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THE USE OF CRYSTALLOGRAPHIC SOFTWARE AS EDUCATIONAL SUPPORT TO MATERIALS SCIENCE AND ENGINEERING

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ABSTRACT

Justified by the lack of proper didatic tools, a systematic review process was executed to verify at what extent existing crystallographic software can support the teaching process and the understanding of crystal structures in materials science and engineering disciplines. A revision protocol was established and executed, where 26 references were selected and analyzed from a total of 804 software from the International Union of Crystallography (IUCr) software database. The research questions were deemed properly answered by this revision, where both a group of top performers (Class A) and gaps not fulfilled by any software, revealed enhancement possibilities and opportunities for development of new software focused on the educational support to materials science and engineering curricula.

1. INTRODUCTION

Motivation behind the development of this research originated from authors' lecturing experience in materials science and engineering classes in undergraduate and postgraduate courses. It is quite common in these classes to encounter students struggling to visualize crystal structures, planes, directions, interstitial positions and atoms neighbourhood.

Many materials properties depend on their crystal structures to a greater or lesser degree, which reinforce the importance of the subject. An example is the mechanical properties of cubic face centered (CFC) or centered body (CCC) crystals, very common among metals. CFC metallic crystals, such as gold, silver, copper and aluminum, are relatively more ductile than CCC crystals, such as iron (at room temperature), niobium, tungsten or molybdenum. This is due to the existence of close-packed planes and directions in the CFC structure, which require less tension for shearing, facilitating plastic deformation. Such planes do not exist in the CCC structure and shearing occurs preferably along plans of greater atomic density (but not close packed) which have close-packed directions. Therefore, stated the relevance of proper comprehension of crystal structures, the problem shifts to limitations of existing representations and didactic strategies.

Most of student difficulties seems to be related to the traditional bi-dimensional representations (on blackboard and slides) of three-dimensional structures, leading to erroneous or partial comprehension of crystal structures concepts. Educational support resources typically adopted in classrooms such as blackboard, books, and multimedia presentations are essentially based in two-dimensional projections, whether flat representations or perspectives. Although images are convenient for the most basic crystal structures, cognitive and geometric limitations render this medium inadequate for proper comprehension of more complex structures.[1-4] Bodner *et al*. [5] used problems of chemistry and crystallography to investigate why certain individuals struggled to understand geometric structures when interpreting static images. Based on results of the Purdue Rotation Visualization, Bodner *et al*.[5] proposes that spatial ability - the proficiency in mentally rotating, reflecting and inverting objects – is crucial to the proper geometric understanding and naturally fluctuates according to gender and on an individual basis as a function of training. Hence, the lack of spatial ability can undermine understanding crystallography essentials or impair the ability to solve practical problems related to the subject.

Another problem evidenced on materials science and engineering books is misinterpretation of the concepts of point lattice and crystalline structure. A crystal is usually defined as a solid composed of atoms, spatially distributed according to an organized (pattern) and periodic (repetitive) arrangement. This is the essence of the concept of crystal, as found in many books on science and engineering of materials or correlates, from the originals to the most recent, namely Barrett[6], Kittel[7], van Vlack[8], Schwarzenbach[9], Padilha[10], Callister and Rethwisch[11], Graef and McHenry[12], Szwacki and Szwacka[13], West[14] and Brostow and Hagg Lobland[15]. Atoms are arranged in such a way that this fundamental pattern is replicated at each point of the space lattice of a particular crystal. The space lattice is what defines this repetition pattern and, as Barrett[6] astutely observed, "the term lattice is often used indiscriminately as a synonym for structure, which is an incorrect and confounding practice."

A crystal structure is then formed by associating a motif or basis of one or more atoms with each lattice point. A particular motif must have unique number, chemical elements, arrangement and atomic orientation. The same designation for the lattice and structure applies only for single atom motifs, which is certainly a confusing aspect, especially when the concepts of lattice and structure are not clear to the student. The term "motif" means a recurring theme or a repeating pattern, so it is fully consistent with the subject matter. Thus, the correlation between lattice and structure can be simplified by the following "equation": Crystal structure = Bravais lattice + motif.

Accordingly, the multiplicity of crystal structures comes from the multiplicity of motifs. Students of materials science and engineering courses surely capture this formulation more easily. It should be noted that the designation "motif"[13] will be favoured over “basis” in this paper. Motif is also used in French[14] and is the obvious translation of “Motif” in German[16].

1.1 Physical and virtual models

Physical and virtual models are traditionally adopted as an alternative to address the previously discussed visualization limitations, allowing to rotate, reflect and reverse perspective views to resolve visual ambiguities and to identify objects within the structure of reference to the structure of reference[5] with more accuracy. Physical models allow the tactile manipulation and exploration of both synesthetic and ludic aspects, as well as the natural sense of depth. The adoption of kits containing self-assembling structures for the construction of three-dimensional models of crystalline structures is still expressive today in the teaching of materials science, particularly due to the intrinsic limitations of two-dimensional representations in achieving an efficient visual mapping. Literature suggests that adoption of physical models can potentially learn enhancements of other media, particularly in the case of high complexity crystalline structures[2,18].

However, the use of physical models is, in practice, limited to simpler structures, as the construction process of complex structures is costly and time-consuming. Although most of these limitations can be mitigated by the recent popularization of 3D printing technologies, 3D printed models are still costly and time-consuming[2]. Traditional physical models also lack flexibility, whenever the visualization of deep internal regions is necessary, due to the difficulty to remove one or more atoms from the assembly without compromising the integrity of the whole model. Other difficult tasks to perform in physical models are visualizing crystal planes and directions. Although stackable models can be printed in 3D to facilitate the exploration of any internal aspect[2], designing such models is not trivial, and there are restrictions on how many aspects can be analyzed with a given model, demanding the creation of additional models.

In summary, most limitations and costs associated with physical models can be tackled by modern visualization technologies. The great advantage is the possibility of exploration and navigation in different scales, angles, perspectives and velocities, without the burden of the physical construction of the model. In addition, virtual models can be "dismantled" disregarding physical integrity. Finally, the use of modern stereoscopic and interactive technologies also allows leveraging aspects typically associated with physical models, such as the natural sense of depth and to some extent tactile stimulation.

However, the construction of virtual models also presents some challenges. Manual construction using CAD or 3D modeling software is impractical due to the great amount of time required for each model as well as software proficiency and specialized knowledge both in materials science and crystal structures. Resta[20] states that instructors and teachers rarely master all those skills. As an alternative, crystallographic software is a viable alternative to build these models.

1.2 Crystallographic software

In short, traditional two-dimensional representations for understanding essential materials science topics are limited[21] and although physical models have been historically adopted as an alternative to circumvent limitations, these models impose production costs and interaction restrictions- scale operations are not possible, while visualizing interior parts often requires impractical structural modifications. Virtual models do not pose such problems, but their use is restricted mostly because teachers and instructors, for the most part, do not have training in 2D or 3D modeling software[20].

Although many of the crystallographic software available today can produce mildly interactive three-dimensional digital crystal structures, creating and manipulating crystals in such tools may require a level knowledge beyond what's provided by materials science's didactic books and the engineering undergraduate curricula, for they will probably adopt the concepts of space groups and internal symmetry. It's important to recall that the translational or complete motif definition assumed in this paper differs from the commonly adopted in crystallography, building crystal structures by simply translating the motif through the lattice points. Crystallographers' motifs, on the other hand, are composed of an asymmetric unit that is part of the structure (region of space), which in combination with the symmetries (space group) of the lattice/crystal gives the complete structure (either the lattice or the crystal)[22].

Therefore, although elemental from the crystallographic perspective, avoiding the concept of space groups and internal symmetry is a didactic strategy often used in introductory classes and engineering textbooks[8,10,23] as it prevents most of the initial difficulties indicated by undergraduate students. This approach is just not practical amongst crystallographers due to the unnecessary complexity and time consumption added even to the most ordinary tasks. Therefore, the translational motif aligns with the one used in engineering and materials sciences' textbooks and should be used in educational software.

1.3 Objectives

The main objective of this research is to verify at what extent the existing crystallographic software supports the teaching process and the understanding of fundamental materials science topics. Therefore, it is necessary to map crystallographic software state of the art, identifying synthesis, visualization, and manipulation functionalities relevant to crystalline structures, as well as positive characteristics related to didactic context. Emphasis will be given to existing gaps, which will contribute to the novelty and value of work.

