

Re: Taxol: modellersDate: Fri, 1 Jan 93 24:11:05 ESTFrom: Francl Michelle M <mf@mcm.brynmawr.edu>Date: 6 Jan 93 12:33:36 -0800From: hcj@guill.unc.edu (Harry C. kfz-heidelberg.de)Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON.DOUGLAS\_W@LILLY.COM>Subject: u : CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremv!andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93 !!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON.DOUGLAS\_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui or doubled messagesDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: data-flow programs for molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@ GAMESS and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSubject: RE:HELPPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe gov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDTFrom: CUNDARIT@MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T 0From: dmschn@bbt.monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harbowy@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDate: Mon, 18 Jan 9 n 93 15:29:22 +0100From: oosten@ruihml.LeidenUniv.nl (A.B. van Oosten)Subject: Re: proton+electron+neutron?Date: wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu O-STATE.EDU>Subject: RE: PC Survey RESULTSDate: wed, 20 Jan 1993 15:4 : JSMCM@royal.crc.uno.edu>Subject: Re: density problemDate: wed, 20 Jan 93 ke to test a program.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.Phys.Em. <pe@inst.f.phys.uni-erlangen.de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milSU Jan 93 13:27:12 GMTFrom: "D. Mathieu" <DEWINDT@FRSAC11.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: force constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFFrom: "BD le RecurrenceDate: Fri, 22 Jan 1993 13:36:26 +0000From: BDIEAL <BDIEAL@camst1.com>Subject: RE: PDB on the MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron From: arne@mango.mef.ki.se (Arne Elofsson)Subject: Re: charmm and SGIS - charmm newsgroup?Date: Sun, 24 Jan 93 15:05:30 -0500From: chm\_ramsay@emunix.emich.eduSubject: CHEMICALC: Subject: This is testDate: 26 Jan 1993 07:25:59 -0600 (CST)From: AHOLDER@VAX1.UMKC.EDUSubject: semiempirical referencesDate: Tue, 26 Jan 93 12:57:38 -0500From: watanabe@tammy.ha ate: 27 Jan 93 08:11:58 From: "P. J. Flory" <P.J.FLORY@UCSC.EDU>Subject: SUPJOINT (S. J. P. J. Flory) <P.J.FLORY@UCSC.EDU>Subject: SUPJOINT (S. J. P. J. Flory) <P.J.FLORY@UCSC.EDU>RequestedDate: 27 3 20:38:08 GMTFrom: "P. J. Flory" <P.J.FLORY@UCSC.EDU>Subject: SUPJOINT (S. J. P. J. Flory) <P.J.FLORY@UCSC.EDU>RequestedDate: 27 3 14:47:36 -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 1993 15:28:31 PSTFrom: WOODOO CHILLE <woodoo@nit2.ucdavis.edu>Subject: Population Analysis in GaussianFrom: mei@ve 1993 14:23:55 +22305823 (EST)Date: Fri, 29 Jan 93 15:07:15 CSTFrom: shepard@dirac.tcg.nsl.gov (Ron Shepard)Subject: excited statesDate: Fri, 29 Jan 1993 16:47:38 -0600From: sliu CHEM.CMU.EDUSubject: RE: Gaussian and excited statesDate: Fri, 29 Jan 93 16:25:12 ESTFrom: louis.ace@umich.eduSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 15 radomski@tdi.comSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 16:25:12 ESTFrom: louis.ace@umich.eduSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 15 : youkha@chem.mcgill.caSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 16:25:12 ESTFrom: louis.ace@umich.eduSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 15 un.nl>Subject: Electronic Periodic TablesDate: 02 Feb 1993 14:36:03 -0500 (EST)From: ZURAW@athena.letia.polaroid.comSubject: 3D structure -> 2D drawingFrom: QINGSONG@minmet.lan. and NanotechnologiesDate: wed, 3 Feb 93 10:46:20 MSTFrom: QINGSONG@minmet.lan.mcgill.caDate: 3 Feb 93 13:04:57Subject: software for calculating zeta potential and e OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals from a G90/G92 CalculationDate: Thu, 4 Feb 93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSO 3 +0100 (NFT)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71127.1231@compuserve.com>Subject: Call for PapersDate: Fri, 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i <bobby\_clark@quickmail.clemson.edu>Subject: E-mail searchDate: 6 Feb 1993 10:08:20 -1812From: "Bobby Clark" <bobby\_clark@quickmail.clemson.edu>Subject: Memory and CPU for Starde 500 (EST)From: spollack@ester.mse.uc.edu (S.K. Pollack)Subject: Phosphazene ModelingDate: Mon, 8 Feb 93 07:58:51 ESTFrom: adit@kodak.COM (Adi Treasurywala)Subject: Coordinates o Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: wed, 10 S.From: Zhou Feng <feng@lisboa.ks.uiuc.edu>Date: wed, 10 Feb 93 16:23:41 -0600Subject: parallel CHARMM?Date: wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG a -2Subject: Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100From: schettler@chemix.mpi-stuttgart.mpg.deSubject: Mac summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus)S /14031@hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program!Date: Fri, 12 Feb 93 09:48:41 CETFrom: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS T. Re: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katsushi Kobayashi <ikob@les.pc.uec.ac.jp>Date: Sat, 13 Feb 1993 14:47:09 +0100 (WET)From: PREINERT@biolan.u ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenneth McGreevy <kgreevy@hpldas1.sid.hp.com>Subject: Re: X windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS TFrom: "w. Todd wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S hu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A Whiteside)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fise feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet Del Bene" <FR042008@YSUB.YSU.EDU>Subject: BSSE calculationDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ravi k Kjemi" <bjerkese@kjemi.unit.no>Subject: Summary. See freq for s and HDate: Sun, 21 Feb 93 20:51:19 +0100 (MET)Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49: : Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wso@chem.mcgill.caSubject: Re: X windows for PC ..Date: Tue, 23 Feb 93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba g)Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 12:21:47 +0900From: Katsushi Kobayashi <ikob@les.pc.uec.ac.jp>Date: Sat, 13 Feb 1993 14:47:09 +0100 (WET)From: PREINERT@biolan.u nl.govSubject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:09 -0500From: feng@gigchem.temple.edu (Feng Chen)Subject: X-windows Server on MS-windowsDate: Thu, 2 d.harvard.edu (jill cheney)Subject: Computer Program to Calculate the Frequency of Simple OxidesFrom: sender@chemcd1.tau.ac.il (Senderowitz Hanoc semiempirical calculations simple oxidesFrom: sender@chemcd1.tau.ac.il (Senderowitz Hanoc)Subject: MOPAC.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19 n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (EST)From: DONALD B. BOYD" <BOYD DONALD B@YALE.EDU>Subject: new book on computational chemistryDate: Tue ate.Edu (Gene Carter)Subject: Co MD parameters.Date: 03 Mar 1993 17:08:17 CSTFrom: "Gene Carter" <GCARTER@YALE.EDU>Subject: Re:Cache on the MacDate: Tue, 2 Mar 9 lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:17 CSTFrom: MARYJO@northeastern.eduSubject: PDB subdir organization?From: Jan Labanowski <jkl@cc1.net>Dat ar 93 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>Subject: Minimum allowable interatomic separationsFrom: sender@chemcd1.tau.ac.il (Senderowitz Hanoc secc.fi.cnr.it)Subject: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 1993Date: Tue, 9 Mar 93 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GROW upl.pdf. Date: Thu, 11 Mar 93 18:54 EDTFrom: <Podosnna%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy. r 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu>Subject: PDB source file...Date: sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq , 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtdscp@hpc.ch.man.ac.uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN ar 1993 13:58:26 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asr.arsusda.gov>Subject: Software st Girona seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01@EBCECS@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa :11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge 23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic .ml)Subject: what about simulated annealing?Date: wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J Subject: 5C&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrf10128@w MO@CHEMNA.DICHI.UNINA.ITSSubject: looking for ACES programFrom: Robert Laird <mbdtdsr1@hpb.ch.man.ac.uk>Subject: Fe-o calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 - ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu

