Results and conclusions of the internet based "Search/match round robin 2002"

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To test the effectiveness of phase identification software, a two-stage search/match round robin using powder X-ray diffraction data was organized, through the internet and world wide web. The first stage provided powder patterns and a vague sample origin, the second stage provided the chemistry and sample history. While the statistics are not robust, it shows that routine phase identification without chemistry can be performed, providing effective modern third generation search/match software is used; the most up to date databases are available; and well trained, experienced scientists perform the analysis. © *2003 International Centre for Diffraction Data.* [DOI: 10.1154/1.1557031]

I. INTRODUCTION

Phase identification from powder X-ray diffraction data is an important and widely used method for qualitative analysis (applied in inorganic, organometallic and organic chemistry, mineralogy, geology, metallurgy, archeometry, criminology, etc). A review is given by Jenkins and Snyder (1996), including historical aspects and description of three generations of search/match algorithms. Manual search/match methods (Hanawalt, 1986 and references therein) show their limits as soon as several major complex phases are mixed, and owing to the fact that the Powder Diffraction File (PDF) will contain close to 300 000 phases, by 2003. Samples from geological or laboratory origin may well be mixtures of two to four major complex phases if not more, and they would be hardly identified manually unless under special circumstances (essentially a previous detailed knowledge of similar mixtures). If the chemical elements constitutive of samples synthesized in a laboratory are generally known, facilitating the search/match, this may not be the case of other samples from geological or archaeologic origin for which a successful search/match without the need for a destructive chemical analysis would be interesting. Modern computer search/match programs coupled with the ICDD Powder Diffraction File (PDF) database (or custom databases) number today at more than 20, applying various algorithms (Smith and Gorter, 1992; Langford and Louër, 1996; Cranswick, 2002). However, their relative efficiency and effectiveness in the hands of their users has not been tested in the public arena. Wasting time because a known compound gave a negative search/match result is something that should not happen nowadays in a well equipped laboratory where

time is counted. Considering the high cost of software and databases, and the common opinion that this, like many areas of crystallography, is "black box" technique, it was concluded that a search/match round robin (SMRR), completely open to academic researchers, manufacturers, developers, etc., would be timely and useful to the community. This is the third round robin of this kind, since in 1977 and 1978, a group at the National Bureau of Standards (NBS), in cooperation with the Computer Sub-Committee of the JCPDS designed a series of sets of X-ray powder diffraction data for the purpose of two successive round robins (Jenkins, 1976; Jenkins and Hubbard, 1978). Each of the sets of data corresponded to a mixture of at least three phases. Some sets of phases were completely inorganic and others were composed only of organic materials. The conclusions, very surprising today, were that hand-searching and computer searching were found equally efficient for mineral and inorganic samples, and hand-searching was found vastly superior to computer searching for organic specimens. The computer programs were of the first generation, and the PDF contained 25 000 phases. Some more recent publications are concerned with the application of search/match software (for instance PDSM) to some of these round robin data (Marquart *et al.*, 1979; Marquart, 1986), however, the mixtures were not unknown, and the program belongs to the second generation. Computer speed and user friendliness have changed enormously since these times. The aim of this paper is to examine the third generation modern software performances facing really unknown and complex mixtures. That third generation being defined in the Jenkins and Snyder (1996) book by the statement: "A new strategy has recently been introduced (Caussin *et al.*, 1989) that has dramatically improved the success rate of the search/match process. The new idea is to search the whole observed pattern with its background (not

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just the $d-I$ list) and to add candidate phases together to compose, rather than decompose, an observed multiphase pattern. The success rate of this procedure is often 100% even for four-phase unknowns with significant amounts of preferred orientation.''

II. PROCEDURE OF THE SMRR-2002

The SMRR-2002 publicly started on May 2, 2002 *via* a main website at http://www.cristal.org/smrr/ (and CCP14 mirrors). The Internet is now considered as the primary tool which allows an entire round robin to be performed in a time effective manner (recent examples are the Structure Determination by Powder Diffratometry round robin or the Size/Strain round robin). Announcements were made in the major crystallographic newsgroups, mailing lists and web pages (see a complete list at the IUCr web site: http://www.iucr.org/). People had the option to propose phase identification results for four different powder patterns representing different fields that use search/match methods. The collection of results occurred in two steps.

Step 1, deadline June 15, 2002—samples without chemistry but with vague origin.

Step 2, deadline June 30, 2002—samples with chemistry information (provided on June 16).

One screen copy for each of the search/match results was requested with each submission with information such as the program name, the ICDD–PDF release, and explanations if people did not get the results by only applying their search/match software (using the Hanawalt search manual, indexing and then finding the compound in the ICSD or CSD databases, etc.). Anonymity was ensured as a basic requirement of the round robin.

