For publications, a summary of experimental details is normally required (often as part of the “supporting information”).

Data from the first page of the docx document supplied with the results of the structure determination should be entered into the template given below. “#” is to be replaced as appropriate.

To safeguard from automatic font substitution operational in some word processors please compare to the authentic picture of such a table on the last page.

Please note greek letters („Symbol” font) and typeface conventions (italics) for certain parameters. Add/delete columns as required. A smaller font size and/or landscape page layout may be used.

Correct format for space group (Hermann-Mauguin) symbols:

<Bravais type><list of principal symmetry elements>

where

<Bravais type> = *P*, (*A*, *B*,) *C*, *I*, *F*, *R* (in *italics*)

<symmetry elements>

 inversion centre: -1

 axes (proper): 1, 2, 3, 4, 6; (screw): 21, 31, 32, 41 etc.;

 (inversion): -1, -2, -3 etc.

 mirror planes *m*;

 glide planes *a*, *b*, *c*, *n*, *d*

Examples: *P* 41/*nmc* *F* *dd*2 *P* -421*m*

**Table #.** Details of the crystal structure determinations of ...

|  | **#** | **#** | **#** |
| --- | --- | --- | --- |
| formula |  |  |  |
| crystal system |  |  |  |
| space group |  |  |  |
| *a* /Å |  |  |  |
| *b* /Å |  |  |  |
| *c* /Å |  |  |  |
| ** /° |  |  |  |
| ** /° |  |  |  |
| ** /° |  |  |  |
| *V* /Å3 |  |  |  |
| *Z* |  |  |  |
| *M*r |  |  |  |
| *F*000 |  |  |  |
| *d*c /gcm-3 |  |  |  |
|  /mm-1 |  |  |  |
| max., min. transmission factors |  |  |  |
| X-radiation, ** /Å | Mo-*K*, 0.71073 Cu-*K*, 1.54184 | Mo-*K*, 0.71073 Cu-*K*, 1.54184 | Mo-*K*, 0.71073 Cu-*K*, 1.54184 |
| data collect. temperat. /K |  |  |  |
| ** range /° |  |  |  |
| index ranges  *h*,*k*,*l* |  |  |  |
| reflections measured |  |  |  |
|  unique [*R*int] |  |  |  |
|  observed [*I***≥**2(*I*)] |  |  |  |
| data / restraints /parameters |  |  |  |
| GooF on *F*2 |  |  |  |
| *R* indices [*F*>4(*F*)] *R*(*F*), *wR*(*F*2) |  |  |  |
| *R* indices (all data) *R*(*F*), *wR*(*F*2) |  |  |  |
| absolute structure parameter |  |  |  |
| largest residual peaks /eÅ-3 |  |  |  |

Example

