

A Hybrid Data Base: Quantum Chemistry Literature Data Base II —New Concept and New Methodology—

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Quantum Chemistry Literature Data Base (QCLDB, http://qcldb2.ims.ac.jp) is a database of those papers published after 1978 which treat only ab initio calculations of atomic and molecular electronic structures. From about thirty core journals they are collected, surveyed, and given proper tags revealing the content and essence by theoretical and computational chemists. Those theoretical works even without reporting any computational results are also collected which are judged to have significant relevance to ab initio calculations, while no semiempirical calculations are included. QCLDB has been maintained by Quantum Chemistry Data Base Group (QCDBG). QCLDB provides information not only to chemists but also to both theoretical and experimental scientists, who want to know the state of the art theoretical aspects of chemical substances and materials. Although the last version, "QCLDB I," has been sustained and utilized steadily for almost a quarter century up to the end of 20th century, new circumstances related to the internet facility imposed re-construction of QCLDB I on QCDBG. A policy of the academic database of references has been established. The policy emphasizes that there should be a balance between data collection as research itself and utility for users. According to the policy, an unprecedented hybrid and highly academic database, QCLDB II, has been constructed and is open to all scientists via the work site.

There have been published a huge number of ab initio electronic structure calculations of molecules and molecular complexes in the journals of a number of different fields worldwide. Scientists who want to know and utilize the results of such calculations have a difficult time finding proper references of a manageable number. Using commercial databases, too much information is collected by the combination of keywords and thus the really necessary information cannot be found. About 30 years ago a group of Japanese chemists headed by Kimio Ohno of Hokkaido University dared to construct a database of references of ab initio calculations. He initiated a project to work up the database in a computer readable form, "Quantum Chemistry Literature Data Base (QCLDB)" on which we have reported in previous papers.[1,2] Richards and co-workers at Oxford had been collecting ab initio papers[3] prior to our start, however they ended their project after ours began.

The data collected in QCLDB were first published in book form in 1982 by Elsevier,[4] and has been supplemented annually as a special issue of *THEOCHEM* (*J. Mol. Struct.*) as shown in Table 1.[4–26] From 2006, the book form is in *J. Comput. Chem. Jpn.*[27,28] Besides the printed version users can use an electronic version with a retrieval program, either by making direct access to a computer at the Institute for Molecular Science (IMS), Okazaki Japan, or by subscribing to the online version from the Japan Association for International Chemical Information (JAICI). From the very beginning we have been occasionally modifying data collection policy and the database format in order to keep up with the rapid progress and expansion of ab initio calculations.

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Table 1. History of QCLDB in 1978–2006

Version	Content	Reference No.
QCLDB I	"Quantum Chemistry Literature Data Base—Bibliography of Ab Initio Calculations for 1978–1980"	
	Supplement 1, "Bibliography of Ab Initio Calculations for 1981"	4
	Supplement 2, "Bibliography of Ab Initio Calculations for 1982"	5
	Supplement 3, "Bibliography of Ab Initio Calculations for 1983"	6
	Supplement 4, "Bibliography of Ab Initio Calculations for 1984"	7
	Supplement 5, "Bibliography of Ab Initio Calculations for 1985"	8
	Supplement 6, "Bibliography of Ab Initio Calculations for 1986"	9
	Supplement 7, "Bibliography of Ab Initio Calculations for 1987"	10
	Supplement 8, "Bibliography of Ab Initio Calculations for 1988"	11
	Supplement 9, "Bibliography of Ab Initio Calculations for 1989"	12
	"Cumulative Substance and Author Indexes of the Bibliography of Ab Initio Calculations for 1978–1989"	
	Supplement 10, "Bibliography of Ab Initio Calculations for 1990"	13
	Supplement 11, "Bibliography of Ab Initio Calculations for 1991"	14
	Supplement 12, "Bibliography of Ab Initio Calculations for 1992"	15
	Supplement 13, "Bibliography of Ab Initio Calculations for 1993"	16
	Supplement 14, "Bibliography of Ab Initio Calculations for 1994"	17
	Supplement 15, "Bibliography of Ab Initio Calculations for 1995"	18
	Supplement 16, "Bibliography of Ab Initio Calculations for 1996"	19
	Supplement 17, "Bibliography of Ab Initio Calculations for 1997"	20
	Supplement 18, "Bibliography of Ab Initio Calculations for 1998"	21
	Supplement 19, "Bibliography of Ab Initio Calculations for 1999"	22
	Supplement 20, "Bibliography of Ab Initio Calculations for 2000"	23
QCLDB II	Supplement 21, "Bibliography of Ab Initio Calculations for 2001"	24
	Supplement 22, "Bibliography of Ab Initio Calculations for 2002"	25
	Supplement 23, "Bibliography of Ab Initio Calculations for 2003"	26
	"Quantum Chemistry Literature Data Base II Bibliography of Ab Initio Calculation for 2004"	27
	"Quantum Chemistry Literature Data Base II Bibliography of Ab Initio Calculation for 2005"	28