III. CHOICE OF THE FOUR SAMPLES

In our opinion, the four selected patterns were not especially hard to identify and correspond to typical real cases. The ICDD PDF database contains identification solutions, or at least close solutions. During the round robin, minimal information was given about the samples since many identifications by search/match methods are frequently made without prior knowledge of the chemical content. There were some pitfalls in the SMRR, mainly for samples 2 and 3 due to nonoptimal ICDD reference data. However, it is not that uncommon for real-life samples to have inexact but close, and therefore valid, solutions in the PDF (identification by similarity to an isostructural compound with slightly different cell parameters and the like). A search/match program should be efficient enough to give the maximum fits. Some explanations about the choice of the four candidates are given here. The bold subtitles below were the only information provided at step 1. These very few details on the sample origins constrained the search/match to specific subsets (mineral for sample 1, organic for sample 3, not mineral for sample 2, and inorganic for sample 4), though most experts in identification would first perform an unrestricted general search.

A. Sample 1: geological sample

The sample contains four major phases: gormanite $[Fe_3Al_4(PO_4)_4(OH)_6 \cdot 2H_2O]$; apatite $[Ca_5(PO_4)_3(OH,F)]$;
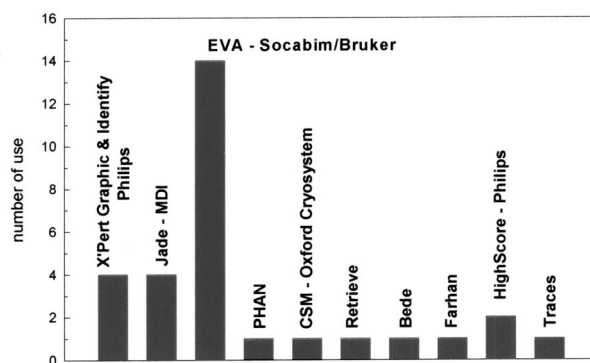

Figure 1. Software used for SMRR-2002, the two steps merged.

siderite $(FeCO_3)$; and quartz (SiO_2). A further difficulty is that of a zero shift in the data but this does not preclude identification. An acceptable set of answers for this sample was (i) apatite (hydroxy- or fluorapatite accepted—respectively, 30 and 33 matching PDF card numbers, most frequently proposed, 15–0876); (ii) siderite (a Mg/Fe solid solution phase was also accepted, not ankerite nor dolomite—38 matching card numbers, most frequently proposed, 29–0696); (iii) gormanite (or souzalite, as this is a series of isostructural compounds—card numbers 36–0403, 33–0863); and (iv) quartz (74 matching cards, most frequent, 46–1045). At step 2, the chemistry was revealed as being Ca, Fe, Al, P, Si, O, C, and H, other traces possible, specimen from Rapid Creek, Yukon, Canada.

B. Sample 2: from a synthetic chemist

The second sample from a synthetic chemist is a pure phase. The compound is isostructural with octadecasil. The template is not quinuclidine, but a linear template whose formula was not revealed to the SMRR organizers. The host remains unchanged. This involves rather important modifications in peak positions, and this sample was ideal for verifying the ability of search/match software to identify a close-enough isostructural compound. It should be clear that such an ability is essential for avoiding enormous waste of time when performing a SDPD (Structure Determination by Powder Diffractometry). The unique acceptable answer for this sample was octadecasil (ICDD card 48–0475). The apparent simplicity of the powder pattern suggested manual search as well, and even indexing. At step 2, the following chemistry details were given: Si, O, maybe F, plus an organic molecule.

C. Sample 3: pharmaceutical sample

Sample 3 contained a 50–50% mixture of the two thalidomide polymorphs (α and β). This could not be fully iden-

TABLE I. ICCD–PDF release.

ICDD–PDF release	2001 up to set 51	2000 up to set 50	1999 up to set 49	Up to set 47	Up to set 46	Up to set 45	Not given
Number of participants	7	7	3	3	1	1	8
%	23.3	23.3	10	10	3.3	3.3	26.7

TABLE II. Summary of participant's results for step 1.

Participant	Samples answered				No. of phases to identify	Software used	No. of right identifications
P1	1	2	3	4	10	EVA	9
P2	1		3	4	9	EVA	6
P3	1	2		4	9	Jade	8
P4	1	2		4	10	HighScore	7
P5	1		3	4	9	EVA	8
P6	1		3	4	9	EVA	8
P7	1		3	4	9	X'Pert Graphic & Identify	7
P8	1	2	3	4	10	Jade	9
P9	1	2	3	4	10	EVA	7
P10	1				4	Farhan	3
P11	1	2		4	9	EVA	6
P12	1	2		4	9	EVA	8
P13	1	2	3	4	10	EVA	8
P14	1	2		4	9	Bede/Hanawalt	7
P15	1	2	3	4	10	EVA	10
P16	1	I^a	3	4	9	EVA	6
P17	1	2	3	4	10	EVA	6
P18				4	4	Jade	4
P19	1		3	4	9	Retrieve	9
P20	1	2	3	4	10	CSM	8
P21	1	2	3	4	10	PHAN	7
P22	1	2		4	9	EVA	7
P23	1	2	3	4	10	Jade	9
P24	1	2	3	4	10	X'Pert Graphic & Identify	3
P25	1		3	4	9	X'Pert Graphic & Identify	7

