# IORTEP

## A Crystallographic Plotting Program

Fortran version by Carroll K. Johnson, 1976 Interactive version by G. C. Lisensky, 2003-2022

To plot a crystal structure you need to enter values for

- the unit cell dimensions (axes in Å, angles in degrees),
- the space group symmetry (equivalent positions and centering),

• a unique name, fractional coordinates and thermal parameters for each atom.

*Example.* Consider the structure of cubane. C<sub>8</sub>H<sub>8</sub> crystallizes in space group  $R\overline{3}$  with unit cell dimensions 5.34 Å and 72.26°. The fractional coordinates are:

Atom	X	У	Z
C1	18711	0.19519	0.10706
C2	0.11546	0.11546	0.11546
H1	32460	0.34680	0.18480
H2	0.21000	0.21000	0.21000

#### Parameters to enter data.

	Parameters	
Title	Space	ce Group
Unit Cell Dimensions. Use Ångstrom (1	00 pm) and degree values.	New
a 0 b 0 c	α 0.0000 β 0.0000 γ 0.0000	Close
Equivalent Positions	Interpreted Symmetry Matrices	s
x, y, z	Equivalent position transformations in matrix T1 R11 R12 R13 x Transform (T2) + (R21 R22 R23) (y) = (Transform T3 R31 R32 R33 z Transform will be listed in the order T1 R11 R12 R13 T2 R21 R22 R23 T3 R3	form, ed x ed y ) ed z 1 R32 R33
Centering Position (such as .	5,.5,0 for a C-centered lattice):	► Interpret
Fractional Coordinates (name, x, y, z, iso	tropic U, comments) Interpreted Fraction	nal Coordinates
Import CIF file Move H to end	Other commands are easier if the coordinate list is sorted by elements.	Include anisotropic Uij

• You can use any text you want for title and space group, but actual names are helpful.

• Press TAB to go from one entry to the next. Click Close when all values are entered.

• Centering positions will be added to the equivalent positions when you click Interpret.

- If you paste text, use Interpret to see if extra characters are correctly removed.
- Remember to Save you work occasionally so you can use Load to continue your work.



Individual atoms are referred to by an ATOM DESIGNATOR CODE:

- The last two digits refer to the symmetry equivalent positions in the order entered.
- The next three digits refer to translations along the *abc* directions, each digit referring to one axis direction. Examples:

555 is no movement,

655 is one unit cell translation along a,

554 is minus one unit cell translation along c, and

656 is one unit cell translation along both *a* and *c*.

• The remaining digit(s) refer to the atoms in the order entered.

Thus 1256504 (think of this as 12 565 04) is the twelfth atom in the original atom list operated on the fourth symmetry element in the equivalent positions list, followed by translation of one unit cell along b.

Sets of atoms are described by atom RUNS.

For example, from 1 to 3 indicates 155501, 255501, 355501.

From 154501 to 365503 thus indicates

154501, 254501, 354501,	155501, 255501, 355501,	165501, 265501, 365501,
154502, 254502, 354502,	155502, 255502, 355502,	165502, 265502, 365502,
154503, 254503, 354503,	155503, 255503, 355503,	165503, 265503, 365503.

What are the bond distances and angles in the molecule?

#### Distances

**Angles** is similar (but use distances first to make sure you are not finding too many values.)

	Distances							
Any atoms in distance of a	Any atoms in the target-run that are within the given distance of any atoms in the origin-run will be used.							
Use the full a ORIGIN atom	Use the full atom designator code to specify ORIGIN atoms (assumed to be 55501 if not given).							
There are 4 a	atoms and 6 sym	metry elem	ents.					
Which atoms	belong to the O	RIGIN-run?						
From atom	155501	to atom	455501					
Which atoms	belong to the T	ARGET-run?	,					
From atom	1	to atom	4					
Maximum dis	atance 2	Å	ngstroms (100 pm) e Distances					

			CODE	x	У	Z					
Distance	fro	m (	155501)	-0.1871,	0.1952,	0.1071	to	1 thru	4		
C1	H1	(	355501)	-0.3246,	0.3468,	0.1848	is	1.0118	Å	(100	pm)
C1	C1	(	155505)	-0.1071,	0.1871,	-0.1952	is	1.5493	Å	(100	pm)
C1	C1	(	155506)	-0.1952,	-0.1071,	0.1871	is	1.5493	Å	(100	pm)
C1	C2	(	255501)	0.1155,	0.1155,	0.1155	is	1.5515	Å	(100	pm)
			CODE	х	У	Z					
Distance	fro	m(	255501)	0.1155,	0.1155,	0.1155	to	1 thru	4		
C2	Н2	(	455501)	0.2100,	0.2100,	0.2100	is	1.1093	Å	(100	pm)
C2	C1	(	155502)	0.1071,	-0.1871,	0.1952	is	1.5515	Å	(100	pm)
C2	C1	(	155503)	0.1952,	0.1071,	-0.1871	is	1.5515	Å	(100	pm)
									-		

Print Window will print the values you find.

