# Structure Tables

|  |  |  |  |
| --- | --- | --- | --- |
|  | {%tc for block in blocklist %} | **{{ block.name }}** | {%tc endfor %} |
| CCDC number | {%tc for block in blocklist %} | {{ block.cif.\_database\_code\_depnum\_ccdc\_archive }} | {%tc endfor %} |
| Empirical formula | {%tc for block in blocklist %} | {{ block.sum\_formula }} | {%tc endfor %} |
| Formula weight | {%tc for block in blocklist %} | {{block.cif.\_chemical\_formula\_weight }} | {%tc endfor %} |
| Temperature [K] | {%tc for block in blocklist %} | {{block.cif.\_diffrn\_ambient\_temperature}} | {%tc endfor %} |
| Crystal system | {%tc for block in blocklist %} | {{ block.cif.\_space\_group\_crystal\_system }} | {%tc endfor %} |
| Space group (number) | {%tc for block in blocklist %} | {{p block.space\_group}} {{ block.itnum }} | {%tc endfor %} |
| *a* [Å] | {%tc for block in blocklist %} | {{block.cif.\_cell\_length\_a }} | {%tc endfor %} |
| *b* [Å] | {%tc for block in blocklist %} | {{block.cif.\_cell\_length\_b }} | {%tc endfor %} |
| *c* [Å] | {%tc for block in blocklist %} | {{ block.cif.\_cell\_length\_c }} | {%tc endfor %} |
| α [°] | {%tc for block in blocklist %} | {{ block.cif.\_cell\_angle\_alpha }} | {%tc endfor %} |
| β [°] | {%tc for block in blocklist %} | {{ block.cif.\_cell\_angle\_beta }} | {%tc endfor %} |
| γ [°] | {%tc for block in blocklist %} | {{ block.cif.\_cell\_angle\_gamma }} | {%tc endfor %} |
| Volume [Å3] | {%tc for block in blocklist %} | {{ block.cif.\_cell\_volume}} | {%tc endfor %} |
| *Z* | {%tc for block in blocklist %} | {{ block.cif.\_cell\_formula\_units\_Z}} | {%tc endfor %} |
| *ρ*calc [gcm−3] | {%tc for block in blocklist %} | {{ block.cif.\_exptl\_crystal\_density\_diffrn}} | {%tc endfor %} |
| *μ* [mm−1] | {%tc for block in blocklist %} | {{ block.cif.\_exptl\_absorpt\_coefficient\_mu}} | {%tc endfor %} |
| *F*(000) | {%tc for block in blocklist %} | {{ block.cif.\_exptl\_crystal\_F\_000}} | {%tc endfor %} |
| Crystal size [mm3] | {%tc for block in blocklist %} | {{ block.crystal\_size}} | {%tc endfor %} |
| Crystal colour | {%tc for block in blocklist %} | {{ block.crystal\_colour}} | {%tc endfor %} |
| Crystal shape | {%tc for block in blocklist %} | {{ block.crystal\_shape }} | {%tc endfor %} |
| Radiation | {%tc for block in blocklist %} | {{ block.radiation}}{%if block.wavelength%} (λ={{ block.wavelength}} Å){%endif%} | {%tc endfor %} |
| 2θ range [°] | {%tc for block in blocklist %} | {{ block.theta\_range}} | {%tc endfor %} |
| Index ranges | {%tc for block in blocklist %} | {{ block.index\_ranges}} | {%tc endfor %} |
| Reflections collected | {%tc for block in blocklist %} | {{ block.cif.\_diffrn\_reflns\_number}} | {%tc endfor %} |
| Independent reflections | {%tc for block in blocklist %} | {{ block.indepentent\_refl}}  *R*int = {{ block.r\_int}} *R*sigma = {{ block.r\_sigma}} | {%tc endfor %} |
| Completeness{%if theta\_full%} to  θ = {{theta\_full}}°{%endif%} | {%tc for block in blocklist %} | {{ block.completeness }} | {%tc endfor %} |
| Data / Restraints / Parameters | {%tc for block in blocklist %} | {{block.data}} / {{ block.restraints}} / {{block.parameters}} | {%tc endfor %} |
| Absorption correction Tmin/Tmax (method) | {%tc for block in blocklist %} | {{ block.t\_min }} / {{ block.t\_max }} ({{ block.cif.\_exptl\_absorpt\_correction\_type or ‘?’ }}) | {%tc endfor %} |
| Goodness-of-fit on *F*2 | {%tc for block in blocklist %} | {{ block.goof }} | {%tc endfor %} |
| Final *R* indexes  [*I*≥2σ(*I*)] | {%tc for block in blocklist %} | *R*1 = {{ block.ls\_R\_factor\_gt}} w*R*2 = {{ block.ls\_wR\_factor\_gt}} | {%tc endfor %} |
| Final *R* indexes  [all data] | {%tc for block in blocklist %} | *R*1 = {{ block.ls\_R\_factor\_all}} w*R*2 = {{ block.ls\_wR\_factor\_ref}} | {%tc endfor %} |
| Largest peak/hole [eÅ−3] | {%tc for block in blocklist %} | {{ block.diff\_dens\_max}}/{{ block.diff\_dens\_min}} | {%tc endfor %} |
| Extinction coefficient | {%tc for block in blocklist %} | {{ block.exti or "---"}} | {%tc endfor %} |
| Flack X parameter | {%tc for block in blocklist %} | {{ block.flack\_x or "---"}} | {%tc endfor %} |