Structure Tables

{% if structure\_figure%}{{structure\_figure}}{%endif%}

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

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

{% if options.atoms\_table %} 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.

**{% endif %}{% 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 %} |  |  |  |  |  |  |

{% endif %}{% if options.bonds\_table %}{%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 %} |  |

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

{{ ba\_symminfo}}{%endif%}{%endif%}

{% endif %}{%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 %} |  |

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

{{ torsion\_symminfo}}{%endif%}{%endif%}

{% if options.hydrogen\_bonds and 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%}{{hydrogen\_symminfo}}{%endif%}{%endif%}