2. SYSTEMATIC REVIEW

Systematic review is a research method aimed at acquiring and evaluating evidence on a central topic, following a procedure defined by a protocol[23]. As proposed by Kitchenham *et al*.[25], systematic review is different from traditional surveying due to deeper methodological concerns. By following a standard protocol and thoroughly documenting the whole process, review extensions are expedited and biases in the process can be more easily detected.

When noting the lack of rigor in systems engineering research, Kitchenham *et al*.[25] adapted the biomedical research protocols and proposed guidelines to address the specific problems of the area. As proposed by the authors, the process follows five iterative phases: problem formulation; primary studies collection; study evaluation; information analysis and results presentation. Nowadays this process is widely used in systems engineering research. Further details on the proposed phases can be found in the development proposed by Kitchenham *et al*.[25]. The following review protocol lays down all methodological details from each phase.

2.1 Revision protocol

This protocol was based on Biolchini *et al*.[24] and Kitchenham *et al*.[25]. It is worth mentioning that all software included in this revision are referenced by an alphanumeric code composed by its shortened name and publication year.

2.1.1 Scope and objectives

- Primary objective: identifying the state-of-the-art of crystallographic software.
- Primary research question: specific software features regarding crystal structure visualization.
- Intervention: specific features.
- Controls: none on the first iteration. Second and third iterations used previous results as controls in addition to participant feedback.
- Population: crystallographic software capable of crystal structure visualization.
- Results: desirable features and major gaps of existing systems, concerning educational applications.
- Envisioned application of review results: selection of a proper software for educational uses or optimum settings and specifications for a new system capable of synthesis and visualization of didactic crystal structures.

2.1.2 Search strategy

- Sources: indexed electronic databases - International Union of Crystallography (IUCr) and Collaborative Computational Project Number 14 (CCP 14).
- Language (interfaces): English is deemed the language of choice for prime scientific work.
- Selected keywords: Visualization, Graphics, Virtual reality, Teaching, Modelling, Materials science.
- Timespan: only software published after 1980 with active development were included in this revision, given compatibility issues and historical relevance.

2.1.3 Software selection criteria

Inclusion criteria: software compatible with current operational systems (Linux, Mac OS X and Windows) and capable of crystal structure visualization.

Exclusion criteria: obsolete, discontinued or incompatible software; launched before 1980; commercial software that evaluation license was not provided by authors.

2.1.4 Software selection process

The first step was building search strings by combining the chosen keywords and their possible synonyms in multiple ways, then testing them in each specified search engine. Inclusion and exclusion criteria were applied by reading the title, abstract and introduction of the references as required.

2.1.4.1 Exploratory survey

Given that no controls were found for the first systematic research iteration, an exploratory survey were performed on the search strings, checking whether they returned any crystallographic software published in a relevant publication, in this case, the Journal of Applied Crystalography. Most relevant software found were CMAK15, JMOL15, VEST14 and MERC15.

2.1.4.2 Search strings

The International Union of Crystallography (IUCr) database[26] provided the following relevant preset keywords: “Visualization”, “Graphics”, “Virtual reality”, “Teaching”, “Modelling” and “Materials science” (“application” category); “Linux”, “MacOs”, “MS Windows” or “Web” (“operational systems” category). Although search engine did not provide timespan filtering, the “Entered” field was adopted to filter software registered in the database before 1980.

All 20 software records registered at the CCP14 database[27] were individually analysed and verified to be previously included in the IUCr database.

2.1.5 *Data extraction, summaries and results*

Selected software was explored by reviewers according to a standard procedure and both basic information (name, authors, project website, original description) and evaluations were registered in a form.

Evaluation parameters (listed on section 2.1.5.1) were based on research objectives and project participant’s expectations. After a few iterations, parameters were systematized in five groups: technology, crystal structure synthesis, visualization, navigation and interactivity, educational features. Software were ranked based on a scoring procedure, where each evaluation parameter received the same amount of points and the total points of each software where compared to the normalized sum of all parameters. This ranking, along with project participant recommendations, where the basis for a software specification.

Additionally, to the more conventional results obtained, a series of interactive charts were also produced by CWD3[28] a dynamic data visualization platform developed exclusively for this project. Built over the D3 specification[29], CWD3 aims to gather better insights and support the systematic review analysis of the crystallographic software process. Source code and data is available online at the project page[28].

2.1.5.1 Software evaluation parameters

Below are listed the 40 Technical Survey Criteria used in CrystalWalk’s Systematic Review, which are divided into 5 main categories: (1) Technological, (2) Synthesis, (3) Visualization, (4) Navigation and Interactivity and (5) Didactic Criteria. Software requirements and specifications are indicated for each criterion in italic bold after the asterisk. For a complete description of survey criteria used in the evaluation, please refer to Bardella *et al*.[28] .

(1) Technological Criteria

The features listed below sought to support an ideal access model for educational software: open, democratic and collaborative.

1.1 Activity Level: based on updating frequency. A high activity level indicates a tendency for a more frequent improvement and continuity of the project.

1.1.1 Update Frequency: *Active or Dynamic

1.2 Application Portability: based on compatibility (operational system and hardware platform) and development rationale (compiled or interpreted).

1.2.1 Development Platform: compiled, interpreted, *embedded interpreter (HTML)

1.3 Use, Distribution and Modification: binary and source code availability.

1.3.1 Use, Distribution, and Modification License: *Open-Source, freeware, shareware, demo, commercial, others

1.3.2 Collaborative Development Model Support: *Yes, No

1.4 Interface Technology Support: supported hardware interfaces and interaction modes.

1.4.1 Base Devices (HID): *Mouse, Keyboard and Trackables

1.4.2 Advanced Interaction Device Support: *3D Monitor and HMD

(2) Synthesis criteria

The features listed below sought to ease access to materials science knowledge for students, teachers and researchers, checking whether the software demands a skill level above the expected for STEM (science, technology, engineering, and mathematics) undergraduate courses, open online courses (MOOCS), technical courses and self-learning.

2.1 Synthesis Method: *lattice + motif (translational), space group + motif (asymmetric)

Accessibility to crystal building features, evaluating the synthesis rationale and restrictions.

2.2 Interactive Synthesis Process: *Yes

Synthesis facilitated by way of graphic elements and representations

2.3 Restriction or Limitation in Synthesis Process: *No

Restrictions to synthesis of particular structures.

2.4 Interactive Atom Selection and Editing: *Yes

Availability of interactive selection and edition methods for atomic elements.

(3) Visualization criteria

The features listed below sought to support crystal structure comprehension to extract useful knowledge from such models.

3.1 Visual Representation: graphic options diversity and support to known materials science visual representations.

3.1.1 Model of Molecular Atomic Representation: *Rigid Spheres, Balls and sticks, space filling model, Wireframe, Polygonal, Others.

3.1.2 Model of Unit Cell Representation: *Whole, partial & interstices

3.1.3 Miller Planes: *Yes

3.1.4 Miller Directions: *Yes

3.1.5 Visualization Support Features: specific visualization methods for crystal structures

3.1.5.1 Multiple Cells: *Yes

3.1.5.2 Section view: *Yes

3.1.5.3 Axis Vectors: *Cartesian or crystallographic

3.1.5.4 Other Auxiliary Resources: *Lattice faces & borders

3.2 Visualization Features: diversity of options given the state of the art on computer graphics.

3.2.1 Visual Perception Features: *Shapes & perspective, color, opacity, luminosity, depth & sound

3.2.2 Projection Type: *Conic & Axonometric

3.2.3 Stereographic Support: *Anaglyph, Side-by-side & HMD

3.2.4 Rendering Modes: *Flat, Sketch/Cartoon, Realistic

(4) Navigation and Interactivity Criteria

Visualization and interaction are intertwined aspects when it comes to support spatial comprehension of crystal structures, easing learning such complex topic.

4.1 Interface: *GUI / Hierarchical menus, GUI, command line

Evaluation of system usability.

4.2 Base Interaction: *Translation, Rotation & Zoom

Diversity of traditional or basic interaction methods.

4.3 Advanced Interaction: availability of smart or assisted interaction methods.

4.3.1 Automatic rotations: *Yes

4.3.2 Guided animations: *Yes

4.3.3 Scale Transition: *Yes

4.3.4 Dynamic Occlusion Management: *Yes

4.3.5 Preconfigured Viewpoints: *Atoms, directions & Orthogonal perspectives

(5) Didactic Criteria

The features listed below sought to check for fundamental support features for educational activities, usually neglected on crystallographic software. This translates to flexibility and usability, considering the target audience (teachers, students, researchers) and features (support to class activities and publishing).