# RTFM!

# Les relations entre le chimiste et le logiciel de calcul.

Alexandre Hocquet  
Nancy Université & CAK  
Nancy, 25 Novembre 2011

# Plan

## 1. Computational chemistry?

## 2. Computational Chemistry List (CCL)?

## 3. CCL en tant que corpus?

## 4. Quelles tensions?

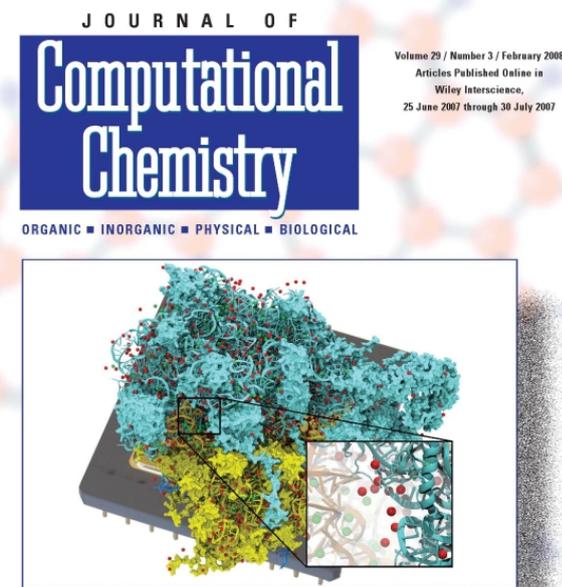
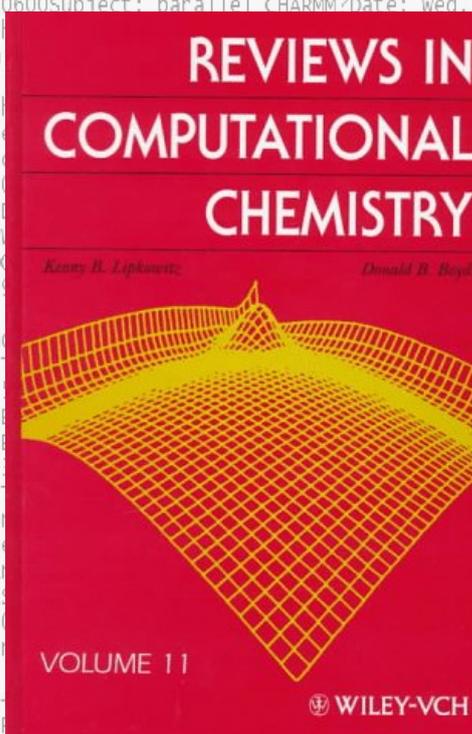
# 1.1 computational chemistry?

## 1.1.1 hardware

## 1.1.2 software

# 1.2. computational chemist?

## 1.3. Qu'en dire?



1930s  
THEORETICAL  
or QUANTUM  
CHEMISTRY

Semi  
empirical 1950s  
ab initio

MOLECULAR  
MECHANICS 1960s

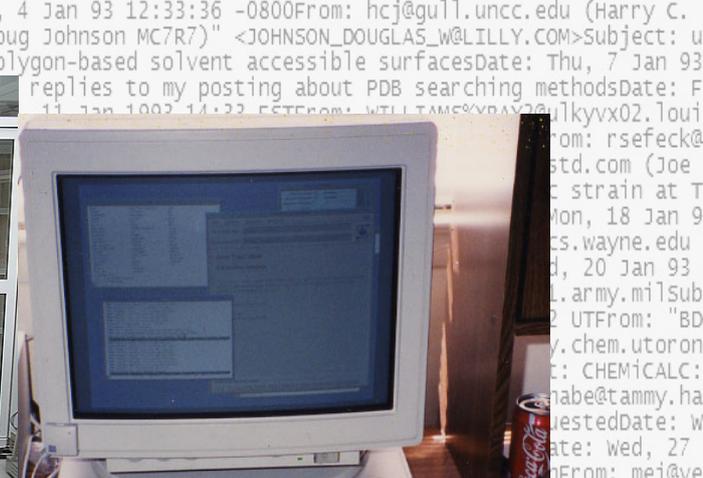
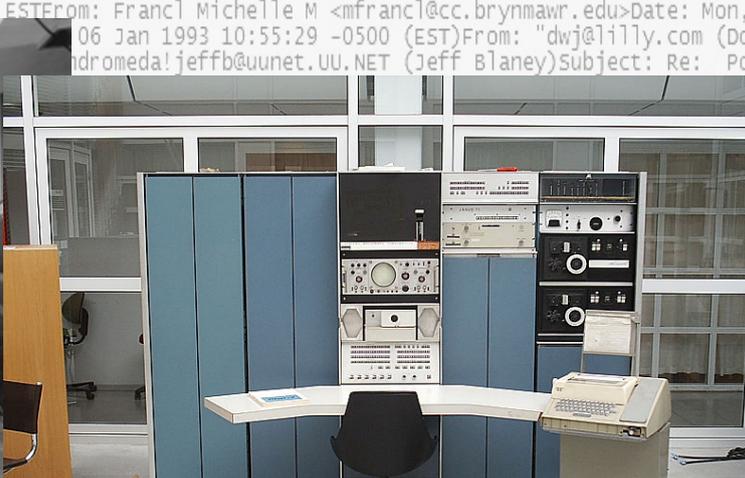
MOLECULAR  
DYNAMICS 1980s