[a] I stands for indexed pattern only.

tified from the ICDD PDF since it contains data (quite old) for only one polymorph (α). While a zero shift is present, this does not preclude identification. Of course, a full correct explanation of the pattern by relying only on the ICDD database is impossible. It was expected that the operators' experience and intelligence would be important for a complete, final proposition. Moreover, it was said at step 2 that the sample was a mixture of polymorphs and the chemical formula was detailed as being $C_{13}H_{10}N_2O_4$.

This example points out the PDF incompleteness, up to the end of 2002, in domains such as organics or organometallics. Addition of powder patterns calculated from the Cambridge Structural Database (CSD) is expected for the end of 2002 but an experienced search/match operator is normally aware that databases can be incomplete. It also makes this a good test of operator expertise in checking for related polymorphs via the relevant structural database. An acceptable answer for sample 3 is thalidomide (ICDD card 19–1946).

(*Note*: the correct formula for Thalidomide is $C_{13}H_{10}N_2O_4$ instead of $C_{13}H_{10}N_2O$ indicated on the 19–1946 ICDD card file, this was even more confusing to some participants who preferred to trust the PDF instead of the organizers.)

D. Sample 4: industrial processing plant sample

That sample is a "typical" lead acid battery cured plate quality control sample for routine identification and quantification of phases. Acceptable answers to sample 4 were (i) massicot (PbO, nine matching ICDD Cards, most frequently

cited, 38–1477); (ii) litharge (PbO, 17 matching ICDD Cards, most frequently given 05–0561); (iii) tetrabasic lead sulfate ($Pb_5O_4SO_4$, ICDD Card 23–0333); (iv) tribasic lead sulfate ($Pb_4O_3SO_4 \cdot H_2O$, ICDD Cards 29–0781 and 88–0552). Very trace phases (lanarkite, anglesite, hydrocerussite, lead sulfate, and lead metal) were also present but it was not expected from participants to identify them, though they can play a significant role in the battery performance. At the SMRR step 2, more details were added with the chemical content (Pb, S, O, trace C, and H): a cured plate from a lead acid battery plant–created by mixing lead oxide with sulphuric acid, pasted on a lead grid and cured at high humidity somewhere between 50 to 90 degrees Celsius.

IV. RESULTS AND DISCUSSION

A. Participation

The first observation which can be clearly made is the poor percentage return of answers. While 248 downloads of the data occurred (a download may be considered a participation, owing to the fact that no download can occur without some willingness to try and participate), only 25 answers were received at the end of step 1. It should be noted that 68% of these answers were received within the 48 h before the deadline of June 15, 2002. During step 2, there were five new participants to the SMRR with the final number of participants reaching 30 at June 30, 2002.

TABLE III. Results by software, step 1.[a]

	Participants	Sample 1			Sample 2			Sample 3			Sample 4		
		Mean	Best	Worst	Mean	Best	Worst	Mean	Best	Worst	Mean	Best	Worst
EVA Socabim/Bruker	P1, P2, P5, P6, P9, P11, P12, P13, P15, P16, P17, P22	3.33/4	4/4	2/4	0.5/1	1/1	0/1	0.75/1	1/1	0/1	2.92/4	4/4	2/4
JADE–MDI	P3, P8, P18 (nr for samples 1,2,3), P23	4/4	4/4	4/4	1/1	1/1	1/1	0.75/1	1/1	0/1	3.25/1	4/4	3/4
HighScore–Philips	P4	3/4			0/1			0/1			4/4		
Graphics & Identify Philips	P7, P24, P25	2.67/4	4/4	1/4	0/1	0/1	0/1	0.67/1	1/1	0/1	2.33/4	3/4	2/4
FARHAN	P10	3/4				nr			nr			nr	
Bede Search/Match	P14	3/4			1/1	(Hanawalt)		0/1			3/4		
Retrieve	P19	4/4			id			1/1			4/4		
CSM Oxford Cryosystems	P20	4/4			1/1			0/1			3/4		
PHAN	P21	3/4			id			1/1			3/4		

[a] The software Traces was used only for step 2.

B. Software used

Three main software packages were used by the participants for step 1 (Figure 1): *Jade*, from MDI, (16%) *X'Pert Graphic & Identify*, from Philips (12%); *EVA* from Socabim/Bruker (48%). While Oxford Cryosystem indicated that their CSM (Crystallographica Search/match) is also part of the new Philips search/match software (Highscore), this does not particularly modify the distribution. Programs used in step 2 do not show strong modification to this distribution 13%–13%–47%, respectively.