QCLDB has been maintained in a main frame computer, and the system of data collection and retrieval has been steadily managed by QCDBG. At around the middle of 1990–2000, rapid progress in computers and internet media made it difficult to keep the system in its original version. Actually there arose three problems. The first was the noticeable increase of references containing ab initio calculations. The second was pervasion of the internet. The third was appearance of commercial databases. It was discussed in QCDBG whether QCLDB should be maintained even under the new circumstances. It was decided to maintain it in an entirely new style with a definite policy. This development, from the original QCLDB I to the second generation QCLDB II, will be described.

Before presenting a detailed explanation of QCLDB II, it is necessary to state the most unique feature of the QCLDB system among the existing databases in chemistry and physical sciences. This is the literature database and it is prepared by a group of ab initio calculation specialists from both in and outside Japan. They have selected, classified, and evaluated work done by authors from different fields. This means that a normalization has been performed for the ensemble of raw data of different quality. We are proud to have prepared a database of high quality.

Fundamental Principles and Policies

We made new policies and rules for re-constructing the database.

(1) Our prime policy is that data production from journals must be the active research of the collectors and reviewers. It is thus important that QCLDB II should maintain balance between internal research goals, and services for end users of the database. When an excessive burden is imposed on the collectors and reviewers to improve the facility, we shall give up improvement for balance. Thus, the term "hybrid" means that there is a balance between the burden on collectors/reviewers and the response to user requests.

(2) QCLDB II is oriented more to chemistry than to quantum theory. This characteristic of QCLDB II is an important difference from QCLDB I. Thus, literature surveyed in data collections should include explicitly the properties of atoms, molecules, and their aggregates. Inclusion or exclusion of related literature (e.g. with theory only and with macroscopic properties) is judged by collectors and reviewers. Journals surveyed for QCLDB II are basically those of chemistry. The QCDBG has the option to select those of peripheral fields such as biochemistry and material science. The core journals are selected by the group. To each journal, collectors and reviewers are assigned.

(3) According to policy (1), the input-data format has been revised (from 2001). Eight items are arranged sequentially. The revised format is in line with the chemistry orientation of QCLDB II. More importantly, bothersome tasks (i.e. construction of molecular formulae) for generating input data have been diminished considerably.

