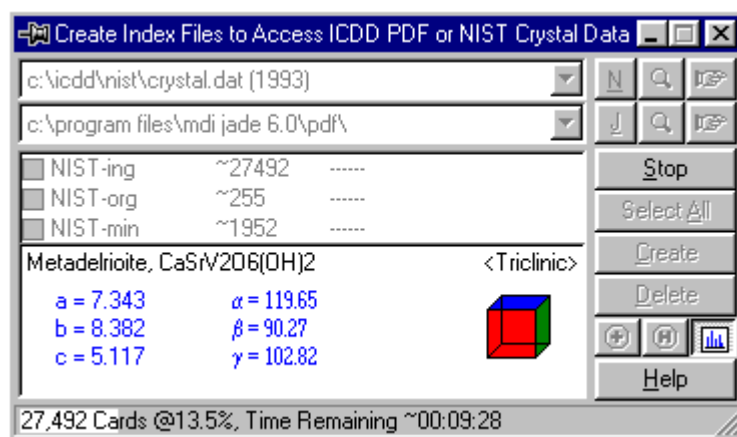



## NIST Crystal Data Access and Retrieval

NIST Crystal Data is a crystal structure database which contains about 200,000 entries of inorganic and organic phases with crystallographic information such as space groups and unit cells as well as literature references. Unlike FIZ ICSD database, there are no atomic coordinates in NIST Crystal Data, and unlike ICDD PDF there are no d-I line lists either for powder XRD patterns. Despite the absence of those two types of informations, you may still find this database useful, for example, in finding structure types and lattice constants for [Cell Refinement](#), [Whole Pattern Fitting](#), and [Rietveld refinement](#). For these reasons, Jade 6 supports this database by providing database indexing and retrieval tools like those for PDF. To create the index files if you have a copy of the crystal data, you need to bring up the [PDF Indexing](#) dialog from the 'PDF | Setup...' menu as shown below,



and select the 'crystal.dat' file on the database list. If it's not on the list, you can click the  button to ask Jade to find it on your PC. When you click the 'Create' button, Jade would then create three subfiles named 'NIST-ing' for the inorganic phases, 'NIST-org' for the organics, and 'NIST-min' for the minerals. These subfiles, which are hereafter referred to as CDF subfiles, could then be selected like any of the PDF subfiles for Boolean retrievals implemented in Jade. An example of a Boolean retrieval of CDF subfile 'NIST-min' is given below:

30 Hits Sorted...	Chemical Form...	PDF-#	CSD#	J	D	P.S.	Space Group	a	b	c
Boehmite	AlOOH	02+8655	NIST	N	X	oA	Amam (63)	3.910	12.780	2.950
Boehmite	AlOOH	00+5011	NIST	N	X	o?		3.790	11.800	2.860
Corundum	Al <sub>2</sub> O <sub>3</sub>	90+2460	NIST	N	X	hR	R-3c (167)	4.756	4.756	12.980
Corundum	Al <sub>2</sub> O <sub>3</sub>	90+1280	NIST	N	X	hR	R-3c (167)	4.758	4.758	12.991
Corundum	Al <sub>2</sub> O <sub>3</sub>	02+5154	NIST	N	X	hR	R-3c (167)	4.760	4.760	13.000
Diaspore	AlOOH	03+3636	NIST	N	X	oP	Pbnm (62)	4.401	9.421	2.845
Diaspore	AlOOH	03+0204	NIST	N	X	oP	Pbnm (62)	4.440	9.380	2.810
Diaspore	AlOOH	01+9094	NIST	N	X	o?		4.360	9.380	2.830
Diaspore	AlOOH	03+2534	NIST	N	X	oP	Pbnm (62)	4.410	9.400	2.840
Diaspore	AlOOH	01+9095	NIST	N	X	oP	Pbnm (62)	4.396	9.426	2.844

Notice that beside the 'N' and 'NIST-CD' designations in the 'J' and 'CSD#' columns, Jade uses the '+' sign (e.g. 03+0108 instead of 03-0108) in the 'PDF-#' column to indicate a CDF phase. That's because these CDF numbers may duplicate the PDF numbers and you can have a mix of both PDF and CDF phases on the same list. This subtle differentiation is also necessary if you want to save a list of hits into an \*.who/own file and restore them in the future.

Since there are no d-I list data in the crystal data, neither can you overlay d-I lists in the zoom window like you could with the PDF, nor can you perform search/match with these CDF subfiles. However, Jade will compute a list of possible reflections when you click a hit on the above dialog, and display them in the zoom window as a set of line markers for phase comparison. You can also bring up the [Calculate d-Spacing](#) and the [XRD Simulation](#) dialogs if you want to see a detailed listing of reflections from the desired unit cell.

In addition to the Boolean retrievals from CDF subfiles, you can search the entire crystal data by their literature references. See the [PDF Retrieval by Literature References](#) topic for more information.