Noticeable is the absence of several well-known search/match packages including *AXES, XPLOT, DRXWin, PADS, TRXDWin, XPOWDER, Powder Suite, LookPDF, NacDIFF,* and *RayfleX*. It is most likely that this disparity of software reflects their commercial distribution, Philips and Bruker being said to occupy the major part of the market, with equal share. Obviously, companies selling search/match software with hardware systems have a marketing advantage over those who don't. Internet awareness of some search/match vendors and sets of users over others may have skewed the results. The Hanawalt search manual was also used by one of the participants (for sample 2). It is moderately surprising that participants did not make more use of Hanawalt or PDF-2 CD-ROM searches. This could indicate an education

TABLE IV. Summary of participant's results for step 2. The new participants (26–30) are in bold and italic.

Participant	Samples answered				No. of phases to identify	Software used	No. of right identifications
P3	1	2		4	9	Jade	**8**
P4	1	2	3	4	10	HighScore	**9**
P5	1	2	3	4	10	EVA	**9**
P7	1			4	8	X'Pert Graphic & Identify	**6**
P8	1	2	3	4	10	Jade	**9**
P9	1	2	3	4	10	EVA	**8**
P10	1				4	Farhan	**3**
P11	1	2	3	4	10	EVA	**8**
P12	1	2	3	4	10	EVA	**8**
P13	1		3	4	9	EVA	**9**
P14	1	2		4	9	Bede/Hanawalt	**7**
P16	1	2	3	4	10	EVA	**8**
P17	1			4	8	EVA	**6**
P19	1	2	3	4	10	Retrieve	**10**
P20	1	2	3	4	10	CSM	**9**
P21	1	*I*[a]	3	4	9	PHAN	**9**
P22	1	2		4	9	EVA	**8**
P23	1	2	3	4	10	Jade	**9**
P24	1	2	3	4	10	X'Pert Graphic & Identify	**6**
P26	*1*	*2*	*3*	*4*	*10*	*EVA*	***10***
P27	*1*	*2*	*3*	*4*	*10*	*Traces*	***8***
P28	*1*			*4*	*8*	*EVA*	***8***
P29	*1*	*2*		*4*	*9*	*X'Pert Graphic & Identify*	***7***
P30	*1*			*4*	*8*	*High Score*	***6***

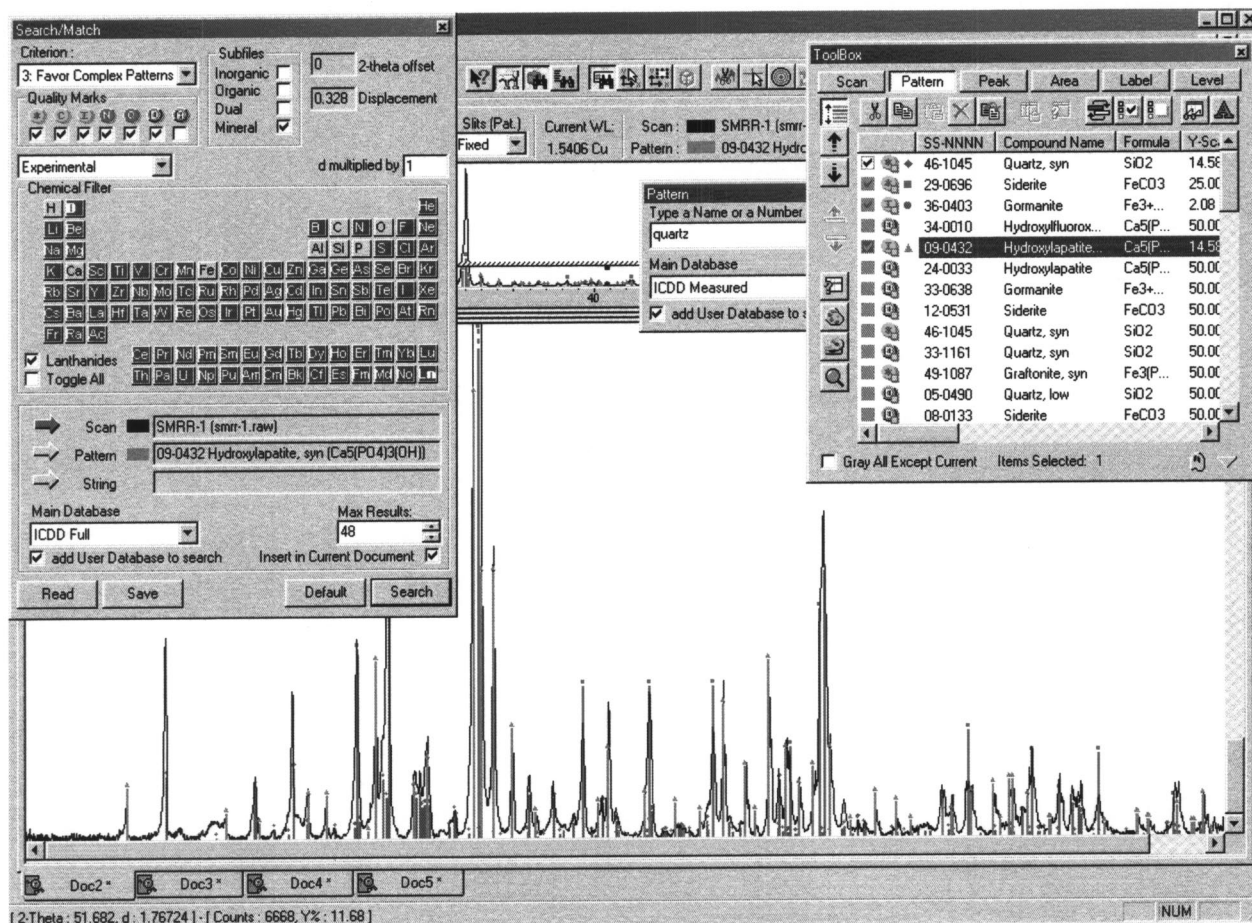[a] *I* stands for indexed pattern only.