5.1 Knowledge Required from User: Basic Materials Sciences

Previous required experience to build and comprehend crystal structures.

5.2 Content Generation & Publication Support

Support to publish models in static or traditional media and interactive formats.

5.2.1 Display support / External portability: *Full application, 3D Model

5.2.2 2D printing support: *Bitmap image

5.2.3 3D printing support: *STL model

5.2.4 Internet Publishing Platform: *Yes

5.3 Didactic Features: additional structured information and support for educational narratives.

5.3.1 Support for didactic narratives: *Yes

5.3.2 Library of crystallographic structures: *Yes

5.3.3 Incremental Construction and Visualization of Structures: *Yes

5.4 End-User Documentation & Support: user support channels, project and system documentation.

5.4.1 Available Support: *Yes

5.4.2 Available Documentation: *Yes

3. RESULTS

3.1 Reference selection

The process started from a total of 804 references and after applying search filters on IUCr[26] and CCP14[27] databases, 604 references were ruled out and another 133 after applying inclusion and exclusion criteria (alleged purpose). Other 19 were excluded due to obsolescence, discontinuation, download or installation restrictions along with 4 duplicates. Two more were discarded as the authors did not agree to supply a trial license. The remaining 42 references were installed and another 16 did not comply with inclusion criteria specified in the revision protocol, as their factual purpose did not reflect the alleged purpose. A total of 26 software, representing 3.23% of the initial reference universe, passed to the analysis phase (Figure 1).

Filtering Category

REFERENCE TOTALS	0 (-100%)	804(100%)
Keyword + Year + OS	-604(-75.12)	200(24.87)
Alleged Purpose	-133(-16.54)	67(8.33)
Discontinued	-19(-2.36)	48(5.97)
Duplicated	-4(-0.49)	44(5.47)
License not provided	-2(-0.24)	42(5.22)
Factual Purpose (as Tested)	-16(-1.99)	26(3.23)
SUBJECTED TO EVALUATION	26	

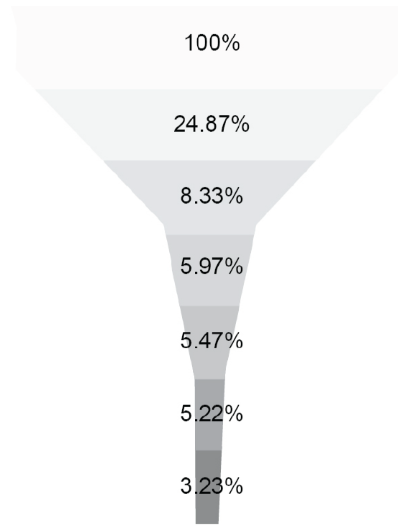

Figure 1. Filtering process of software references from IUCr and CCP14 databases. Source: authors.

3.2 Data presentation

As described in Section 2, references were individually rated based on the sum of points of each 40 individual criteria of the technical survey and ranked both by categories and total points, which facilitated further detailed analysis and comparisons. Based on its general ranking, references were then grouped in three classes: Class A comprising of top 6 references while Class B and Class C mid and lower tiers. Charts bellow illustrate these procedures.

Complete evaluation data is presented at Appendix A of this paper. According to the analysis model, Figure 2 shows the top performers in the general ranking and Figure 3 highlights neglected criteria. Class A references follow the same color code as Figure 2, while Class B references are displayed in white and Class C in black.

3.3 Analysis

Class A group comprises the top performers in the general ranking (Figure 2) including CMAK15 (1st), JMOL15 (2nd) and VEST14 (3rd) as top performing software. CMAK15 (1st) and JMOL15 (2nd) presented more stability in positioning along categories among the top three software and they also complied to five of eight neglected criteria, while VEST14 (3rd) complied only to three. DIAM15 (4th), DRAW11 (7th) and CARI04 (7th) stand out for complying to some of the most neglected criteria in this analysis. Eight criteria were not satisfied by any software, representing development gaps to be tackled by future research.

When considering the full ranking one can see the considerable discrepancy (the ‘valley’ in the plot) in the Visualization category, particularly across Class B and C software, which confirms that visualization is considered a secondary concern in most software. By removing the top four software of this category (CMAK15, VEST14, DIAM15 and XCRY14) this valley becomes evident. Although this discrepancy (‘valley’) seem less abrupt on the Didactic and Navigation categories, it is still notable.

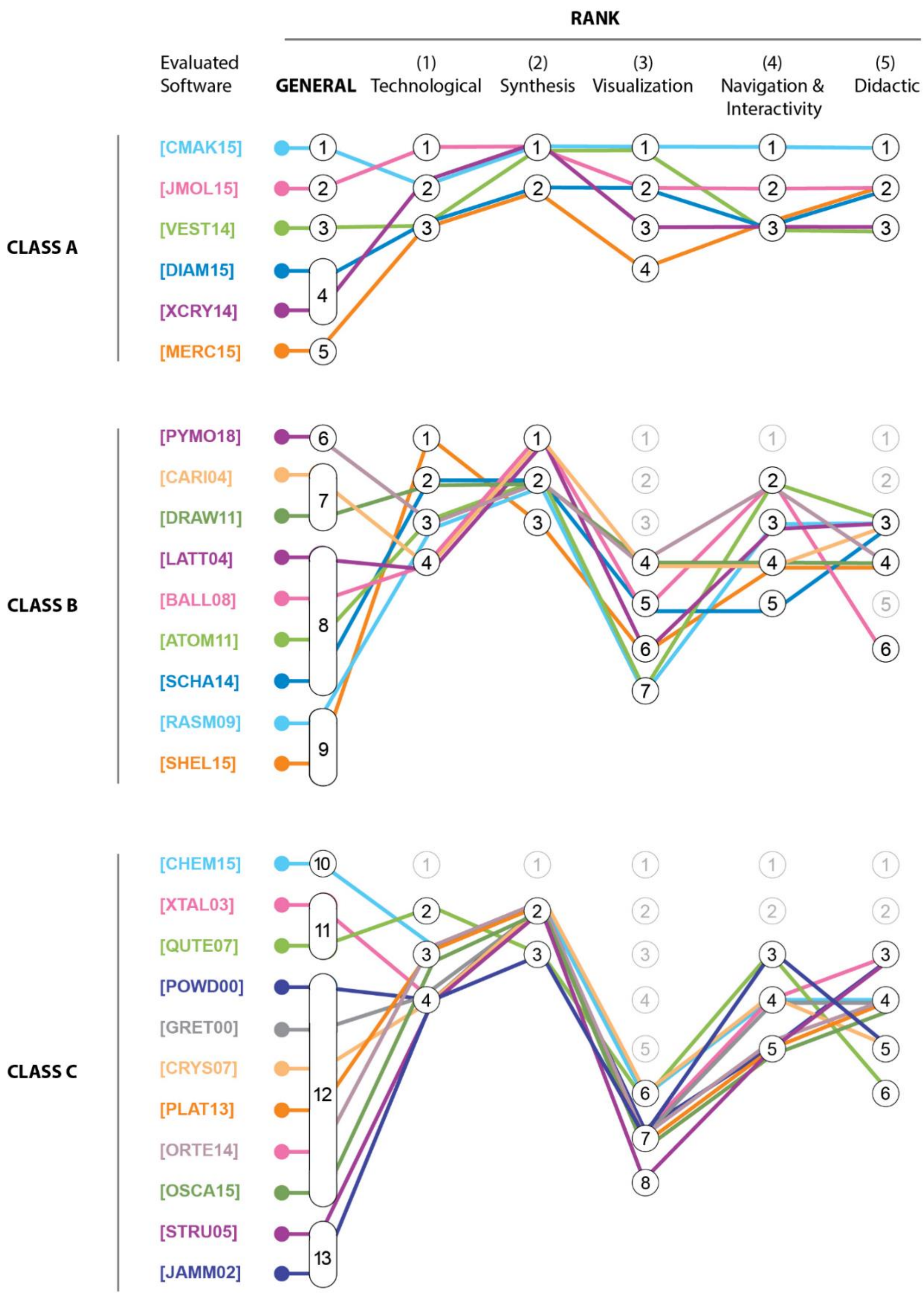

Figure 2. Software analysis summary, according to performance in each category. Source: authors.