Table 2. Core Journals Covered in QCLDB II

CODEN	Abbreviated journal names	Data collected[a)]
ACIEF5	*Angew. Chem. Int. Ed.* (since 2000)	184
BCSJA8	*Bull. Chem. Soc. Jpn.*	2
CHCOFS	*Chem. Commun.* (since 1997)	77
CHPLBC	*Chem. Phys. Lett.*	465
CJCHAG	*Can. J. Chem.*	40
CMPHC2	*Chem. Phys.*	213
IJQCB2	*Int. J. Quantum Chem.*	317
INOCAJ	*Inorg. Chem.*	233
JACSAT	*J. Am. Chem. Soc.*	559
JCCHDD	*J. Comput. Chem.*	98
JCPSA6	*J. Chem. Phys.*	912
JMOSB4	*J. Mol. Struct.*	600
JOCEAH	*J. Org. Chem.*	319
JPCAFH	*J. Phys. Chem. A* (since Vol. 101, 1997)	971
JPCBFK	*J. Phys. Chem. B* (since Vol. 101, 1997)	682
JPOCEE	*J. Phys. Org. Chem.*	57
MOPHAM	*Mol. Phys.*	103
OBCRAK	*Org. Biomol. Chem.* (since 2003)	34
ORGND7	*Organometallics* (Washington, DC.)	185
PLRAAN	*Phys. Rev. A*	272
PPCPFQ	*Phys. Chem. Chem. Phys.* (since 1999)	174
PRBMDO	*Phys. Rev. B*	937
SUSCAS	*Surf. Sci.*	152
TCACFW	*Theoret. Chem. Acc.* (since Vol. 96, 1997)	62
THEODJ	*THEOCHEM*	440

a) Number of articles collected in 2005.

Process of Construction and Data Accumulation of QCLDB II

An important work of our group is selection of core journals. The selection cannot be made automatically. Impact factor is a criterion for assessing the quality of chemistry journals. But, a larger value does not mean necessarily that the journal contains highly academic research results. Through discussion of the academic quality of chemistry journals, we selected the 26 journals shown in Table 2. We make it a rule to check whether our selection is appropriate or not every year, considering the number of papers annually collected from each journal.

Table 3 shows the information which is collected from the literature. In author names, special symbols such as umlauts (ö) may be omitted (e.g., from Löwdin to Lowdin). Journal names are given in CODENs in Table 2. Year is the publication year. Substance formula is given as C6H6, C5H8O and H2O for C_6H_6, C_5H_8O and H_2O, respectively. Our general rules follow the style of the formula index of Chemical Abstracts, except for the expression of the assignment of charge (vide infra). Carbon atoms come first, hydrogen atoms next, and then other atoms follow them in alphabetical order. Charged species (cations and anions) are signified with the charge number, with 1 omitted (e.g., not H4N+1, but H4N+ for NH_4^+). Element names are expressed in the usual way, with one or two letters (upper and lower case). Until 2001, a capital letter followed by a period was used as the second character of the element symbols in QCLDB I. For example, NA. represents Na. No such

Table 3. Information Collected from Articles

Author names
Journal names
Year
Substance formula
IUPAC names or common names of the compound
Computational methods
Basis sets
Physical properties (codes in Table 4)
Comments

convention is employed in QCLDB II on the web. IUPAC names or common names of the compound such as benzene, 1-methoxy-1,3-butadiene, and water are used. For molecular complexes, monomer and/or complex formulae are used (e.g., H2O, H3N and H5NO for water–ammonia complex, C2H4 for polyethylene, and ClNa for NaCl crystal), and may be explicitly identified here. Names of complex systems are sometimes difficult to specify (e.g. an O_2 molecule adsorbed on the step site of a MgO surface). Braces { } are introduced in this item to allow flexible presentations, e.g. {an O_2 molecule on a MgO surface}. Informal but informative contents are welcome in the braces. Use of the braces complements the lack of information for large systems in the substance formula. In computational methods, key codes were used for the data up to 2000. From 2001, popular abbreviations in the literature are used. Namely keywords in Gaussian and GAMESS programs are good examples. In basis sets, key codes were used for data up to 2000. Popular abbreviations such as 6-31+G(d) and DZP are used from 2001. Also in physical properties, key codes shown in Table 4 are used. In comments, any supplementary information considered to be important by the abstractor is included. This item must involve free keywords representing what the authors intended, found out, and postulated. The comment is the central content in QCLDB II. The quality of QCLDB II is determined mainly by this. This is required by policy (1): data are collected in the literature survey as a first step of research.