- DRUG DESIGN  
- QSAR 1990s

# 1.1. Computational chemistry : ordinateurs pour la chimie

## Héritage de la chimie théorique

Re: Taxol: molmod1.chem.mcmaster.ca Fri, 1 Jan 1993 14:11:05 EST From: Francis Michelle M <mfranc4@bryn.mawr.edu> Subject: Taxol  
06 Jan 1993 10:55:29 -0500 (EST) From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON.DOUGLAS\_W@LILLY.COM> Subject: u  
dromeda!jeffb@uunet.UU.NET (Jeff Blaney) Subject: Re: Polygon-based solvent accessible surfaces Date: Thu, 7 Jan 93 12:33:36 -0800 From: ahcj@gull.uncc.edu (Harry C  
replies to my posting about PDB searching methods Date: Fri, 11 Jan 1993 14:23 EST From: WILLIAMS%YAY2@u.wisc.edu (Willi  
kyvxo2.loui  
from: rsefeck@  
std.com (Joe  
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d, 20 Jan 93  
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nabe@tammy.ha  
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Feb 93 17:57  
g@minmet.lan.  
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ject: MOLSOL  
ciam.unibo.i



1993 14:23:55 +22305823 (EST) Date: Fri, 29 Jan 93 15:07:11  
CHEM.CMU.EDU Subject: RE: Gaussian and excited states Date:  
radomski@mond1.ccrs.uga.edu Date: Mon, 1 Feb 1993 12:04:28  
: youkha@biosym.com Subject: Summary: Internals & Non-Born  
un.nl Subject: Electronic Periodic Tables Date: 02 Feb 1993  
and Nanotechnologies Date: Wed, 3 Feb 93 10:46:20 MST From:  
OF TOLEDO" <DSMITH@uoft02.utoledo.edu> Subject: Re: Plotting orbitals from a G90/G92 Calculation Date: Thu, 4 Feb 93 11:27  
3 +0100 (NFT) Date: 05 Feb 93 09:28:33 EST From: Elliot King <71127.1231@compuserve.com> Subject: Call for Papers Date: Fri,  
<bobby\_clark@quickmail.clemson.edu> Subject: E-mail search Date: 6 Feb 1993 10:08:20 -1812 From: "Bobby Clark" <bobby.clark@quickmail.clemson.edu> Subject: Memory and CPU for Starde  
500 (EST) From: "collin@esthac.edu" <collin@esthac.edu> Subject: Phosphate Hydrolysis of ATP Date: 8 Feb 93 09:51 EST From: "adi@kodak.com (Adi Treasurywala)" Subject: Coordinates o  
Date: Tue, 9 Feb 93 13:33:33 EST From: "MIAMI" <MIAMI@u.wisc.edu> Subject: Parallel workstations and servers Date: Wed, 10  
s. From: Zhou Feng <feng@lisboa.ks.uiuc.edu> Date: Wed, 10 Feb 93 16:23:41 -0600 Subject: parallel CHARMM? Date: Wed, 10 Feb 93 15:46:43 -0800 From: rickl@biosym.com Subject: DIBUG 4  
-2 Subject: Re: ZINDO program Date: 11 Feb 1993 13:06:18 +0100 From: schettler@chemix.mpi-stuttgart.mpg.de Subject: Mac summery From: theresa@si.fi.ameslab.gov (Theresa Windus) S  
/14031%hkux@u.wisc.edu Subject: Plotting program! Date: Fri, 12 Feb 93 09:48:41 CET From: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS  
t: Re: X Windows for Mac Date: Sat, 13 Feb 1993 14:47:09 +0100 (WET) From: PREINERT@biolan.u  
ell.edu Subject: MPW Fortran? Date: Tue, 16 Feb 93 13:28:40 EST From: Kenneth McGreevy <kgreevy@hpldas1.sid.hp.com> Subject: Re: X windows for PC .. Date: Tue, 16 Feb 93 11:29:01 PS  
TFrom: "w. Todd wipke" <wipke@secs.ucsc.edu> Subject: Final Call Summer Undergraduate Research Fellowship (SURF) Date: Wed, 17 Feb 93 14:15:16 -0500 (EST) From: "DR. DOUGLAS A. S  
Thu, 18 Feb 93 17:02:32 PST From: fisher@scripps.edu (Cindy Fisher) Date: Thu, 18 Feb 93 17:02:32 PST From: fisher@scripps.edu (Cindy Fisher) Date: Thu, 18 Feb 93 17:02:32 PST From: fisher@scripps.edu (Cindy Fisher)  
feld charges Date: Fri, 19 Feb 93 11:53:05 -0500 (EST) From: "jalet@u.wisc.edu" <jalet@u.wisc.edu> Subject: G92 calculation Date: Fri, 19 Feb 93 11:53:05 -0500 From: G. Ravishanker <ravi  
k kjemi" <bjerkes@kjemi.uio.no> Subject: Summary: Scaled freq for s and HDate: Sun, 21 Feb 1993 20:51:19 +0100 (MET) Subject: Long Time-scale Dynamics Date: Mon, 22 Feb 93 16:49:  
: Carl JugDate: Tue, 23 Feb 93 15:08:43 PST From: wsonnen@alnitak.usc.edu (Wayne Sonnen) Subject: dna base charges Date: 23 Feb 93 15:38:36-2300 From: "Alexandre MICU P16A" <alex@ba  
g) Subject: X-window terminal emulator for Mac Date: Thu, 25 Feb 93 17:19:09 -0500 From: feng@gl.chem.temple.edu (Feng Chen) Subject: X-windows Server on MS-Windows Date: Thu, 2  
ni.gov Subject: X-window terminal emulator for Mac Date: Thu, 25 Feb 93 17:19:09 -0500 From: feng@gl.chem.temple.edu (Feng Chen) Subject: X-windows Server on MS-Windows Date: Thu, 2  
d.harvard.edu (Jill Cheney) Subject: Computer Program to Evaluate Wigner 3j Coefficients Date: Fri, 26 Feb 1993 22:08:57 +0100 From: ole.swang@kjemi.uio.no Subject: language questi  
semiempirical calculations simple oxides From: sender@chemdc1.tau.ac.il (Senderowitz Hanoc) Subject: MOPAC6.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00 Date: Mon, 1 Mar 1993 15:25:19  
n.desubject: Re: MOPAC6.0 Date: Sun, 28 Feb 93 13:44:41 GMT-2:00 Date: Mon, 1 Mar 1993 15:25:19  
ate.Edu (Gene Carter) Subject: Co MD parameters. Date: Tue, 2 Mar 93 17:22:53 CST From: Greg Landrum <landrum@chemres.tn.cornell.edu> Subject: Re: Cache on the Mac Date: Tue, 2 Mar 9  
lling Software: Does anyone have STELLA? Date: 04 Mar 1993 17:08:31 -0500 (EST) From: MARYJO@northeastern.edu Subject: PDB subdir organization? From: Jan Labanowski <jkl@cc1.net> Dat  
ar 93 17:30:16 GMT Date: Sun, 7 Mar 93 12:36 EST From: <SML108@PSUMV.PSU.EDU> Subject: Minimum allowable interatomic separations From: sender@chemdc1.tau.ac.il (Senderowitz Hanoc  
secc.fi.cnr.it Subject: MO Theory Made Visible Date: Tue Mar 9 11:23:12 1993 Date: Tue, 9 Mar 93 10:52:25 -0500 From: gallion@auriga.rose.brandeis.edu (steve gallion) Subject: GROW  
upl.pdf. Thu, 11 Mar 93 18:54 EDT From: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU> Subject: Software for PC Date: Fri, 12 Mar 93 04:51:15 GMT From: jim@quanta.phy.  
r 1993 02:33:09 -0800 (PST) From: Thomas Nhan <tom@cassandra.chem.washington.edu> Subject: PDB source file... Date: Sun, 14 Mar 93 11:06:13 +0100 From: doelz@comp.bioz.unibas.ch (Re  
MA.ACS.OHIO-STATE.EDU) Subject: partial charges for fictive atoms in G92 Date: Mon, 15 Mar 1993 12:55 EST From: HSUS@chemv2.mps.ohio-state.edu Subject: Problem with vibrational freq  
, 15 Mar 1993 21:55:05 -0600 (CST) From: Chris Parkinson <mbdtscp@hpc.ch.man.ac.uk> Subject: MM2 code for UNIX systems Date: Tue, 16 Mar 93 11:49:33 GMT Subject: Re: MM2 code for UN  
ar 1993 13:58:36 -0400 From: ZSHI@ac.dal.ca Subject: Information about IBM RS6000 Date: 17 Mar 93 16:18:00 EDT From: "STEPHEN R. HELLER" <srheller@asr.usda.gov> Subject: Software  
st Girona seminar on Molecular Similarity Date: Thu, 18 Mar 93 10:40:05 CET From: ZSYAMP01%EBCECAL@OHSTVMA.ACS.OHIO-STATE.EDU Subject: First Congress of the ISTCP (pa  
:11 -0500 Subject: Keep the noise down, please Date: 19 Mar 93 11:37:00 EST From: nauss@wrair-emh1.army.mil Subject: Program called GRID Date: Fri, 19 Mar 93 14:33:18 EST From: Ge  
23 -0600 (CST) From: Andy Holder <AHOLDER@VAX1.UMKC.EDU> Subject: Announcing AMPAC 4.5 Date: 21 Mar 1993 17:36:57 -0600 (CST) From: Andy Holder <AHOLDER@VAX1.UMKC.EDU> Subject: Semic  
.mil Subject: what about simulated annealing? Date: Wed, 24 Mar 93 14:11:32 +0100 From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner) Subject: efg in g92 From: "Christopher J  
ject: 5C&A Conference speakers - thanks Date: Thu, 25 Mar 93 10:18:48 -0500 From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson) Subject: Batching files in MOPAC From: zrf10128@w  
MO@CHEMNA.DICHI.UNINA.IT Subject: looking for ACES program From: Robert Laird <mbdtssl@hpb.ch.man.ac.uk> Subject: Fe-O calculation Date: Mon, 29 Mar 93 15:49:03 BST From: rafapa@obel  
uk> Subject: Polyrate query Date: Tue, 30 Mar 1993 19:31:32 +0200 From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz) Subject: NBO analyses Date: Tue, 30 Mar 1993 16:04:42 -  
ulz) Subject: Stephen R. Wilson Date: Thu, 1 Apr 1993 16:33:29 +0200 From: oles@gollum.uio.no Subject: Biosym Date: 01 Apr 1993 11:43:13 -0600 (CST) From: CUNDRIT@memstvx1.memst.edu