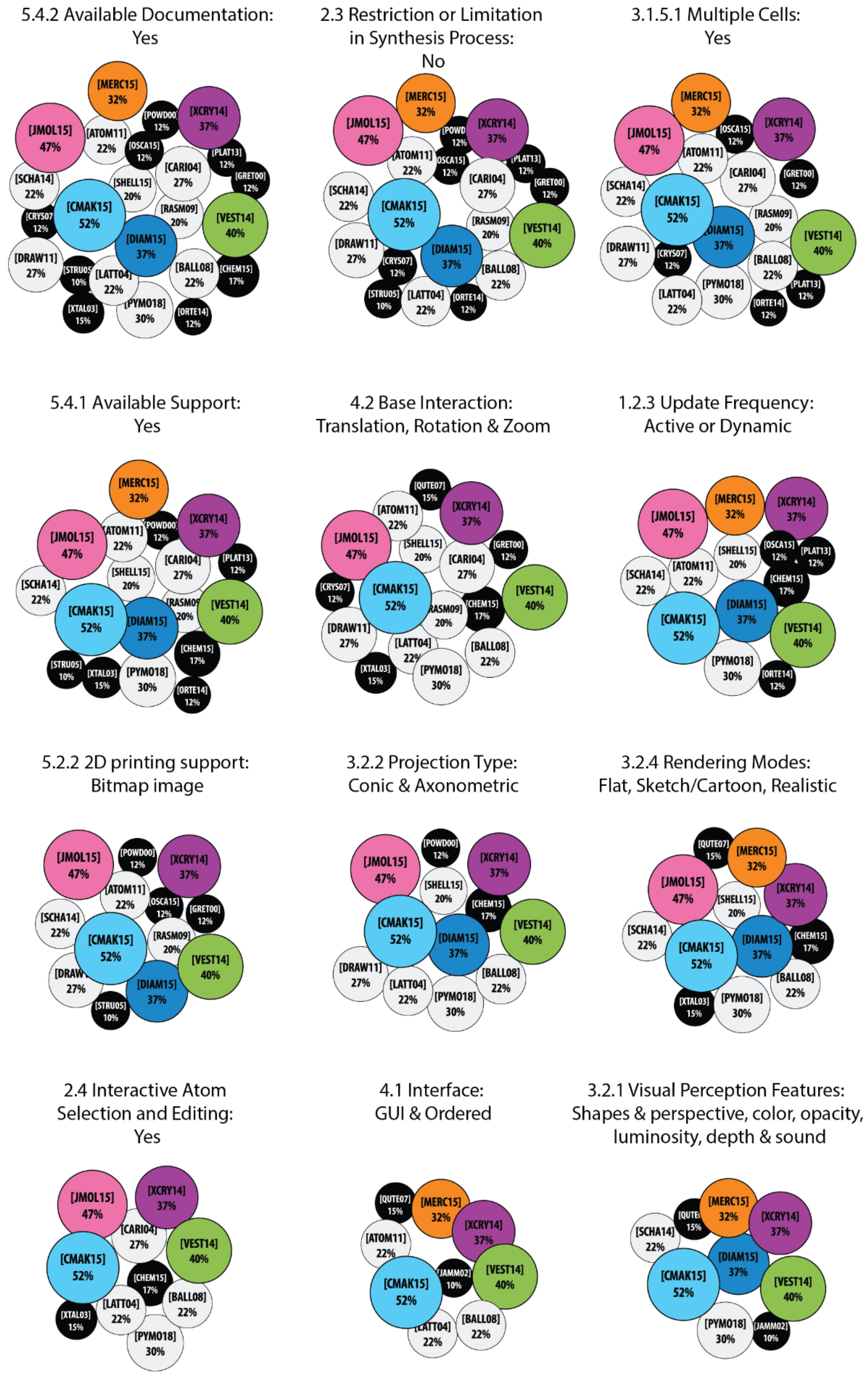

Figure 3. Software analysis summary, according to neglected criteria (Ref.26, adapted) 1st page.

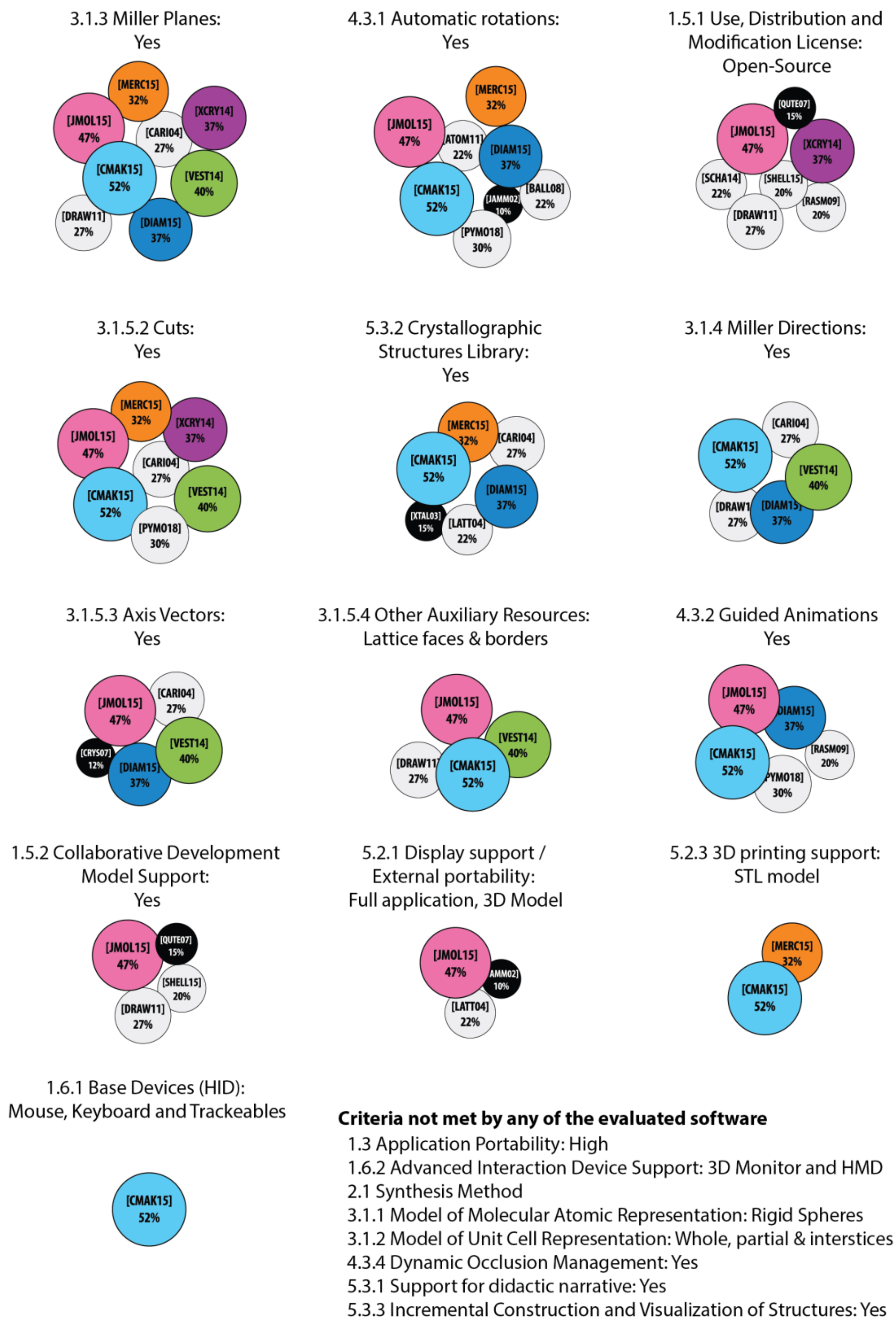

Figure 3. Software analysis summary, according to neglected criteria. (Ref.26, adapted). 2nd page/

3.4 Final remarks

A revision protocol was established and executed, where 26 references were selected and analyzed from a total of 804 software. All search strings were documented, allowing reproduction and expansion of this revision as needed, leveraging the proposed classification.

The research questions were deemed properly answered by this revision. Desirable educational features were identified, along with the most relevant existing software, which will serve as references for comparisons and evaluations of new software. The five criteria categories expedited the software analysis process and the reporting of results. This survey may also be useful as insightful direction for the enhancement of the analyzed references but also as the grounds for the development of new software with focus on educational and visualization performance improvement.

