

3. CIF DATA DEFINITION AND CLASSIFICATION

Table 3.1.7.1. Abbreviations in CIF data names

Terms for which abbreviations are defined are sometimes found unabbreviated.

Abbreviation	Term	Abbreviation	Term	Abbreviation	Term
abbrev	abbreviation	eqn	equation	oper	operation
abs	absolute (configuration, not structure)	esd	standard uncertainty (estimated standard deviation) (<i>see su</i>)	org	organism
absorpt	absorption			orient	orientation
alt	alternative	expt	experiment	origx	orthogonal coordinate matrix (PDB files)
amp	amplitude	exptl	experimental	os	operating system
AN	accession number	fom	figure of merit	param	parameter
anal	analyser	fract	fractional	pd	powder diffraction
aniso	anisotropic*	Fsqd	<i>F</i> squared	PDB	Protein Data Bank
anisotrop	anisotropic*	gen	generation	PDF	Powder Diffraction File
anom	anomalous	gen	generator	perp	perpendicular
ASTM	American Society for Testing and Materials	gen	genetic	phos	phosphate
asym	asymmetric	geom	geometric	pk	peak
atten	attenuation	H-M	Hermann–Mauguin	polarisn	polarization
au	arbitrary units	ha	heavy atom	poly	polymer
auth	author	hbond	hydrogen bond	pos	position
av	average	hist	history	prep	preparation
ax	axial	horiz	horizontal	proc	processed
B	<i>B</i> form of atomic displacement parameter (a.d.p.)	I	intensity	prof	profile
		ICSD	Inorganic Crystal Structure Database	prot	protein
backgd	background*	id	identifier	ptnr	partner
beg	begin	illum	illumination	publ	publication
bg	background*	imag	imaginary	R	agreement index
biol	biology	inc	increment	rad	radius
bkg	background*	incl	include	recd	received
bond	bonding	info	information	recip	reciprocal
Bsol	<i>B</i> form of a.d.p. for solvent	instr	instrument	ref	reference
calc	calculated	Int	international	refine	refinement
calib	calibration (pd)	ISBN	International Standard Book Number	refln	reflection
cartn	Cartesian	iso	isotropic	reflns	reflections
CAS	<i>Chemical Abstracts Service</i>	iso	isomorphous	res	resolution
char	characterization (pd)	ISSN	International Standard Serial Number	restr	restraints
chem	chemical	IUCr	International Union of Crystallography	rev	revision
chir	chirality	IUPAC	International Union of Pure and Applied Chemistry	Rmerge	agreement index of merging
clust	cluster			rms	root mean square
coef	coefficient	len	length	rot	rotation
com	common	lim	limit	S	goodness of fit
comp	component	loc	lack of closure	samp	sample
conc	concentration	ls	least squares	scat	scattering factor
conf	conformation	max	maximum	seq	sequence
config	configuration	MDF	Metals Data File	sigl	$\sigma(I)^*$
conform	conformant	meanI	mean intensity	sigmaI	$\sigma(I)^*$
conn	connectivity	meas	measured	sint	$\sin \theta$
cons	constant	mid	middle (between max and min)	sint/lambda	$\sin(\theta)/\lambda^*$
CSD	Cambridge Structural Database	min	minimum	sol	solvent
db	database	mod	modification	spec	specimen
defn	definition	mods	modifications	src	source
detc	detector	mon	monomer	std	standard
der	derivative	monochr	monochromator (pd)*	stol	$\sin(\theta)/\lambda^*$
dev	standard deviation	mono	monochromator (pd)*	struct	structure
dict	dictionary	nat	natural	su	standard uncertainty
dif	difference*	NBS	National Bureau of Standards (now National Institute of Standards and Technology)	suppl	supplementary
diff	difference*			sys	systematic
diffr	diffractometer			tbar	mean path length
diffm	diffraction	NCA	number of connected atoms	temp	temperature
displace	displacement	ncs	noncrystallographic symmetry	tor	torsion angle
dist	distance	netI	net intensity	tran	transformation*
divg	divergence	NH	number of connected hydrogen atoms	transf	transformation*
dom	domain	nha	non-hydrogen atoms	transform	transformation*
dtime	deadtime	norm	normal	tvect	translation vector (PDB files)
ens	ensemble	nst	nonstandard	vert	vertical
eq	equatorial*	nucl	nucleic acid	wR	weighted agreement index
equat	equatorial*	num	number	wt	weight
equiv	equivalent	obs	observed		

* Terms with multiple definitions.

It is clear that the location specified for the local dictionary is only meaningful for applications running on the same computer or network, and therefore the ability to validate against this local dictionary is not portable. On the other hand, it may be that the local data names used by the authors of this CIF are not intended to have meaning outside their own laboratory.

3.1.8.2. The dictionary register

COMCIFS maintains a register of dictionaries known to it, including the identifying name and version strings within those dictionaries. The register also includes the location of each dictionary, expressed at present as a URL designed to allow retrieval

by file transfer protocol (ftp) from the IUCr server. Changes in the location of a particular dictionary file can be made by modifying the entry in the register, avoiding the problem of specifying a URL in a data file that would then become outdated if the dictionary was moved. Dictionary applications can consult the register (according to a protocol outlined below) to locate and retrieve the dictionaries needed for validating data files. It is of course essential that the validation software knows how to locate the register. The location is at present given by the URL <ftp://ftp.iucr.org/pub/cifdics/cifdic.register>.

The problem of changing URLs has therefore not disappeared completely, but is at least confined to the need to maintain one single address.