In QCLDB I, sometimes collectors took great pains extracting molecular formulae of calculated molecular complexes. For instance, in some papers, only vague compound names are described, and molecular formulae cannot be elucidated. As for large systems, such as porphyrin complexes and surface–adsorbate interacting systems, molecular formulae do not have significant meaning. Thus, when the formulae are unclear in the literature, they may be omitted from QCLDB II data. Also when only small molecules H_2, H_2O, HCl, NH_3, H_2S,… are calculated as a benchmark test of theory and methodology, those may be omitted in the formula section. In order to compensate for the omission, detailed explanations are reported in the compound name and comment frames. Besides formal compound names non-standard but suggestive descriptions of calculated systems are allowed by the use of braces { }. Examples of usage of braces are {typical small molecules}, {H2 adsorbed on SiO surface}, and {model molecules of single-walled carbon nanotubes}.

Data collectors are experts of chemistry and data collection is the first step of their research. Therefore, data accumulated in

Table 4. Codes for Properties

Key code	Contents
Onel:	One-electron properties, dipole, quadrupole moment, charge density map, orbital assignment, and interaction
Geom:	Properties involving change of geometry, potential energy surface, geometry optimization, conformation analysis, vibrational analysis, stereochemistry
Dynm	Dynamic properties, polarizability, hyperpolarizability, scattering factor
Vbro	Vibronic interaction, Jahn–Teller splitting, Lambda-type doubling, nonadiabatic coupling
Excd	Excited states (bound states), photochemistry, intersystem crossing, excimer, energy relaxation, photochemical reaction
Ionz	Ionization, ionization potential, electron affinity
Intn	Molecular interaction, dimer, charge-transfer complex, hydrogen-bond, surface–adsorbate interaction
Reac	Chemical reaction, transition state, reaction coordinate, rate constant
Magn	Magnetic properties, *g*-value, coupling constant
Spec	Spectroscopic data, UV, NMR, IR, ESR, MASS, photoelectron spectra
Thrm	Thermodynamic properties, heat of formation, binding energy, heat capacity, entropy, free energy
Relv	Relativistic effects, one-, two-, or four-component relativistic calculations
Fild	Solvent effect and external field effect, self-consistent reaction field, Madelung potential
PELS	Miscellaneous

Table 5. An Example of Input Records

ID:	68905
Authors:	Ishimoto T, Tachikawa M, Yamauchi M, Kitagawa H, Tokiwa H, Nagashima U
Journal:	CHPLBC, **Volume**: 372, **Pages**: 503–507, **Year**: 2003
Substances:	HPd4-, DPd4-, HPd6-, DPd6-
Compounds:	{hydrogen-absorbing Pd cluster anions}
Methods:	HF, MP2
Basis sets:	3-21G(d, p), LANL2DZ
Properties:	geom, onel
Comments:	isotope effect of hydrogen-absorbing Pd ultra-fine particle, multi-component MO theory, MC MO, hydrogen and deuteron as quantum waves, geometry optimization, exponent of hydrogen and deuteron wave, Mulliken population analysis, X-ray powder diffraction

QCLDB accurately contain the essence of publications in the core literature. That is, the content of QCLDB is not a mere list of apparent keywords. QCLDB is not comprehensive but is oriented toward quality literature, and from the collected data users may find target information from the well analyzed description.

Table 5 shows an example of a input record where each item is arrayed sequentially. In the compound name entry, calculated species are shown in braces, because the interacting systems cannot be expressed by IUPAC nomenclature. They are of chemical significance, and are informative for QCLDB users. The presentation is believed to offer as a whole what users want to know.

According to the rules of data input, QCLDB data are collected and reviewed by participating chemists every half year. Collectors and reviewers are assigned to core journals in Table 2. We have the responsibility to match the assignment of core journals with the research interests of collectors and reviewers. When collectors finish their tasks, they contact reviewers via e-mail to request examination of the collected data. The collection and review system has been maintained from QCLDB I and seems to assure the quality of the accumulated data.