Figure 2. Search/match result for sample 1 by participant 26, using the EVA software.

issue in the powder diffraction community, as well as the high level of trust that users put on a single search/match program. Financial constraints on individual laboratories in the variety of products that can be afforded may also play a part. It may be interesting to compare the current search/match software list to that, already quite large, listed in the Powder Diffraction journal in 1986: *FREVEL MATCH, PDIDENT, JCPDS Johnson/Vand Search/Match, Mini Search, DC26, AFPY*, and *AFPB, WAIT, SEARCH, XRDQUAL, μPDSM, MICRO-ID*. Some of them were provided without charge by the ICDD. If the algorithms have survived and evolved, the names all died.

C. Database release

Table I shows the ICDD–PDF release used by participants of which 56% use a release from 1999 or onwards. This number may be higher as 27% of the participants did not give information on their PDF version used. All publicly announced round robins of this nature run the risk of having very skewed statistics due to accepting receipt of any responses that arrive, rather than having the ability of dictating the scope, number, expertise and detail of responses.

Such a table allows an explanation of why at least 16% of the participants could not identify sample 2, because of using an old ICDD release not including the octadecasil 48–0475 card. This emphasizes the importance of having the

most up to date databases possible for performing reliable phase identification using Powder X-ray diffraction.

D. Participants results for step 1

Participants had the option of only responding to samples they found to be of interest. With this flexibility in mind, 92% of the participants give at least their answers for three samples at step 1. A summary of the results is proposed in Table II (information on the full submissions is available at http://sdpd.univ-lemans.fr/smrr/). Of the proposed four samples in the SMRR-2002, the total number of phases requested to find among these samples was 10.

The distribution of the 10 requested phases is the following:
sample 1, four phases;
sample 2, one phase;
sample 3, one phase (β-thalidomide not requested, because not in PDF);
sample 4, four phases.

The best result at step 1 was from participant P15, having proposed the correct 10 phases for the four samples using the EVA software (Socabim/Bruker). The number of answers received at the end of step 1 is not sufficient to discuss the results without taking into account each user's experience.