4. CONCLUSIONS

The rigorous crystallographic software state-of-the-art research presented in this article allowed exposing several gaps and development possibilities for accessible and novel educational crystal structure synthesis and visualization methods. Software references were evaluated according to several criteria defined by the research questions relevant to this project.

Although the available crystallographic software is capable of producing useful 3D crystal structure models, existing synthesis and visualization procedures are not suited for educational applications, demanding a specific level of crystallography's knowledge to be able to use the software and deal with the parameters. Additionally, interfaces are not user-friendly and usually developed by researchers for very specific and strict purposes. Finally, it is worth mentioning that proprietary closed source codes present a challenge for customization attempts aiming user experience enhancements or integration of existing tools. In short, no available software satisfied all listed criteria, revealing a fertile research field.

According to the results of this systematic review, in order to empower teachers, instructors, students and even researchers, it is therefore necessary to create novel specific tools for educational applications, characterized by ease of use, integration, accessibility and low cost. This effort is aligned to the modernization scenario envisioned by UNESCO[20]. This leading organization advocates that the computerization is a necessary condition for educational enhancement, which will in turn allow the transition from a reproductive to an independent learning model that promotes creativity and leadership. In order to achieve this, UNESCO recommends enduring and active technical development and maximal exploration of new technologies potentials, possibly achieved by public and private investments on hardware upgrades, more research and development of software and human resource improvements.

APPENDIX A –

SYSTEMATIC REVIEW SOFTWARE EVALUATION DATA

See following pages

TABLE 1 - TECHNOLOGICAL SURVEY CRITERIA						
	1.1 Activity Level	1.2 Application Portability				
Sotware	1.1.1 Update Frequency	1.2.1 Application portability	1.2.2 Development Platform	1.2.3 Supported Operating Systems	1.2.4 Requires Installation	1.2.5 Multi-platform
CMAK15	Active	Medium	Compiled (Not specified)	Windows; Mac	Yes	No (Desktop)
JMOL15	Dynamic	Medium	Interpretado (Java)	Independent (JRE comp.)	Yes/Plugin	Yes (Desktop; Emb.)
VEST14	Active	Medium	Compiled (C++)	Windows; Linux; Mac	Yes	No (Desktop)
DIAM15	Dynamic	Low	Compiled (Not specified)	Windows	Yes	No (Desktop)
XCRY14	Active	Medium	Interpreted (TCL/Tk)	Windows; Linux; Mac	Yes	No (Desktop)
MERC15	Active	Low	Compiled (Not specified)	Windows; Linux; Mac	Yes	No (Desktop)
PYMO18	Active	Medium	Interpreted (Python)	Windows; Linux; Mac	Yes	Yes (Desktop; Mobile; Emb.)
DRAW11	Not active	Medium	Compiled/C++	Windows; Linux; Mac	Yes	No (Desktop)
CARI04	Not active	Medium	Compiled (Not specified)	Windows; Linux	Yes	No (Desktop)
BALL08	Not active	Low	Compiled (Not specified)	Windows	Yes	No (Desktop)
LATT04	Not active	Medium	Interpreted (Java)	Independent (JRE comp.)	Yes/Plugin	Yes (Desktop; Emb.)
SCHA14	Active	Medium	Compiled (FORTRAN)	Windows; Linux	Yes	No (Desktop)
ATOM11	Active	Medium	Compiled (Not specified)	Windows; Linux; Mac	Yes	No (Desktop)
SHEL15	Active	Low	Compiled (C++)	Windows; Linux; Mac	Yes	No (Desktop)
RASM09	Not active	Medium	Compiled (C++)	Windows; Linux; Mac	Yes	No (Desktop)
CHEM15	Active	Low	Compiled (Not specified)	Windows; Linux	Yes	No (Desktop)
QUTE07	Not active	Medium	Compiled (C++)	Windows; Mac	Yes	No (Desktop)
XTAL03	Not active	Low	Compiled (Not specified)	Windows	Yes	No (Desktop)
CRYS07	Not active	Low	Compiled (PASCAL)	Windows	Yes	No (Desktop)
POWD00	Not active	Low	Compiled (Delphi)	Windows; Other (DOS)	Yes	No (Desktop)
PLAT13	Active	Medium	Compiled (FORTRAN)	Windows; Linux	Yes	No (Desktop)
GRET00	Not active	Low	Compiled (Delphi)	Windows	Yes	No (Desktop)
ORTE14	Active	Medium	Compiled (FORTRAN)	Windows	Yes	No (Desktop)
OSCA15	Dynamic	Low	Compiled (Not specified)	Windows	Yes	No (Desktop)
STRU05	Not active	Low	Compiled (Not specified)	Windows	Yes	No (Desktop)
JAMM02	Not active	Medium	Interpreted (Java)	Independent (JRE comp.)	Yes/Plugin	Yes (Desktop; Emb.)

TABLE 1 - TECHNOLOGICAL SURVEY CRITERIA (CONTINUATION)						
Sotware	1.3 Use, Distribution, and Modification		1.4 Interface Technology Support		Survey score	
	1.3.1 Use, Distribution, and Modification License Type	1.3.2 Collab. Dev. Model Support	1.4.1 Base Devices (HID)	1.4.2 Advanced Interaction Device Sup.	Total	Normalized
CMAK15	Commercial: Binary; Closed source; Demo: Binary; Closed source	No	Mouse; Keyb.; Trackeable (LeapMotion)	Yes (3D Monit.)	2	5
JMOL15	Free software (GNULesser)	Yes	Mouse; Keyb.	No	3	7,5
VEST14	Commercial: Binary; Closed source; (Students) Freeware: Binary; Closed source	No	Mouse; Keyb.	No	1	2,5
DIAM15	Commercial: Binary; Closed source; Demo: Binary; Closed source	No	Mouse; Keyb.	No	1	2,5
XCRY14	Free software (GNU)	No	Mouse; Keyb.	No	2	5
MERC15	Commercial: Binary; Closed source; Demo: Binary; Closed source	No	Mouse; Keyb.	Yes (3D Monit.)	1	2,5
PYMO18	Commercial: Binary; Closed source; (Students) Python License; Open source	Commercial: No; Source code: Yes	Mouse; Keyb.	Yes (3D Monit.)	1	2,5
DRAW11	Free software (GNU2)	Yes	Mouse; Keyb.	No	2	5
CARI04	Commercial: Binary; Closed source; Demo: Binary; Closed source	No	Mouse; Keyb.	No	0	0
BALL08	Freeware: Binary; Closed source	No	Mouse; Keyb.	No	0	0
LATT04	N/A: Binary; Source avail.	No	Mouse; Keyb.	No	0	0
SCHA14	Free software (GNU)	No	Mouse; Keyb.	No	2	5
ATOM11	Commercial: Binary; Closed source; Demo: Binary; Closed source	No	Mouse; Keyb.	Yes (3D Monit.)	1	2,5
SHEL15	Free software (GNU)	Yes	Mouse; Keyb.	Yes (3D Monit.)	3	7,5
RASM09	Free software (GNU)	No	Mouse; Keyb.	No	1	2,5
CHEM15	Commercial: Binary; Closed source; Demo: Binary; Closed source	No	Mouse; Keyb.	No	1	2,5
QUTE07	Free software (GNU2)	Yes	Mouse; Keyb.	No	2	5
XTAL03	Freeware: Binary; Closed source	No	Mouse; Keyb.	No	0	0
CRYS07	Commercial: Binary; Closed source; Demo: Binary; Closed source	No	Mouse; Keyb.	No	0	0
POWD00	Freeware: Binary; Closed source	No	Mouse; Keyb.	Yes (3D Monit.)	0	0
PLAT13	(Original Fortran): Código-fonte; (Port Windows); Commercial: Binary; Closed source; (Students) Freeware: Binary; Closed source	No	Keyb.	No	1	2,5
GRET00	Freeware: Binary; Closed source	No	Mouse; Keyb.	No	0	0
ORTE14	(Original Fortran): Source code avail.; (Port Windows); Commercial: Binary; Closed source; (Students) Freeware: Binary; Closed source	No	Mouse; Keyb.	No	1	2,5
OSCA15	Commercial: Binary; Closed source; (Students) Freeware: Binary; Closed source	No	Mouse	No	1	2,5
STRU05	Freeware: Binary; Closed source	No	Mouse; Keyb.	No	0	0
JAMM02	N/A: Binary; Closed source	No	Mouse	No	0	0