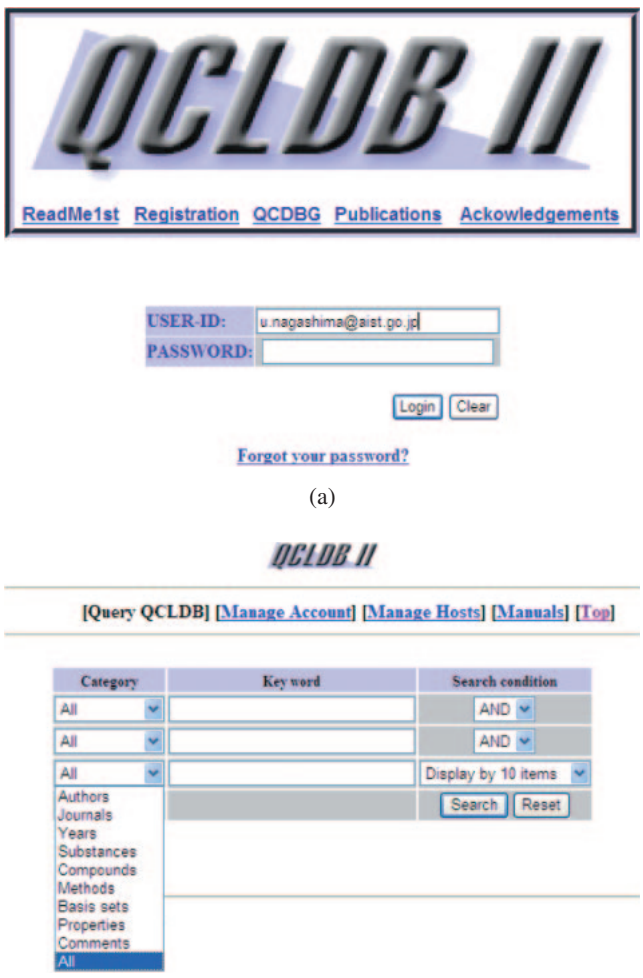


Figure 1. (a) Top window of QCLDB II. (b) Query QCLDB page.

Example 1

Category	Key word	Search condition
Authors	Nagashima$	AND
Substances	Pd$	AND
Basis sets		Display by 10 items
		Search Reset

Example 2

Category	Key word	Search condition
Compounds	$porphy$	AND
Methods	$SAC-CI$	AND
All	$magnetic$	Display by 10 items
		Search Reset

(a)

Example 1

<<< Back | Display by 10 items | Next >>>

1 of 2
ID: 68905
Authors: Ishimoto T, Tachikawa M, Yamauchi M, Kitagawa H, Tokiwa H, Nagashima U
Journal: CHPLBC
Volumes: 372
Pages: 503-507
Years: 2003
Substances: HPd4-, DPd4-, HPd6-, DPd6-
Compounds: (hydrogen-absorbing Pd cluster anions)
Methods: HF, MP2
Basis sets: 3-21G(d, p), LANL2DZ
Properties: geom, onel
Comments: isotope effect of hydrogen-absorbing Pd ultra-fine particle, multi-component MO theory, MC MO, hydrogen and deuteron as quantum waves, geometry optimization, exponent of hydrogen and deuteron wave, Mulliken population analysis, X-ray powder diffraction

[New Search][TOP]

2 of 2
ID: 19190
Authors: BLOMBERG M R A, SIEGBAHN P E M, NAGASHIMA U, WENNERBERG J
Journal: JACSAT
Volumes: 113
Pages: 424
Years: 1991
Substances: C2H6, CH4, H2, Fe, Co, Ni, Rh, Pd, C2H6Fe, C2H6Co, C2H6Ni, C2H6Rh, C2H6Pd, CH4Fe, CH4Co, CH4Ni, CH4Rh, CH4Pd, H2Rh, H2Pd
Compounds:
Methods: MSCF
Basis sets: GEXT
Properties: ONEL, GEOM, INTN
Comments: ACTIVATION OF ALKANE CARBON-HYDROGEN AND CARBON-CARBON BONDS BY TRANSITION METAL ATOMS

