 groups and ammonium H atoms were refined isotropically on calculated positions using a riding model. Methyl CH3, ammonium NH3+ and hydroxyl H atoms were allowed to rotate but not to tip to best fit the experimental electron density. Positions of pyramidal (sp3 hybridized) amine H atoms and water H atoms were refined isotropically, X-H and H…H distances were restrained to expected target values and were further restrained based on hydrogen bonding considerations. *U*iso values were constrained to 1.5 times the *U*eq of their pivot atoms for methyl, hydroxyl and ammonium NH3+ groups and 1.2 times for all other hydrogen atoms. {%endif%}

## {% if refinement\_details %}

{{ refinement\_details }}

{% endif %}

This report and the CIF file were generated using FinalCif. [{{literature.finalcif|ref\_num}}]

## Bibliography

{%p for num, ref in references.items() %}

[{{ num|e }}]{{ “\t” }}{{ ref.richtext|e}}

{%p endfor %}

## Table 1 Crystal data and structure refinement for {{ cif.block.name }}

|  |  |
| --- | --- |
| Empirical formula | {{ sum\_formula }} |
| Formula weight | {{cif.\_chemical\_formula\_weight }} |
| Temperature [K] | {{cif.\_diffrn\_ambient\_temperature}} |
| Crystal system | {{ cif.\_space\_group\_crystal\_system }} |
| Space group (number) | {{p space\_group}} {{ itnum }} |
| *a* [Å] | {{cif.\_cell\_length\_a }} |
| *b* [Å] | {{cif.\_cell\_length\_b }} |
| *c* [Å] | {{cif.\_cell\_length\_c }} |
| α [°] | {{cif.\_cell\_angle\_alpha }} |
| β [°] | {{cif.\_cell\_angle\_beta }} |
| γ [°] | {{cif.\_cell\_angle\_gamma }} |
| Volume [Å3] | {{cif.\_cell\_volume}} |
| *Z* | {{cif.\_cell\_formula\_units\_Z}} |
| *ρ*calc [gcm−3] | {{cif.\_exptl\_crystal\_density\_diffrn}} |
| *μ* [mm−1] | {{cif.\_exptl\_absorpt\_coefficient\_mu}} |
| *F*(000) | {{cif.\_exptl\_crystal\_F\_000}} |
| Crystal size [mm3] | {{crystal\_size}} |
| Crystal colour | {{crystal\_colour}} |
| Crystal shape | {{crystal\_shape }} |
| Radiation | {{radiation}}{%if wavelength%} (λ={{wavelength}} Å){%endif%} |
| 2θ range [°] | {{theta\_range}} |
| Index ranges | {{index\_ranges}} |
| Reflections collected | {{cif.\_diffrn\_reflns\_number}} |
| Independent reflections | {{indepentent\_refl}}*R*int = {{r\_int}}*R*sigma = {{r\_sigma}} |
| Completeness{%if theta\_full%} to θ = {{theta\_full}}°{%endif%} | {{completeness}} |
| Data / Restraints / Parameters | {{data}} / {{restraints}} / {{parameters}} |
| Goodness-of-fit on *F*2 | {{ goof }} |
| Final *R* indexes [*I*≥2σ(*I*)] | *R*1 = {{ls\_R\_factor\_gt}}w*R*2 = {{ls\_wR\_factor\_gt}} |
| Final *R* indexes [all data] | *R*1 = {{ls\_R\_factor\_all}}w*R*2 = {{ls\_wR\_factor\_ref}} |
| Largest peak/hole [eÅ−3] | {{diff\_dens\_max}}/{{diff\_dens\_min}} |
| {%tr if exti %} |  |
| Extinction coefficient | {{exti}} |
| {%tr endif %} |  |
| {%tr if flack\_x %} |  |
| Flack X parameter | {{flack\_x}} |
| {%tr endif %} |  |

## {%p if atomic\_coordinates %}

## Table 1 Atomic coordinates and Ueq [Å2] for {{ cif.block.name }}

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Atom** | ***x*** | ***y*** | ***z*** | ***U*eq** |
| {%tr for atom in atomic\_coordinates %} |  |  |  |  |
| {{ atom.label }} | {{ atom.x }} | {{ atom.y }} | {{ atom.z }} | {{ atom.u\_eq }} |
| {%tr endfor %} |  |  |  |  |

*U*eq is defined as 1/3 of the trace of the orthogonalized *Uij* tensor.

{%p endif %}

{%p if displacement\_parameters %}

## Table 1 Anisotropic displacement parameters (Å2) for {{ cif.block.name }}. The anisotropic displacement factor exponent takes the form: −2π2[*h*2*(a\*)*2*U*11*+ k*2*(b\*)*2*U*22 + … + *2hka\*b\*U*12 ]

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Atom** | ***U*11** | ***U*22** | ***U*33** | ***U*23** | ***U*13** | ***U*12** |
| {%tr for atom in displacement\_parameters %} |  |  |  |  |  |  |
| {{ atom.label }} | {{ atom.U11 }} | {{ atom.U22 }} | {{ atom.U33 }} | {{ atom.U23 }} | {{ atom.U13 }} | {{ atom.U12 }} |
| {%tr endfor %} |  |  |  |  |  |  |

{%p endif %}

{%p if bonds %}

## Table 1 Bond lengths and angles for {{ cif.block.name }}

|  |  |
| --- | --- |
| **Atom–Atom** | **Length [Å]** |
| {%tr for b in bonds %} |  |
| {{ b.atoms }} | {{ b.dist }} |
| {%tr endfor %} |  |
|  |  |
| **Atom–Atom–Atom** | **Angle [°]** |
| {%tr for a in angles %} |  |
| {{ a.atoms }} | {{ a.angle }} |
| {%tr endfor %} |  |

{%r if options.without\_h %}Bonds and angles to hydrogen atoms were omitted.

{%r endif %}{% if ba\_symminfo %}{{r ba\_symminfo }}{% endif %}

{%p endif %}

{%p if torsions%}

## Table 1 Torsion angles for {{ cif.block.name }}

|  |  |
| --- | --- |
| **Atom–Atom–Atom–Atom** | **Torsion Angle [°]** |
| {%tr for t in torsions %} |  |
| {{ t.atoms }} | {{ t.angle }} |
| {%tr endfor %} |  |

{%r if options.without\_h %}Bonds and angles to hydrogen atoms were omitted.

{%r endif %}{% if torsion\_symminfo %}{{r torsion\_symminfo }}{% endif %}

{%p endif %}

{%p if hydrogen\_bonds %}

## Table 1 Hydrogen bonds for {{ cif.block.name }}

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **D–H⋯A [Å]** | **d(D–H) [Å]** | **d(H⋯A) [Å]** | **d(D⋯A) [Å]** | **<(DHA) [°]** |
| {%tr for h in hydrogen\_bonds %} |  |  |  |  |
| {{h.atoms}} | {{h.dist\_dh}} | {{h.dist\_ha}} | {{h.dist\_da}} | {{h.angle\_dha}} |
| {%tr endfor %} |  |  |  |  |

{% if hydrogen\_symminfo %}{{r hydrogen\_symminfo }}{% endif %}

{%p endif %}