TABLE 2 - SYNTHESIS SURVEY CRITERIA						
Software	2.1 Synthesis Method	2.2 Interactive Synthesis Process	2.3 Restriction or Limitation in Synthesis Process	2.4 Interactive Atom Selection & Editing	Survey score	
					Total	Normalized
CMAK15	Wyckoff positions	No	No	Yes	2	5
JMOL15	Wyckoff positions	No	No	Yes	2	5
VEST14	Wyckoff positions	No	No	Yes	2	5
DIAM15	Wyckoff positions	No	No	No	1	2,5
XCRY14	Wyckoff positions	No	No	Yes	2	5
MERC15	Wyckoff positions	No	No	No	1	2,5
PYMO18	Wyckoff positions	No	Yes (req. external parametrization)	Yes	1	2,5
DRAW11	Wyckoff positions	No	No	No	1	2,5
CARI04	Wyckoff positions	No	No	Yes	2	5
BALL08	Wyckoff positions	No	No	Yes	2	5
LATT04	Wyckoff positions	No	No	Yes	2	5
SCHA14	Wyckoff positions	No	No	No	1	2,5
ATOM11	Wyckoff positions	No	No	No	1	2,5
SHEL15	Wyckoff positions	No	Yes (req. external app ShelX)	No	0	0
RASM09	Wyckoff positions	No	No	No	1	2,5
CHEM15	Wyckoff positions	No	Yes (req. external parametrization)	Yes	1	2,5
QUTE07	Wyckoff positions	No	Yes (req. external parametrization)	No	0	0
XTAL03	Wyckoff positions	No	Yes (req. external parametrization)	Yes	1	2,5
CRYS07	Wyckoff positions	No	No	No	1	2,5
POWD00	Wyckoff positions	No	No	No	1	2,5
PLAT13	Wyckoff positions	No	No	No	1	2,5
GRET00	Wyckoff positions	No	No	No	1	2,5
ORTE14	Wyckoff positions	No	No	No	1	2,5
OSCA15	Wyckoff positions	No	No	No	1	2,5
STRU05	Wyckoff positions	No	No	No	1	2,5
JAMM02	Wyckoff positions	No	Yes (req. external parametrization)	No	0	0

TABLE 3 - VISUALIZATION SURVEY CRITERIA

Software	3.1 Visual Representation					
	3.1.1 Molecular Atomic Representation Model	3.1.2 Model of Unit Cell Representation	3.1.3 Miller Planes	3.1.4 Miller Directions	3.1.5 Visualization Support Features	
					3.1.5.1 Multiple Cells	3.1.5.2 Sections
CMAK15	Balls and sticks; Space Filling; Others (Skeletal; Polyhedral)	Whole	Yes	Yes	Yes	Yes
JMOL15	Balls and sticks; Space Filling; Others (Skeletal)	Whole	Yes	No	Yes	Yes
VEST14	Balls and sticks; Space Filling; Others (Skeletal)	Whole	Yes	Yes	Yes	Yes
DIAM15	Balls and sticks; Space Filling; Others (Skeletal)	Whole	Yes	Yes	Yes	No
XCRY14	Balls and sticks; Space Filling; Others (Skeletal)	Whole	Yes	No	Yes	Yes
MERC15	Balls and sticks; Space Filling; Others (Skeletal)	Whole	Yes	No	Yes	Yes
PYMO18	Balls and sticks; Space Filling; Others (Skeletal)	Whole	No	No	Yes	Yes
DRAW11	Balls and sticks; Others (Skeletal; Polyhedral)	Whole	Yes	Yes	Yes	No
CARI04	Balls and sticks; Space Filling; Others (Polyhedral)	Whole	Yes	Yes	Yes	Yes
BALL08	Balls and sticks; Others (Polyhedral)	Whole	No	No	Yes	No
LATT04	Space Filling	Whole	No	No	Yes	No
SCHA14	Balls and sticks; Space Filling; Others (Skeletal; Ortep)	Whole	No	No	Yes	No
ATOM11	Balls and sticks; Space Filling; Others (Skeletal; Polyhedral)	Whole	No	No	Yes	No
SHEL15	Balls and sticks	Whole	No	No	No	No
RASM09	Balls and sticks; Space Filling; Others (Skeletal)	Whole	No	No	Yes	No
CHEM15	Balls and sticks; Space Filling; Others (Skeletal)	Whole	No	No	No	No
QUTE07	Balls and sticks; Space Filling; Others (Skeletal)	Whole	No	No	No	No
XTAL03	Balls and sticks; Space Filling; Others (Ortep; Polyhedral)	Whole	No	No	No	No
CRYS07	Balls and sticks; Space Filling	Whole	No	No	Yes	No
POWD00	Balls and sticks	Whole	No	No	No	No
PLAT13	Balls and sticks; Others (Skeletal; Ortep)	Whole	No	No	Yes	No
GRET00	Balls and sticks	Whole	No	No	Yes	No
ORTE14	Balls and sticks; Others (Skeletal; Ortep)	Whole	No	No	Yes	No
OSCA15	Balls and sticks; Others (Skeletal; Ortep)	Whole	No	No	Yes	No
STRU05	Others (Polyhedral)	Whole	No	No	No	No
JAMM02	Balls and sticks; Space Filling; Others	Whole	No	No	No	No

TABLE 3 - VISUALIZATION SURVEY CRITERIA (CONTINUATION)				
Software	**3.1 Visual Representation (cont.)**		**3.2 Visualization Features**	
	3.1.5 Visualization Support Features (cont.)		**3.2.1 Visual Perception Features**	**3.2.2 Projection Type**
	3.1.5.3 Axis Vectors	**3.1.5.4 Other Auxiliary Resources**		
CMAK15	Cartesian (xyz)	Borders & Faces	Shapes & perspective; Color; Opacity; Luminosity; Depth	Conic & Axonometric
JMOL15	Cartesian (xyz); Crystallographic (abc)	Borders & Faces	Shapes & perspective; Color; Opacity; Luminosity	Conic & Axonometric
VEST14	Cartesian (xyz); Crystallographic (abc)	Borders & Faces	Shapes & perspective; Color; Opacity; Luminosity; Depth	Conic & Axonometric
DIAM15	Cartesian (xyz); Crystallographic (abc)	Borders	Shapes & perspective; Color; Opacity; Luminosity; Depth	Conic & Axonometric
XCRY14	Cartesian (xyz)	Borders	Shapes & perspective; Color; Opacity; Luminosity; Depth	Conic & Axonometric
MERC15	Crystallographic (abc)	Borders	Shapes & perspective; Color; Opacity; Luminosity; Depth	Axonometric
PYMO18	Cartesian (xyz)	No	Shapes & perspective; Color; Opacity; Luminosity; Depth	Conic & Axonometric
DRAW11	Crystallographic (abc)	Borders & Faces	Shapes & perspective; Color; Opacity; Luminosity	Conic & Axonometric
CARI04	Cartesian (xyz); Crystallographic (abc)	Borders	Shapes & perspective; Color; Opacity; Luminosity	Axonometric
BALL08	Cartesian (xyz)	Borders	Shapes & perspective; Color	Conic & Axonometric
LATT04	Cartesian (xyz)	Faces	Shapes & perspective; Color; Opacity; Luminosity	Conic & Axonometric
SCHA14	No	No	Shapes & perspective; Color; Opacity; Luminosity; Depth	Axonometric
ATOM11	Crystallographic (abc)	Faces	Shapes & perspective; Color	Axonometric
SHEL15	Crystallographic (abc)	Borders	Shapes & perspective; Color; Opacity; Luminosity	Conic & Axonometric
RASM09	No	No	Shapes & perspective; Color	Axonometric
CHEM15	Cartesian (xyz)	No	Shapes & perspective; Color; Opacity; Luminosity	Conic & Axonometric
QUTE07	No	No	Shapes & perspective; Color; Opacity; Luminosity; Depth	Axonometric
XTAL03	Crystallographic (abc)	Borders	Shapes & perspective; Color; Opacity; Luminosity;	Axonometric
CRYS07	Cartesian (xyz); Crystallographic(abc)	Borders	Shapes & perspective; Color	Axonometric
POWD00	Crystallographic (abc)	Borders	Shapes & perspective; Color	Conic & Axonometric
PLAT13	Cartesian (xyz)	No	Shapes & perspective; Color; Opacity; Luminosity;	Axonometric
GRET00	Crystallographic (abc)	Borders	Shapes & perspective; Color	Axonometric
ORTE14	Cartesian (xyz)	No	Shapes & perspective; Color	Axonometric
OSCA15	Cartesian (xyz)	No	Shapes & perspective; Color	Axonometric
STRU05	No	No	Shapes & perspective; Color	Axonometric
JAMM02	Cartesian (xyz)	No	Shapes & perspective; Color; Opacity; Luminosity; Depth	Axonometric