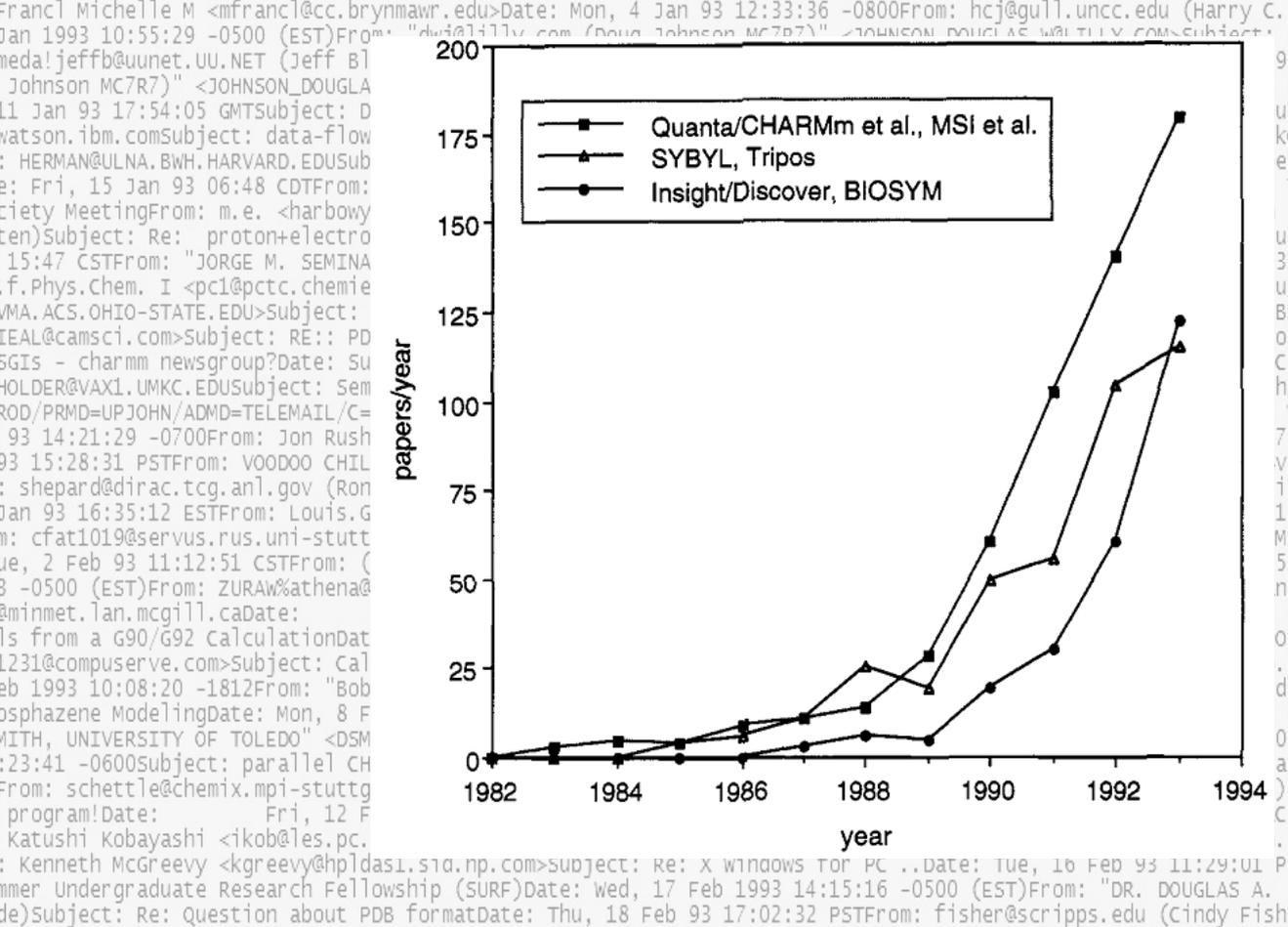
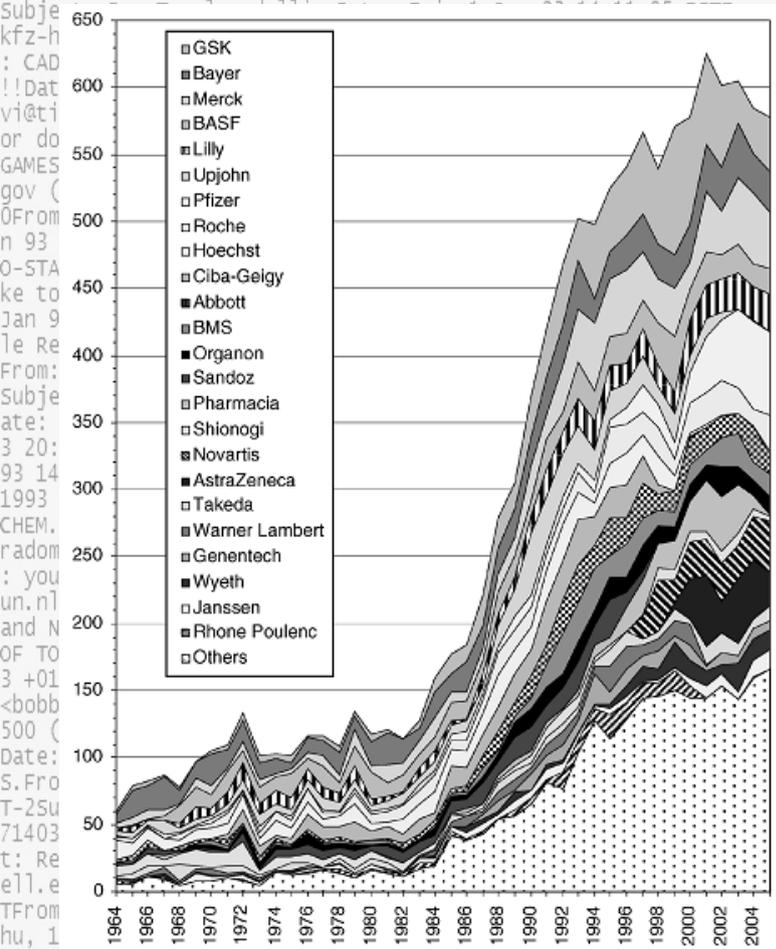
# 1.1.1. Computational chemistry & Hardware