During step 1, nine different software packages were used in this search/match round robin. Table III presents the
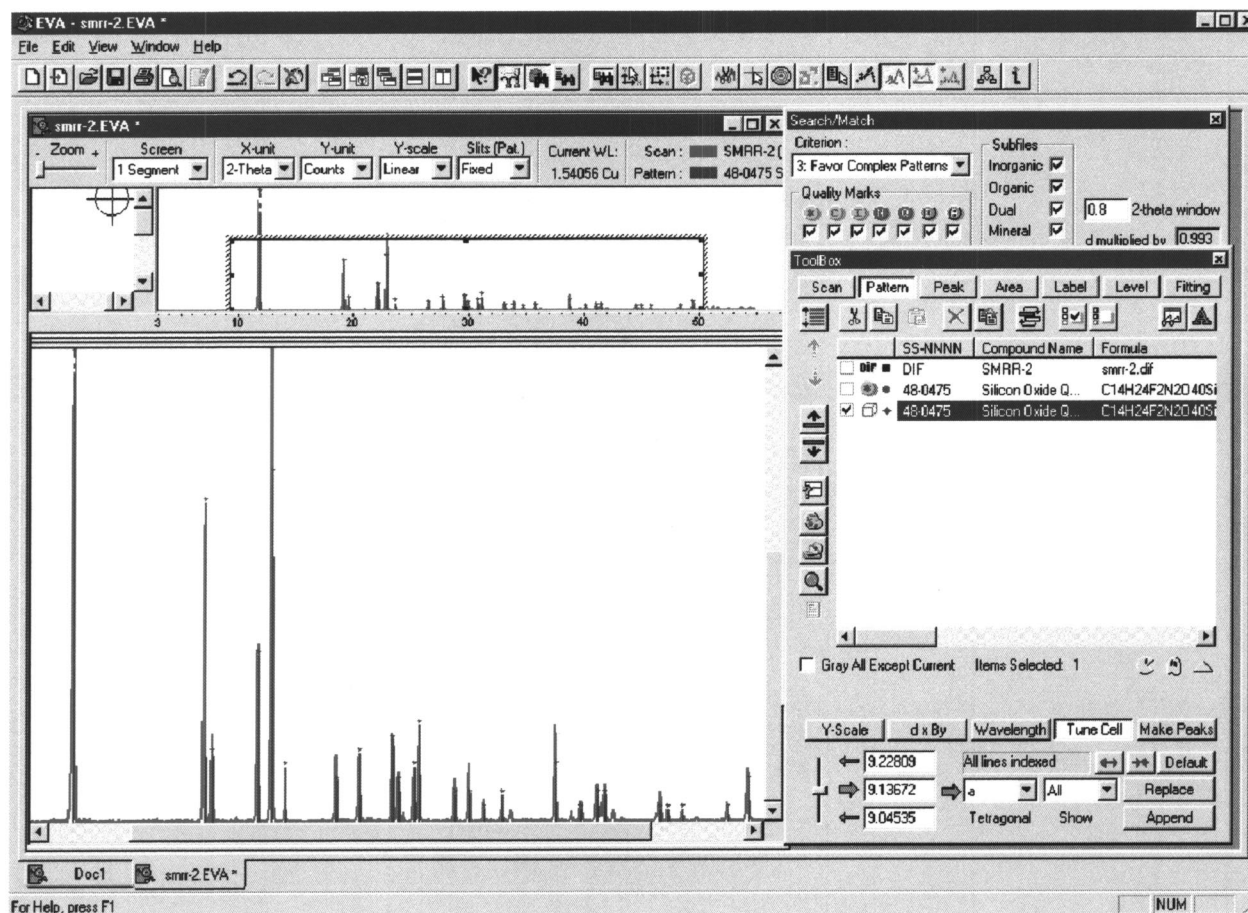
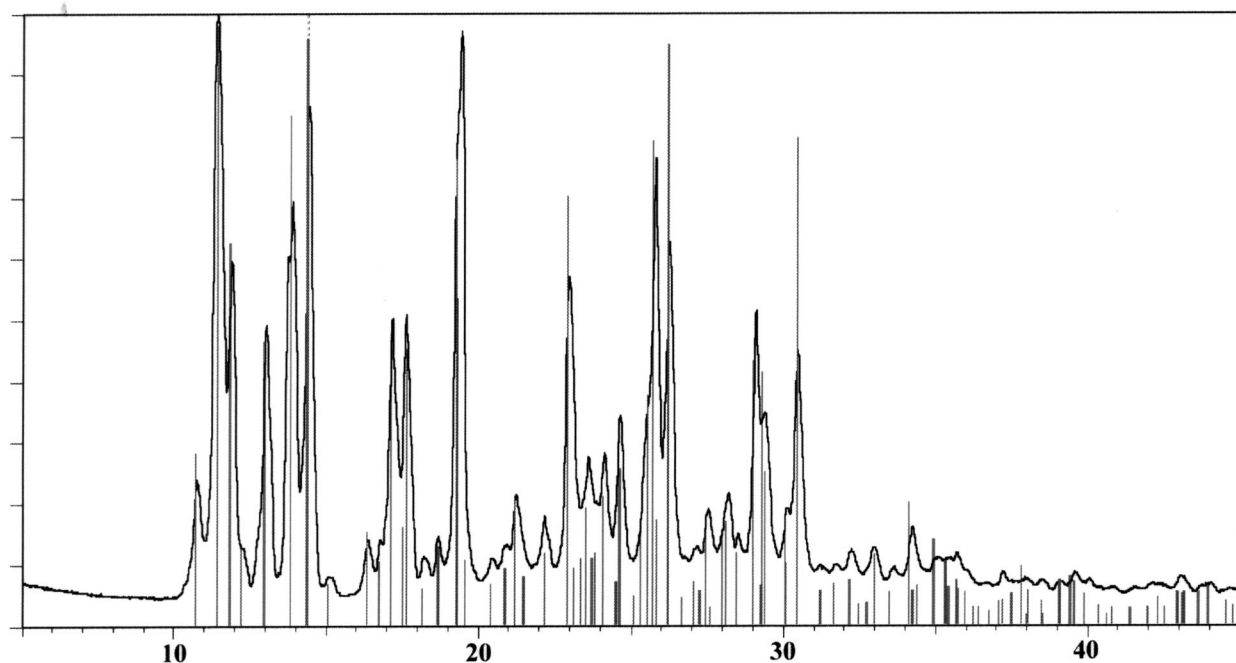Figure 3. Search/match result for sample 2 by participant 15, using the EVA software.