TABLE 3 - VISUALIZATION SURVEY CRITERIA (CONTINUATION)				
Software	**3.2 Visualization Features (cont.)**		**Survey score**	
	3.2.3 Stereographic Support	**3.2.4 Rendering Modes**	**Total**	**Normalized**
CMAK15	Anaglyph; Side-by-side; Stereogram	Flat; Sketch/Cartoon; Realistic	8	20
JMOL15	Anaglyph; Side-by-side; Stereogram	Flat; Sketch/Cartoon; Realistic	7	17,5
VEST14	No	Flat; Realistic	8	20
DIAM15	Anaglyph; Side-by-side; Stereogram	Flat; Sketch/Cartoon; Realistic	7	17,5
XCRY14	Anaglyph	Flat; Sketch/Cartoon; Realistic	6	15
MERC15	Anaglyph; Side-by-side; Stereogram	Flat; Sketch/Cartoon; Realistic	5	12,5
PYMO18	Anaglyph; Side-by-side; Stereogram	Flat; Sketch/Cartoon; Realistic	5	12,5
DRAW11	No	Flat	5	12,5
CARI04	No	Flat	5	12,5
BALL08	Anaglyph	Flat; Sketch/Cartoon; Realistic	3	7,5
LATT04	No	Realístico	2	5
SCHA14	Anaglyph	Flat; Sketch/Cartoon; Realistic	3	7,5
ATOM11	Anaglyph; Side-by-side; Stereogram	Flat; Sketch/Cartoon	1	2,5
SHEL15	Anaglyph; Side-by-side; Stereogram	Flat; Sketch/Cartoon; Realistic	2	5
RASM09	Stereogram	Flat; Sketch/Cartoon	1	2,5
CHEM15	No	Flat; Sketch/Cartoon; Realistic	2	5
QUTE07	No	Flat; Sketch/Cartoon; Realistic	2	5
XTAL03	No	Flat; Sketch/Cartoon; Realistic	1	2,5
CRYS07	No	Sketch/Cartoon	2	5
POWD00	Stereogram	Sketch/Cartoon	1	2,5
PLAT13	Anaglyph	Sketch/Cartoon	1	2,5
GRET00	No	Sketch/Cartoon	1	2,5
ORTE14	Anaglyph; Side-by-side; Stereogram	Flat; Sketch/Cartoon	1	2,5
OSCA15	No	Flat; Sketch/Cartoon	1	2,5
STRU05	No	Flat	0	0
JAMM02	Anaglyph	Flat; Sketch/Cartoon	1	2,5

TABLE 4 - NAVIGATION AND INTERACTIVITY SURVEY CRITERIA

Software	4.1 User Interface		4.2 Base Interaction	4.3 Advanced Interaction		
				4.3.1 Automatic rotations	4.3.2 Guided animations	4.3.3 Scale Transition
CMAK15	GUI; Hierarchical menus	Friendly	Zoom; Translation; Rotation	Yes	Yes	No
JMOL15	GUI; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	Yes	Yes	No
VEST14	GUI; Hierarchical menus	Friendly	Zoom; Translation; Rotation	No	No	No
DIAM15	GUI; No Hierarchical menus	Unfriendly	Zoom; Rotation	Yes	Yes	No
XCRY14	GUI; Hierarchical menus	Friendly	Zoom; Translation; Rotation	No	No	No
MERC15	GUI; Hierarchical menus	Friendly	Zoom; Rotation	Yes	No	No
PYMO18	GUI; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	Yes	Yes	No
DRAW11	GUI; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	No	No	No
CARI04	GUI; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	No	No	No
BALL08	GUI; Hierarchical menus	Friendly	Zoom; Translation; Rotation	Yes	No	No
LATT04	GUI; Hierarchical menus	Friendly	Zoom; Translation; Rotation	No	No	No
SCHA14	Text; No Hierarchical menus	Unfriendly	Zoom; Rotation	No	No	No
ATOM11	GUI; Hierarchical menus	Friendly	Zoom; Translation; Rotation	Yes	No	No
SHEL15	GUI; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	No	No	No
RASM09	GUI; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	No	Yes	No
CHEM15	GUI; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	No	No	No
QUTE07	GUI; Hierarchical menus	Friendly	Zoom; Translation; Rotation	No	No	No
XTAL03	Text; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	No	No	No
CRYS07	GUI; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	No	No	No
POWD00	GUI; No Hierarchical menus	Unfriendly	Zoom; Rotation	No	No	No
PLAT13	Text; No Hierarchical menus	Unfriendly	Zoom; Rotation	No	No	No
GRET00	GUI; No Hierarchical menus	Unfriendly	Zoom; Translation; Rotation	No	No	No
ORTE14	Text; No Hierarchical menus	Unfriendly	Zoom; Rotation	No	No	No
OSCA15	GUI; No Hierarchical menus	Unfriendly	Zoom; Rotation	No	No	No
STRU05	GUI; No Hierarchical menus	Unfriendly	Zoom; Rotation	No	No	No
JAMM02	GUI; Hierarchical menus	Friendly	Zoom; Rotation	Yes	No	No

TABLE 4 - NAVIGATION AND INTERACTIVITY SURVEY CRITERIA (CONTINUATION)				
Software	4.3 Advanced Interaction (cont.)		Survey score	
	4.3.4 Dynamic Occlusion Management	4.3.5 Preconfigured Viewpoints	Total	Normalized
CMAK15	No	Yes (Directions & Orthogonal Perspectives)	4	10
JMOL15	No	Yes (Directions & Orthogonal Perspectives)	3	7,5
VEST14	No	Yes (Directions & Orthogonal Perspectives)	2	5
DIAM15	No	Yes (Directions & Orthogonal Perspectives)	2	5
XCRY14	No	No	2	5
MERC15	No	Yes (Directions & Orthogonal Perspectives)	2	5
PYMO18	No	Yes (Directions & Orthogonal Perspectives)	3	7,5
DRAW11	No	No	1	2,5
CARI04	No	Yes (Directions & Orthogonal Perspectives)	1	2,5
BALL08	No	Yes (Directions & Orthogonal Perspectives)	3	7,5
LATT04	No	No	2	5
SCHA14	No	Yes (Directions & Orthogonal Perspectives)	0	0
ATOM11	No	No	3	7,5
SHEL15	No	Yes (Directions & Orthogonal Perspectives)	1	2,5
RASM09	No	Yes (Directions & Orthogonal Perspectives)	2	5
CHEM15	No	Yes (Directions & Orthogonal Perspectives)	1	2,5
QUTE07	No	No	2	5
XTAL03	No	Yes (Directions & Orthogonal Perspectives)	1	2,5
CRYS07	No	Yes (Directions & Orthogonal Perspectives)	1	2,5
POWD00	No	Yes (Directions & Orthogonal Perspectives)	0	0
PLAT13	No	Yes (Directions & Orthogonal Perspectives)	0	0
GRET00	No	Yes (Directions & Orthogonal Perspectives)	1	2,5
ORTE14	No	Yes (Directions & Orthogonal Perspectives)	0	0
OSCA15	No	Yes (Directions & Orthogonal Perspectives)	0	0
STRU05	No	Yes (Directions & Orthogonal Perspectives)	0	0
JAMM02	No	Yes (Directions & Orthogonal Perspectives)	2	5