-Supercomputers : 60s

-Minicomputers + Graphic terminals : 70s

-Graphic workstations ; Personal Computers : 80s

**Developer et User ne sont pas la même personne.**



# 1.1.2. Computational Chemistry & Software

## -Portabilité, Diffusion, Publication, Copyright (licence), Maintenance...

## -80s, 90s : Commercialisation du monde académique

## -Business models

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 Fax: +1-314-647-9241

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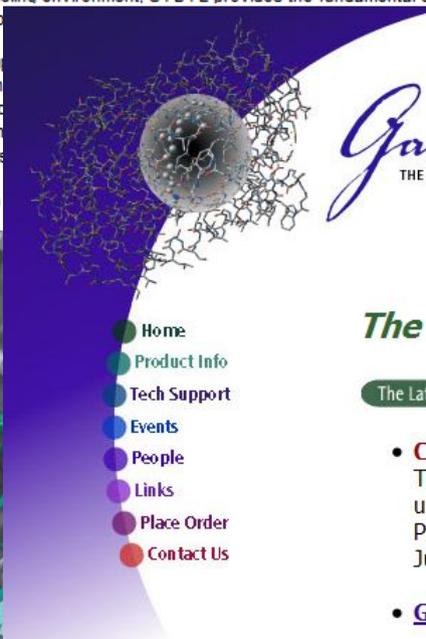
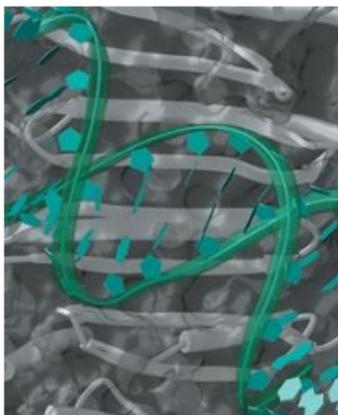
## SYBYL

### Computational Informatics Software for Molecular Modelers

SYBYL<sup>®</sup> is a suite of computational informatics software designed to enhance the drug discovery workflows and decision-making of today's computational chemists and molecular modelers. An industry standard for over 20 years and the basis for Tripos' expert molecular modeling environment, SYBYL provides the fundamental components for understanding molecular structure and pro

Computational chemists understand the *in silico* discovery programs. They realize the science. Well-designed and frequently used between success and failure. Tripos' pre with its ever-growing suite of technologies

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 THE OFFICIAL GAUSSIAN 03 WEB SITE