Figure 4. Search/match result for sample 3 by participant 11, using CSD data (α- and β-thalidomide).
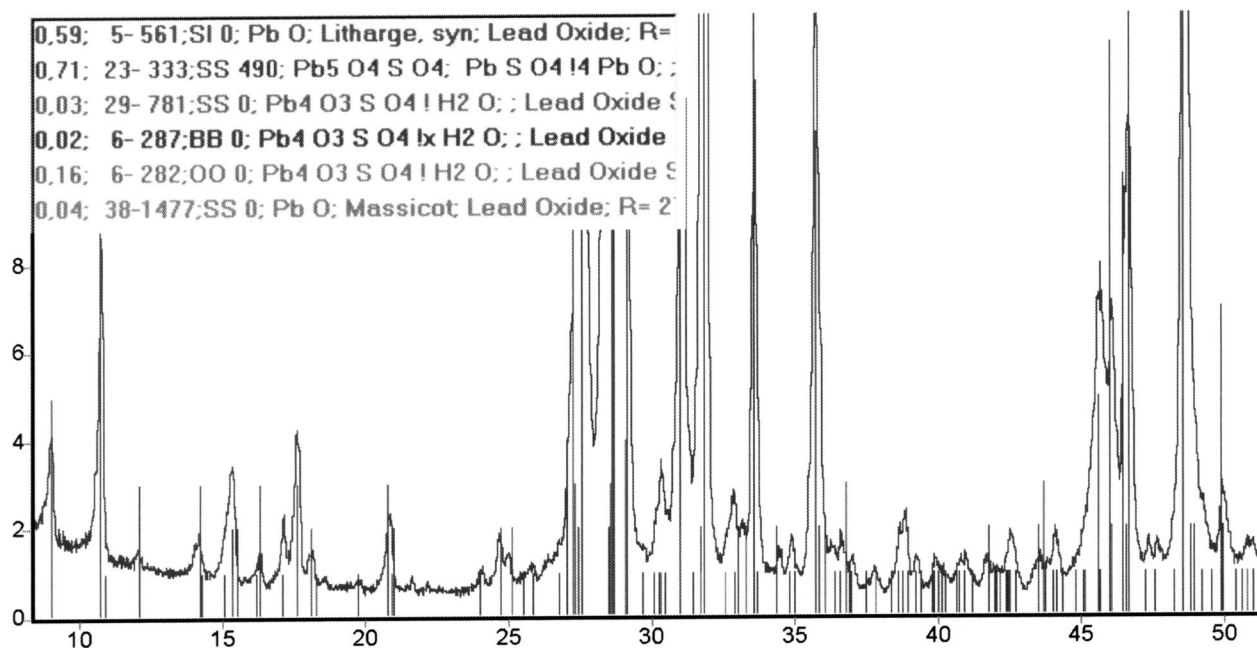
Figure 5. Search/match result for sample 4 by participant 19, using the Retrieve software.

results of step 1 against the software used. The mean number of phases identified for each sample is given below (nr=no result provided; id=incomplete database precluding sample 2 identification), and also the numbers given by the best performer (mixing the software versions) and the worst one.

This first step of the SMRR, without knowledge about chemistry, is interesting in several ways. Indeed, it is often a clear advantage to be able to identify phases in a sample without doing any chemical analysis; this can save time and money, as well as the sample itself. Of course, performing a chemical analysis of a fine powder which is actually a phase mixture will give only a global composition and no details on the individual phases. A synthetic chemist would normally know already what elements are inside the sample unless there were errors in labelling or degradation of starting

materials. However, it is not uncommon that phase identification is required on materials where reliable information is not initially available. These results as a whole indicate that in the absence of details about the chemistry, but including information allowing to select a subset (mineral, inorganic, organic), the performance of the above search/match software is quite high. In the hands of competent users, the above programs appear to be able to identify 3–4 phases in a mixture of up to 4 major phases.

From the series of EVA users, the performance appears to depend a lot on the performer training, and this seems to be particularly true for the more difficult sample 2 (no exact match possible–only close match) and sample 3 (no complete match possible–only one of the two polymorphs is in the PDF). Other points to take into account to define the

TABLE V. Results by software, step 2.