[New Search][TOP]

Example 2

<<< Back | Display by 10 items | Next >>>

1 of 1
ID: 76498
Authors: Hada M
Journal: JACSAT
Volumes: 126
Pages: 486-487
Years: 2004
Substances: C22H14FeN6, C30H30FeN6, C24H18FeN7
Compounds: bis(cyanide)porphyrinato iron(III), bis(cyanide)(meso-tetraethyl)porphyrinato iron(III), (cyanide)(imidazole)porphyrinato iron(III)
Methods: B3LYP, SAC, SAC-CI
Basis sets: 6-311G, largerbasissets
Properties: magn, geom, onel, excd
Comments: SAC-CI calculation of Fermi contact term, 13C CN calculated magnetic shifts, spin-polarization, ground and low lying excited states, trans-ligand effect, ferric electronic configurations

[New Search][TOP]

(b)

Figure 2. (a) Two examples of a basic search on QCLDB II. (b) Answer windows of QCLDB II.

Example of Retrieval

QCLDB II is open to all scientists worldwide. Users first access the top page of **QCLDB II** on the web with a standard browser, and input their USER-IDs to login, as shown in Figure 1a. All users must register when they login to the QCLDB II on the web for the first time. Account name is the user e-mail address.

Query QCLDB page in Figure 1b is to search the literature. Each record in QCLDB II contains the data categorized in Table 3. The categories and input keywords may be selected. QCLDB II looks for records including the keywords in the data of the selected categories. All data in the records preceded by the total number of hits will be output.

Users can carry out retrieval using keywords as shown in Figure 2a. First, a category is selected to examine from the pull down menu on the left hand side. Default is "ALL" which surveys all categories. Next, a keyword in the text box in the middle is input. A search condition from among "AND," "OR," and "NOT" is chosen from the pull down menu on the right hand side. Then, another target category is selected from the pull down menu in the left hand side, and another keyword in the text box in the middle is input. The above steps may be

repeated if necessary. The way of displaying the result from the pull down menu in the bottom right may be chosen. Default is "Display by 10 hits." Click the "Search" button. All letters in the text boxes are case insensitive except substance category.

Answer Window is shown in Figure 2b. The input keywords are marked by red font. If the number of records is too many for the user, the user can specify additional keywords to refine the records to an adequate size.

In Figure 2a, a user is interested in theoretical and computational studies of adsorption mechanisms on a palladium surface. The number of hits in terms of two keywords, "adsorption" and "Pd" is 110 in the present QCLDB II (March, 2010). On the other hand, those of Google scholar and Google (keywords: "adsorption," "Pd," and "ab initio MO") are 16000 and 30900, respectively. Using the QCLDB II output list, relevant literature may be targeted effortlessly in the library. The examples show that effective retrieval of theoretical and computational chemical literature is achieved in QCLDB II.

Statistical Analysis of the Number of QCLDB Data

From the starting year of QCLDB, the number of QCLDB data accumulated in one year has gradually increased except for 2006 as shown in Figure 3. The decrease of the collected data arises from policy (1). Since QCLDB I, *Phys. Rev. A*, *Can. J. Chem.*, *Mol. Phys.*, *Surf. Sci.* (CODEN: PLRAAN, CJCHAG, MOPHAM, and SUSCAS, respectively) have been core journals, which contained 567 publications in 2005. Scrutinizing the literature collected so far, we assessed either that content is distant from chemistry or that the quantity of collected data are too small. We excluded these four journals from core journals. It is noteworthy that the increase was sharp around 1990. The software, Gaussian (http://www.gaussian.com/), contributed largely to the sharp increase, particularly since calculations by density functional theory (DFT) in a version from Gaussian92 have become practical. Among many DFT methods, B3LYP[29,30] has been used most frequently. Figure 3 shows clearly that the number of papers with B3LYP calculations has occupied a large part of the total over the last ten years, while the number of Hartree–Fock calculations was larger than that of B3LYP calculations before 2000.