## The Official Gaussian Website

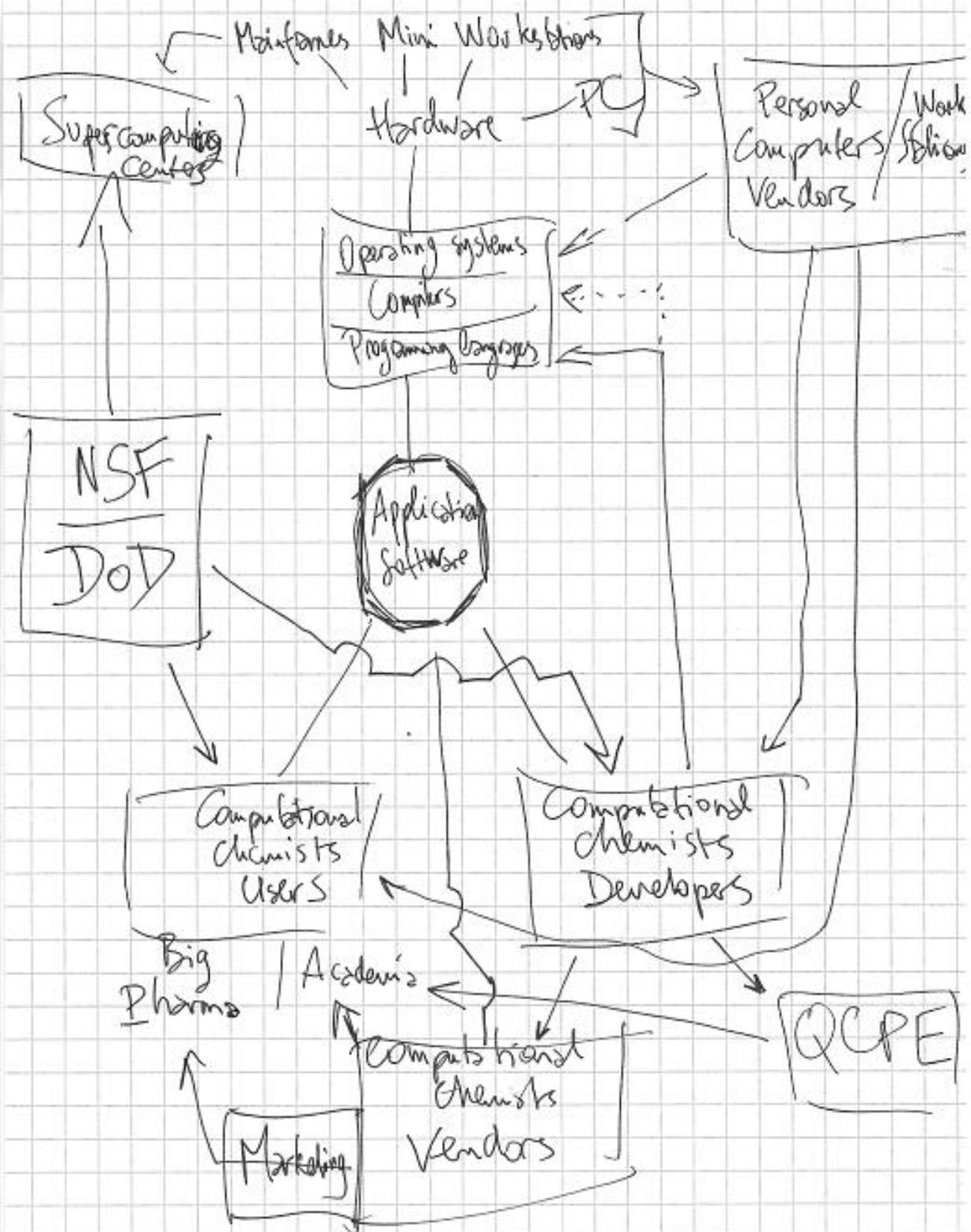
### The Latest News

- **Congratulations to Keiji Morokuma** on being awarded the [Imperial Prize](#) of the Japan Academy. This well-deserved honor is in recognition of "the integrated impact of chemistry in [his] work in understanding structure, function and reactivity of molecules by theoretical/computational approaches." Professor Morokuma will be presented the prize by Japanese Emperor Akihito in a ceremony in Tokyo June 9th. [Additional information](#)
- [Gaussian Workshop in Sydney in September](#)
- **Gaussian 03 Revision E.01 available:**
  - Read the [release notes](#) for more details.
  - Includes support for Intel Macs ([details](#))
  - The AMD Opteron and EM64T platforms now have separate versions of *Gaussian 03*. For maximal performance, be sure to purchase and install the appropriate version for your hardware. You can use the:

**cat /proc/cpuinfo**

ing.subject: X-Window terminal emulator for macDate: d.harvard.edu (jill cheney)Subject: Computer Program semiempirical calculations simple oxidesFrom: sender@n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993Date: 02 Mar 1993 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: secc.fi.cnr.itSubject: MO Theory Made VisibleDate: Thu, 11 Mar 93 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu>Subject: PDB source file...Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (ReMA.ACS.OHIO-STATE.EDU)Subject: partial charges for fictive atoms in g92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational frequency, 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtsr@hpc.ch.man.ac.uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UNIX 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asrr.arsusda.gov>Subject: Software for the first Girona seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCECAL@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (part 1) -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semicircular subject: what about simulated annealing?Date: wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J. Subject: 5C&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrf10128@awmop@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsr1@hpb.ch.man.ac.uk>Subject: Fe-0 calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel.uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -0500From: ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNARIT@memstvx1.memst.edu