#### Load to resume your work later. (Use Inventory to see this page again.)

			iORTEP			
Parameters	Inventory	Distances	Choose	Bond	Graph	Quick Start
Load	Save	Angles	Kind	Orient	Print Window	Key
Cell paramet 5.34, 5.34, Origin for p Orthonormal x vector, 0.18726592 0.0000000 Symmetry mai T1 R: 1).0000 2).0000 4).0000 - 5).0000 6).0000 Atoms: name 1) Cl 2) C2 3) H1 4) H2 Selected ato Bond instruct	ters: 5.34, 72.25999 projection axis reference vect y vector, , -0.06486512, , 0.19001204, trices for spac 11 R12 R13 1x 0y 02 .0 0x 0y 1z .0 0x 0y 1z .0 0x 1y 02 .0 0x 0y -1z .0 0x 0y 02 .0 0x 0y 00 .0 0x 00 .	<pre>, 72.25999, 72.25 in crystal coord ors based on crys z vector 0.04014409 -0.20090899 0.06915873 e group R3bar T2 R21 R22 R23 000 0x 1y 0z 000 1x 0y 0z 000 0x 0y 1z 000 0x -1y 0z 000 0x 0y -1z z colo 519 0.10706 colo 546 0.11546 colo 680 0.18480 colo 000 0.21000 colo</pre>	999 inates: 0.00000 tal axes: T3 R31 R32 1 .0000 0x 0y .0000 0x 1y .0000 1x 0y .0000 0x 0y .0000 0x -1y .0000 -1x 0y or type r 1 shaded quad r 1 shaded quad r 4 hollow r 4 hollow	<pre>, 0.00000, 0.00 R33 1z 0z 0z -1z 0z 0z 0z comments</pre>	000	

**Choose** to select the atoms to be plotted. If no atoms are selected then none will be plotted.

	Choose						
Which method t Atom Number	o select atoms to s	be plotted?					
Choose	Remove						
Distances							
Choose	Remove	Grow					
Unit Cell							
Choose	Choose Remove Save before trying Unit Cell						
	Clear All	Close					
	Choose						
Any atoms in the ru	n will be used.						
Use the full atom de atoms (assumed to There are 4 atoms a	esignator code to spe be 55501 if not give and 6 symmetry elem	ecify Help n). nents.					
Which atoms should From atom 15550	d be added? )1 to atom	455501					
	Clo	se Choose					

```
Choose (Atom numbers)
```

```
Selected atoms: 155501, 255501, 355501, 455501
```

Save frequently so you can revert back if something unexpected happens. ORTEP parameter files are very small.

1	Grow					
	Grow selects atoms within the specified distance of previously selected atoms.					
Choose (Grow) to find the rest of the molecule.	Translations and symmetry are ignored for ORIGIN atoms so the selection can propagate.					
The distance must be	There are 4 atoms and 6 symmetry elements.					
additional molecules.	Which atoms belong to the ORIGIN-run?					
(Not recommended for	From atom 155501 to atom 455501					
polymers!)	Which atoms belong to the TARGET-run?					
	From atom 1 to atom 4					
	Maximum distance       2       Ångstroms (100 pm)         Use distances command first to decide maximum bond distance.       Close       Grow					

```
Selected atoms:
155501, 255501, 355501, 455501, 155505, 155506, 155502, 155503
255504, 355505, 355506, 355502, 155504, 355503, 455504, 355504
```

**Orient (Best Plane)** makes the view plane the least squares best plane for the molecule. This often provides an excellent orientation.

**Orient (Rotate)** is useful for adjusting the orientation. Try 5 or 10 degrees and repeatedly press RETURN for small adjustments.



The origin atom is the in-plane center of the plot. 0 is usually the best choice but you might want to rotate around a central metal atom instead.

The orientation is saved in the ORTEP file; save a file for each view you wish to keep.

#### Orient (Vectors) to specify the exact view.

	Orient by Vectors
The coordinate system will b The first vector will be the h The second vector forms a p The plotted plane can be eit	be specified by means of two vectors. orizontal axis. blane with the first vector. her parallel or perpendicular to the chosen plane. Plotted plane
REFERENCE VECTORS	Perpendicular     O     Parallel
screen horizontal along screen vertical along vert out of screen along vect	vector U U ector U x V (U x V) x U cor U x (U x V) U x V
Parallel First vector	U Second Vector V Plotted plane
Example 155501 to 165	501 155501 to 156501 ab
Help 155501 to 156	5501 155501 to 155601 bc
Vector U origin 155501	Vector U terminus 165501
Vector V origin 155501	Vector V terminus 156501
	Cancel

**Bond** defines the bonds in the molecule. You should previously have used the **Distances** command so you have some idea of what distances to call a bond.

You will normally need to have different commands to specify distances for metals and ligands, for carbons, and for hydrogen.

It is often useful to indicate coordination bonds by using a 2-line bond and covalent bonds by using more lines.

If solid color is selected, the background of the bond will be the chosen color; if solid color is not selected the lines themselves will be the chosen color.

Bond instructions

1) From atoms 1 thru 2 to 1 thru 4 within 0.9 thru 2.0 Å, connected with 0.04 Å radius bond of 6 lines of color 2.

Any atoms in the target-run that are within the given distance of any atoms in the origin-run will be connected. Use only the atom number to specify atoms (all symmetries will be used). There are 4 atoms. Which atoms belong to the ORIGIN-run?

Edit bond instruction 1

From atom	1		to atom	2	2			
Which atoms belong to the TARGET-run?								
From atom	1		to atom	1	4			
Maximum dist	ance	2		Ån	Ångstroms (100 pm)			
Minimum dista	ance	0.9		Ån	gstroms	(100	pm)	
Bond radius (try values 0.04 Ångstroms (100 pm) between .01 and .06)?								
Number of line each bond (2-	es for 6)?	5			lines	coord 5 fo	lination and r covalent.	
Bond Color								
•	$\bigcirc$	0						
Solid color with black lines Close Change								

**Kind** selects the atom types and colors.

To show the ellipses you need to enter anisotropic thermal parameters on the parameter pages.

If solid color is selected, the body of the atom will be the chosen color; if solid color is not selected the lines themselves will be the chosen color.

You should make every element a different color or style. Key can be used to provide a legend to go with Graph.

Atoms:

1)

2)

3)

4)

Graph

Name

Code

name

Perspective

C1

C2

Η1

Н2



Hint: You can have many command windows open and changes in one will update the other windows. If things seem slow, try having fewer windows open.

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