Concluding Remarks

Since 1978, QCLDB I has been maintained without suspension. At the end of the twentieth century, we were obligated to adjust to the progress quantum chemistry and the internet and to relieve the burden of data collectors and reviewers.

We believe that the renovated database, QCLDB II, was successfully initiated from 2001. Also, data of QCLDB I and II are believed to be comprehensive and of high quality under steady continuation. QCLDB deals primarily with electronic structure which is the most fundamental information of atoms, molecules and their aggregates. In this regard, the role of QCLDB will become increasingly important in many fields of physical chemistry, biochemistry, cosmochemistry, and analytical chemistry as well as in theoretical and computational chemistry. QCLDB is a result of the literature survey of the research of participating chemists. The decentralized QCLDB II matches well with the internet structure. The system is shown in Scheme 1.

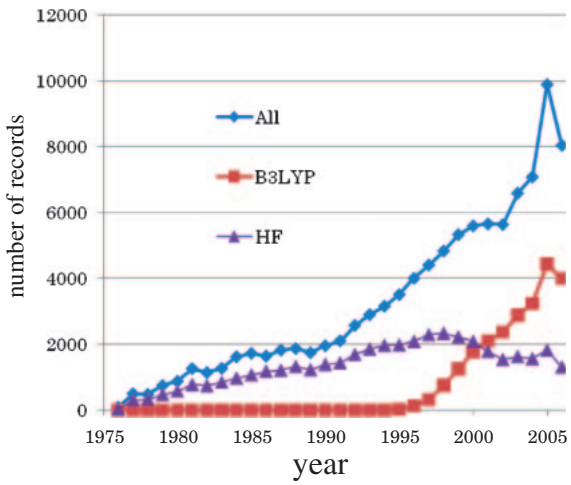
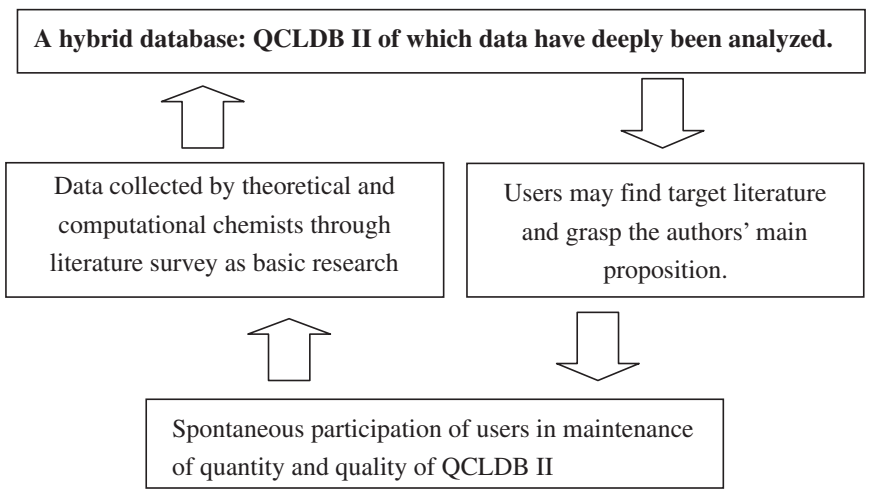


Figure 3. Number of total records in QCLDB and of the records selected by keywords "B3LYP" and "HF."



Scheme 1. A non-commercial and highly academic hybrid database sustained over 25 years. The term "hybrid" means that there is a balance between the burden of collectors/reviewers and the response to user requests.

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