Re: [unclear] Date: Fri, 12 Jan 93 14:11:05 EST From: [unclear]  
 kfz-heidelberg.de>Subject: Energy contribution of hbonds?Date: 06 Jan 1993  
 : CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda.ije  
 !!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@illy.com (Doug Johnson  
 vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan  
 or doubled messagesDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.  
 GAMESS and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMA  
 gov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri,  
 0From: dms@ngp.cit.umd.eduFrom: [unclear] Graphics Society M  
 n 93 15:29:22 +0100From: oostener@mil.leidenuniv.nl (A.B. van Oosten)Sub  
 O-STATE.EDU>Subject: RE: PC Survey RESULTSDate: wed, 20 Jan 1993 15:47  
 ke to test program Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.Phys  
 Jan 93 13:17:00From: [unclear] Mathieu" <DEWINDT@FRSAC11.BITNET@OHSTVMA.AC  
 le RecurrenceDate: Fri, 22 Jan 1993 13:36:26 +0000From: BDIEAL <BDIEAL@ca  
 From: arne@mango.mef.ki.se (Arne Elofsson)Subject: Re: charmm and SGIs -  
 subject: This is testDate: 26 Jan 1993 07:40:58 +0600 (CST)From: AHOLDER@  
 ate: 27 Jan 1993 14:47:36 -0500From: [unclear] DOWELROD/PRV  
 3 20:38:08 GMTSubject: RE: XWD->Mac conversion...Date: wed, 27 Jan 93 14:  
 93 14:47:36 -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 1993 15:2  
 1993 14:23:55 +03593 (EST)From: [unclear] 07:15 CSTFrom: shepa  
 CHEM.CMU.EDU>Subject: Re: Gaussian and excited statesDate: Fri, 29 Jan 93  
 radomski@mond1.ccr.c.uga.eduDate: Mon, 1 Feb 1993 12:04:28 +0100From: cfat  
 : youkha@biosym.comSubject: summary: Internals & Non-BondsDate: Tue, 2 Feb  
 un.nl>Subject: [unclear] Date: 26 Feb 93 14:36:03 -0500  
 and NanotechnologiesDate: wed, 3 Feb 93 10:46:20 MSTFrom: QINGSONG@minmet  
 OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals from  
 3 +0100 (NFT)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71117.1231@cc  
 <bobby\_c1@kku.edu>Date: 05 Feb 1993 14:47:36 -0500 (EST)From: [unclear] Feb 1993  
 500 (EST)From: spollack@ester.mse.uc.edu (S.K. Pollack)Subject: Phosphaze  
 Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, U  
 S.From: Zhou Chengshou@uic.edu Date: wed, 10 Feb 93 16:23:41  
 T-2Subject: [unclear] Date: 10 Feb 1993 16:23:41  
 /14031@hkuxa.hku.hk@OHSTVMA.AC.S.OHIO-STATE.EDUSubject: MO Plotting progr  
 t: Re: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katush  
 ell.edu>Subject: [unclear] Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenne  
 TFrom: "wipke@secs.ucsc.edu" <wipke@secs.ucsc.edu>Subject: Final Call Summer Ur  
 hu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A whiteside)Subj  
 feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet Del Bene" <FR04  
 k Kjemi" <[unclear]@[unclear]>Subject: [unclear] and  
 : Carl JugDate: Tue, 23 Feb 93 15:18:43 PSTFrom: wsonnen@nitak.usc.edu  
 g)Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 17:21 EDTFrom: <PC  
 ni.gov>Subject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:  
 d.harvard.edu>Subject: [unclear] Date: Thu, 25 Feb 93 17:  
 semiempirical calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Se  
 n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (E  
 ate.Edu (Gordon Carter)Subject: Co MD parameters Date: Tue, 2 Mar 93 17:22  
 lling software Date: Sun, 7 Mar 93 17:08:31 -0500  
 ar 93 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU  
 secc.fi.cnr.it>Subject: MO Theory Made visibleDate: Tue Mar 09 11:23:12 19  
 uplingDate: Tue, 9 Mar 1993 11:23:12 ESTFrom: [unclear] NYUACF1.BITNET@OF  
 r 1993 02:11:23 +0000 (EST)From: [unclear] [unclear] chem.washingt  
 MA.AC.S.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92D  
 , 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtscp@hpc.ch.n  
 ar 1993 13:00:00 (EST)From: [unclear] Information about IBM  
 st Girona seminar on molecular similarityDate: Thu, 18 Mar 93 10:  
 :11 -0500subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 EST  
 23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcir  
 .milsubject: what about simulated annealing?Date: wed, 24 Mar 93 14:11:32  
 ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -05  
 MO@CHEMNA.DICHI.UNINA.ITSUBject: looking for ACES programFrom: Robert Lai  
 uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@  
 ulz)subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: c



## 1.2 Computational

### Chemist

-Developers : écrivent le

code puis le diffusent

-Users : utilisent le code

-Vendors : vendent le code

-NSF, DoD : financent des

projets

-Supercomputers : allouent

des ressources de calcul

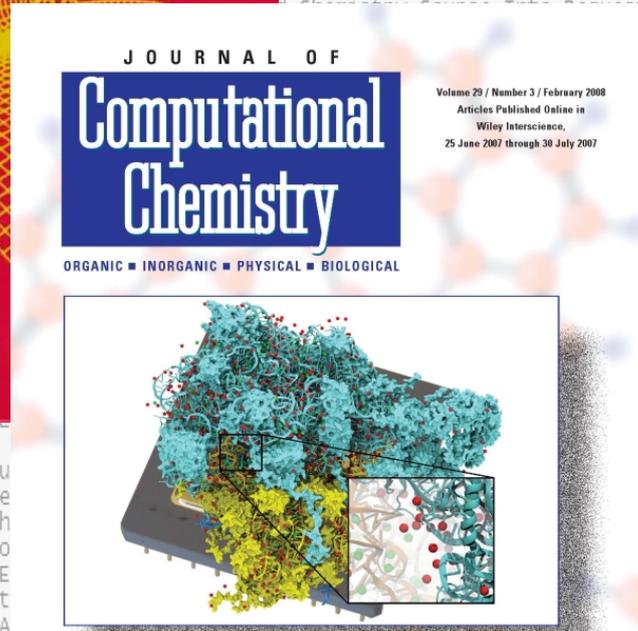
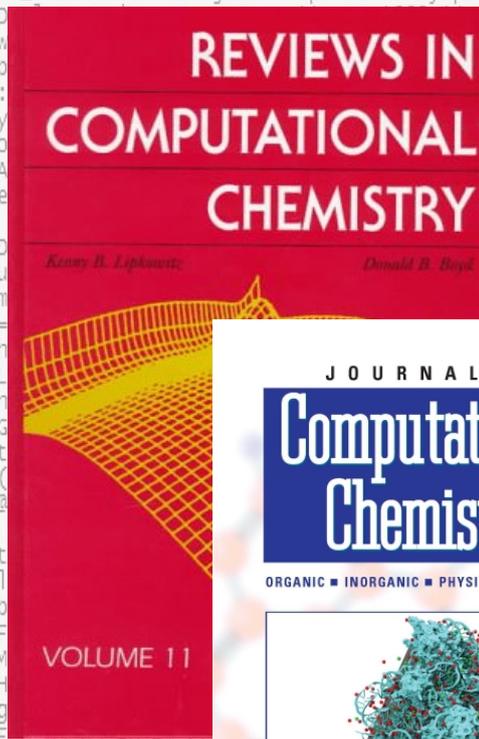
-Hardware vendors +

Operating systems :

vendent l'infrastructure

# 1.3 Comment cette communauté scientifique a traité le problème du software dans ce contexte ?

- science/technologie
- formes d'innovation
- software en société



EDITORS: CHARLES L. BROOKS III • GERNOT FRENKING • SHIGEYOSHI SAKAKI

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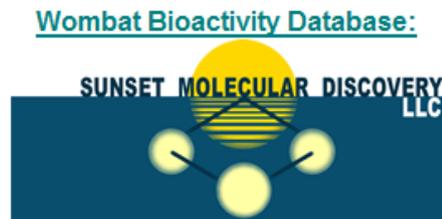
# 2. Computational Chemistry List (CCL)

## 2.1. Principe

## 2.2. Genèse et contexte de création

## 2.3. Histoire

**CCL.NET**  
computational chemistry list, ltd.



<http://www.ccl.net/index.shtml>

### CCL Home

Messages in a queue: 0 (approx. wait time: 00:00 hours)