	Participants	Sample 1			Sample 2			Sample 3			Sample 4		
		Mean	Best	Worst	Mean	Best	Worst	Mean	Best	Worst	Mean	Best	Worst
EVA Socabim/Bruker	P5, P9, P11, P12, P13, P16, P17, P22, P26, P28	3.6/4 (+0.27)	4/4	3/4	0.5/1	1/1	0/1	0.7/1 (−0.05)	1/1	0/1	3.3/4 (+0.38)	4/4	3/4
JADE–MDI	P3, P8, P23	4/4	4/4	4/4	1/1	1/1	1/1	0.66/1 (−0.09)	1/1	0/1	3/4 (−0.25)	3/4	3/4
HighScore–Philips	P4, P30	3.5/4 (+0.5)	4/4	3/4	0.5/1 (+0.5)	1/1	0/1	0.5/1 (+0.5)	1/1	0/1	4/4 (−1)	4/4	2/4
Graphics & Identify Philips	P7, P24, P29	2.67/4	4/4	1/4	0.66/1 (+0.66)	1/1	0/1	0.33/1 (−0.33)	1/1	0/1	2.67/4 (+0.33)	3/4	2/4
FARHAN	P10	3/4			nr			nr			nr		
Bede Search/Match	P14	3/4			1/1	(Hanawalt)		0/1			3/4		
Retrieve	P19	4/4			id			1/1			4/4		
CSM Oxford Cryosystems	P20	4/4			1/1			0/1			3/4		
Phan	P21	4/4 (+1)			id			1/1			3/4		
Traces	P27	4/4			0/1			1/1			3/4		

performance are the man–machine interface, the user-friendliness of the software, its simplicity and the facility of catch in hand, which of course are rather difficult to evaluate inside a round robin. These last points could perhaps explain the lack of answers from users of very largely distributed software packages. Moreover, informal verbal and E-mail feedback indicated that at least some nonsubmissions were due to search–match software defaults not giving obviously good answers; which combined with time constraints to continue trying to identify the phases, meant no submission was provided. Some participants used the facility of tuning cell parameters included in some programs, so as to obtain a perfect fit for sample 2 (for which some proposed the correct indexing, even if they could not retrieve that 48–0475 card). Also, the zero point which affects some data was detected and corrected by many participants.

From these very limited results, a ''best program'' cannot be selected (moreover a dozen programs have not participated in the SMRR and there are not enough participants using the same package) for step 1. While third generation search/match programs such as Jade, EVA, CSM, and Philips HighScore give users an advantage over older algorithms, the human element seems to still be of great importance in obtaining a reliable phase identification result. Readers will have to make their own conclusion on which software may be best for their needs, but will have to keep in mind that the present range of software is not an effective substitute for good staff experience and training.

There were five more participants for step 2 and one new software package (Traces). The results are gathered in Table IV. The new participants (26–30) are in bold and italic.

Some excellent participants at step 1 obviously decided not to participate in step 2. This may be because they did not find better identifications using chemical information. This is probably the case with participant 15, who provided the most effective and accurate set of results at step 1. This could be also the case of participant 1, who missed only massicot in sample 4. With hindsight, many participants may have preferred massicot to be declared a trace phase.

The most confusing case in this SMRR is sample 3 for which the maximum of information was given at step 2: a mixture of $C_{13}H_{10}N_2O_4$ polymorphs. Only one participant (P11) proposed the identification of the two thalidomide polymorphs based on the CSD data. It should be remembered that only one of the polymorphs was required because of the incompleteness of the PDF. However, this again reinforces the importance of the human operator using imagination and intelligence in phase ID, instead of placing complete trust in the ICDD reference database.

Overall, the results are generally improved at step 2 as a consequence of the chemistry knowledge. This resulted in two new participants who identified all 10 required phases: P19 (who updated his PDF release from set 47 to set 49) and P26, a new participant. Selected search/match results from the best participants are shown in Figures 2–5. The mean number of phases identified for each sample is given on Table V (nr=no result provided; id=incomplete database precluding sample two identification), and also the numbers given by the best performer (mixing the software versions) and the worst one. Table V can be compared to Table III– step 1. Mean score evolution is indicated between parentheses.

V. CONCLUSION

Due to the lack of manual searches, the following conclusions contrast considerably with those of the 1976–1978 two previous search/match round robins. While the statistics are not robust, from the 30 returns, it is nevertheless concluded that high quality phase identification without the need for chemistry can be routinely performed providing (i) modem third generation search/match software is used, (ii) the search/match database is as up to date as possible, and most importantly, (iii) competent operators with good intuition, imagination, and training are available to make use of the available software and databases.

These conclusions may seem obvious and unexciting. However, they may not be obvious to the decision makers, given the policies of many laboratories in minimizing expenditure on consumables and expendables such as databases, software, and trained scientists. It should be remembered that 88% of the data downloaders preferred not to submit an answer. Does this imply that these 218 participants were finding the problems nontrivial, that they considered their software not adequate for the problem, or that they finally had not enough time?

Caussin, P., Nusinovici, J., and Beard, D. W. (**1988**). ''Using digitized X-ray powder diffraction scans as input for a new PC-AT Search/match program,'' Adv. X-Ray Anal. **31**, 423–430.

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