TABLE 5 - DIDACTIC SURVEY CRITERIA						
Software	**5.1 Knowledge Required from User**	**5.2 Content Generation & Publication Support**				**5.3 Didactic Features**
		5.2.1 Display support / External portability	**5.2.2 2D printing support**	**5.2.3 3D printing support**	**5.2.4 Internet Publishing Platform**	**5.3.1 Didactic narratives support**
CMAK15	Crystallography (Space Groups)	3D Model (VRML; QTR; POV)	Bitmap & Vectorial Image	Yes (STL)	No	Text/ Annotations
JMOL15	Crystallography (Space Groups)	Full Application; Widget	Bitmap & Vectorial Image	No	No	Text/ Annotations
VEST14	Crystallography (Space Groups)	3D Model (VRML; POV)	Bitmap & Vectorial Image	No	No	Text/ Annotations
DIAM15	Crystallography (Space Groups)	3D Model (POV)	Bitmap & Vectorial Image	No	No	Text/ Annotations
XCRY14	Crystallography (Space Groups)	No	Bitmap & Vectorial Image	No	No	No
MERC15	Crystallography (Space Groups)	3D Model (POV)	Bitmap Image	Yes (STL)	No	No
PYMO18	Crystallography (Space Groups)	3D Model (VRML)	Bitmap Image	No	No	No
DRAW11	Crystallography (Space Groups)	3D Model (POV)	Bitmap & Vectorial Image	No	No	No
CARI04	Crystallography (Space Groups)	No	Bitmap Image	No	No	Text/ Annotations
BALL08	Crystallography (Space Groups)	No	Bitmap Image	No	No	No
LATT04	Crystallography (Space Groups)	Full Application; Widget	Bitmap Image	No	No	No
SCHA14	Crystallography (Space Groups)	No	Bitmap & Vectorial Image	No	No	Text/ Annotations
ATOM11	Crystallography (Space Groups)	3D Model (VRML; POV)	Bitmap & Vectorial Image	No	No	No
SHEL15	Crystallography (Space Groups)	No	Bitmap Image	No	No	No
RASM09	Crystallography (Space Groups)	3D Model (VRML; POV)	Bitmap & Vectorial Image	No	No	No
CHEM15	Crystallography (Space Groups)	No	No	No	No	Text/ Annotations
QUTE07	Crystallography (Space Groups)	No	Bitmap Image	No	No	No
XTAL03	Crystallography (Space Groups)	No	Bitmap Image	No	No	No
CRYS07	Crystallography (Space Groups)	3D Model (VRML; POV)	Bitmap Image	No	No	No
POWD00	Crystallography (Space Groups)	3D Model (POV)	Bitmap & Vectorial Image	No	No	No
PLAT13	Crystallography (Space Groups)	3D Model (POV)	Vectorial Image (PS)	No	No	No
GRET00	Crystallography (Space Groups)	3D Model (POV)	Bitmap & Vectorial Image	No	No	No
ORTE14	Crystallography (Space Groups)	3D Model (POV)	Vectorial Image	No	No	No
OSCA15	Crystallography (Space Groups)	3D Model (POV)	Bitmap & Vectorial Image	No	No	No
STRU05	Crystallography (Space Groups)	3D Model (VRML; POV)	Bitmap & Vectorial Image	No	No	No
JAMM02	Crystallography (Space Groups)	Full Application; Widget	Vectorial Image	No	No	Text/ Annotations

TABLE 5 - DIDACTIC SURVEY CRITERIA						
Software	5.3 Didactic Features (cont.)		5.4 End-User Documentation & Support		Survey score	
	5.3.2 Library of Crystallographic structures	5.3.3 Incremental Construction and Visualization of Structures	5.4.1 Available Support	5.4.2 Available Documentation	Total	Normalized
CMAK15	Yes	No	Paying customers only (Forum; Trackers; E-mail; Phone)	Yes (Manual; Tutorials)	5	12,5
JMOL15	No	No	Yes (Forum; Trackers)	Yes (Manual; Tutorials)	4	10
VEST14	No	No	Yes (Forum)	Yes (Manual)	3	7,5
DIAM15	Yes	No	Yes (Forum; E-mail)	Yes (Manual)	4	10
XCRY14	No	No	Yes (Forum)	Yes (Manual)	3	7,5
MERC15	Yes	No	Paying customers only (Forum; Trackers; E-mail)	Yes (Manual; Tutorials)	4	10
PYMO18	No	No	Yes (Forum; Trackers); Paying customers only (E-mail)	Yes (Manual; Tutorials)	2	5
DRAW11	No	No	No	Yes (Manual)	2	5
CARI04	Yes	No	Paying customers only (Forum; Trackers; E-mail)	Yes (Manual)	3	7,5
BALL08	No	No	No	Yes (Manual)	1	2,5
LATT04	Yes	No	No	Yes (Manual)	3	7,5
SCHA14	No	No	Yes (E-mail)	Yes (Manual)	3	7,5
ATOM11	No	No	Paying customers only (E-mail)	Yes (Manual)	3	7,5
SHEL15	No	No	Yes (Forum; Trackers)	Yes (Manual)	2	5
RASM09	No	No	Yes (Forum; Trackers)	Yes (Manual; Tutorials)	3	7,5
CHEM15	No	No	Paying customers only (E-mail)	Yes (Manual)	2	5
QUTE07	No	No	No	No	0	0
XTAL03	Yes	No	Yes (E-mail)	Yes (Manual)	3	7,5
CRYS07	No	No	No	Yes (Manual)	1	2,5
POWD00	No	No	Yes (E-mail)	Yes (Manual)	3	7,5
PLAT13	No	No	Paying customers only (E-mail)	Yes (Manual)	2	5
GRET00	No	No	No	Yes (Manual)	2	5
ORTE14	No	No	Paying customers only (E-mail)	Yes (Manual)	2	5
OSCA15	No	No	No	Yes (Manual)	2	5
STRU05	No	No	Paying customers only (E-mail)	Yes (Manual)	3	7,5
JAMM02	No	No	No	No	1	2,5

TABLE 6 - CRITERIA SUMMARY													
Software	Overall Rank	Survey General score		Survey 1 score		Survey 2 score		Survey 3 score		Survey 4 score		Survey 5 score	
		Total	Norm.% (/40*100)	Total	Norm.% /40*100	Total	Norm.% /40*100	Total	Norm.% /40*100	Total	Norm.% /40*100	Total	Norm.% /40*100
CMAK15	1	21	52,5	2	5	2	5	8	20	4	10	5	12,5
JMOL15	2	19	47,5	3	7,5	2	5	7	17,5	3	7,5	4	10
VEST14	3	16	40	1	2,5	2	5	8	20	2	5	3	7,5
DIAM15	4	15	37,5	1	2,5	1	2,5	7	17,5	2	5	4	10
XCRY14	4	15	37,5	2	5	2	5	6	15	2	5	3	7,5
MERC15	5	13	32,5	1	2,5	1	2,5	5	12,5	2	5	4	10
PYMO18	6	12	30	1	2,5	1	2,5	5	12,5	3	7,5	2	5
DRAW11	7	11	27,5	2	5	1	2,5	5	12,5	1	2,5	2	5
CARI04	7	11	27,5	0	0	2	5	5	12,5	1	2,5	3	7,5
BALL08	8	9	22,5	0	0	2	5	3	7,5	3	7,5	1	2,5
LATT04	8	9	22,5	0	0	2	5	2	5	2	5	3	7,5
SCHA14	8	9	22,5	2	5	1	2,5	3	7,5	0	0	3	7,5
ATOM11	8	9	22,5	1	2,5	1	2,5	1	2,5	3	7,5	3	7,5
SHEL15	9	8	20	3	7,5	0	0	2	5	1	2,5	2	5
RASM09	9	8	20	1	2,5	1	2,5	1	2,5	2	5	3	7,5
CHEM15	10	7	17,5	1	2,5	1	2,5	2	5	1	2,5	2	5
QUTE07	11	6	15	2	5	0	0	2	5	2	5	0	0
XTAL03	11	6	15	0	0	1	2,5	1	2,5	1	2,5	3	7,5
CRYS07	12	5	12,5	0	0	1	2,5	2	5	1	2,5	1	2,5
POWD00	12	5	12,5	0	0	1	2,5	1	2,5	0	0	3	7,5
PLAT13	12	5	12,5	1	2,5	1	2,5	1	2,5	0	0	2	5
GRET00	12	5	12,5	0	0	1	2,5	1	2,5	1	2,5	2	5
ORTE14	12	5	12,5	1	2,5	1	2,5	1	2,5	0	0	2	5
OSCA15	12	5	12,5	1	2,5	1	2,5	1	2,5	0	0	2	5
STRU05	13	4	10	0	0	1	2,5	0	0	0	0	3	7,5
JAMM02	13	4	10	0	0	0	0	1	2,5	2	5	1	2,5

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