Page supported by:



[Computational Science & Engineering Online](#)  
... a laboratory without walls for scientific computing

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Supporting CCL,  
Uploading file to  
CCL Site, Security  
Policy, Privacy  
Policy, About Us  
Contact Us

Drug Discovery  
Training

Drug Discovery

ACS-COMB Division supports CCL

Subject: RE: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Kathleen  
ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenneth McGreevy <kgreevy@hp1das1.sid.hp.com>Subject: Re: X Windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PST  
From: "w. Todd Wipke" <wipke@secs.ucsc.edu>Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S  
thu, 18 Feb 93 14:22:08 PSTFrom: rww@autodesk.com (Robert A Whiteside)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fische  
feld chargeDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ravi@  
k.kjemi> <kjerkesek@kemi.uio.no>Subject: Summary: Scaled Pref for 5 and 10Date: Sun, 21 Feb 1993 20:51:19 +0100 (MET)Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49:  
: Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.usc.edu (wayne sonnen)Subject: dna base chargesDate: 23 Feb 93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba  
g>Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 17:21 EDTFrom: <Podosnna%nyuacf1.bitnet@ohstvm.acs.ohio-state.edu>Subject: X-window terminal emulator for MacDate: Thu,  
ni.govSub: <Gallion@brandeis.edu>Subject: Cache on the MacDate: Tue, 2 Mar 9  
d.harvard.edu (Jill Cheney)Subject: Computer Programs to Evaluate Wigner 3j CoefficientsDate: Fri, 26 Feb 1993 22:08:57 +0100From: tole.wiangekjem.uio.noSubject: language questi  
semiempirical calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoch)Subject: MOPAC6.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19  
n.desubject: Experts know-how wanted!Date: 02 Mar 1993 08:17:18 -0500 (EST)From: "DONALD B. BOYD" <BOYD.DONALD.B@LILLY.COM>Subject: new book on computational chemistryDate: Tue  
ate.edu (John P. O'Neil)Subject: STALLA 2.0Date: 02 Mar 1993 12:22:49 GMT-0500From: "John P. O'Neil" <John.P.O'Neil@univ.illinois.edu>Subject: Cache on the MacDate: Tue, 2 Mar 9  
lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (EST)From: MARYJO@northeastern.eduSubject: PDB subdir organization?From: Jan Labanowski <jkl@cc1.net>Dat  
ar 93 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SMLL08@psu.edu>Subject: Minimum allowable interatomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoc  
suppl.dat.criitSubject: MM2 code for UNIX systemsDate: Tue, 9 Mar 93 10:52:25 -0500From: gallion@brandeis.edu (steve gallion)Subject: GROV  
r 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu>Subject: PDB source file...Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re  
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq  
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ar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq  
st Girona Seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01%EBCECAL@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa  
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uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDRIT@memstvx1.memst.edu

# Attack of the killer workstations

- From: [jle@world.std.com](mailto:jle@world.std.com) (Joe M Leonard)
- Subject: Attack of the killer workstations
- Date: Tue, 10 Dec 91 20:04:44 -0500

Reviewing the recent discussion regarding C vs. Fortran and structured vs. spaghetti coding, isn't it reasonable to consider the time of the programmer as more important than the code's runtime (within reason)? Given that approx. \$20k workstations are comparable to Cray machines, isn't 10-ish% overhead more than worth the human time savings through better-thought-out programming (structured, modular, OO, etc.)? I hope the day's past for really needing to count cycles in loops - as one can wait for the next version of workstation xxx to gain appreciable speedups.

Obviously, this isn't the case for mpp machines, for which the consensus is that one must rethink and/or reimplement algorithm's in order to use the hardware to advantage. Still, this might prove to be an example where clearer coding styles might turn out to be a win after all...

Joe Leonard  
[jle@world.std.com](mailto:jle@world.std.com)

## 2.1. Mailing List: discussion list

Communication asynchrone. Internet. Email. Subscription. 90s.

Moderation Influe sur la reactivite. Communauté déclarée.

Pas d'édition. Pas d'anonymat. Échange privé ou public.

Active readers (Lurkers)

1991	CCL is born	E-mail Listserver and FTP archives for computational chemists are established at OSC as a hobby project of Jan Labanowski.
1994	CCL gets Gopher	CCL Introduces Gopher interface to messages and its FTP site. CCL grows in number of <a href="#">subscribers</a> and <a href="#">messages</a> .
1995	CCL gets WEB	CCL Introduces WEB interface to messages and its FTP site.
		
1996	CCL gets money from NSF	After your help with support letters, CCL got a 3-year grant from the National Science Foundation ( <a href="#">NSF</a> )
1996	CCL gets domain	Just in case, Jan Labanowski personally registers the domain <a href="#">ccl.net</a> since the good domains are being bought by the millions by domain name investors.
1996	CCL buys small iron	After deliberations and all the advice not to ( <i>...buy something solid if you have money...</i> ) CCL decided to operate from PCs running Linux and Apache Web Server.

m: hcj@gull.uncc.edu (Harry C. ...  
 \DOUGLAS\_W@LILLY.COM>Subject: u  
 ble surfacesDate: Thu, 7 Jan 93  
 out PDB searching methodsDate: F  
 m: WILLIAMS%XRAY2@ulkyvx02.loui  
 an 93 13:38:09 ESTFrom: rsefeck@  
 500From: jle@world.std.com (Joe  
 E.EDUSubject: Steric strain at T  
 diradicals/TSDate: Mon, 18 Jan 9  
 : landman@hal.physics.wayne.edu  
 ity problemDate: wed, 20 Jan 93  
 m: nauss@wrair-emh1.army.milSU  
 : 22 Jan 93 13:06:32 UTFFrom: "BD  
 From: system@alchemy.chem.utoron  
 rix.emich.eduSubject: CHEMICALC:  
 :08 -0500From: watanabe@tammy.har  
 try Course Info RequestedDate: W  
 iodic Table WidgetDate: wed, 27  
 Analysis in GaussianFrom: mei@ve  
 an 1993 16:47:38 -0600From: sliu  
 ed statesDate: Fri, 29 Jan 93 15  
 Feb 93 19:26:49-0500From: SBPM  
 lectricDate: Mon, 1 Feb 93 17:57  
 awing?From: QINGSONG@minmet.lan.  
 calculating zeta potential and e  
 <moore@ncsc.org>Subject: MOLSOL  
 )From: ivan@gandalf.ciam.unibo.i  
 oject: Memory and CPU for Starde  
 asurywala)Subject: Coordinates o  
 ations and serversDate: wed, 10  
 ickl@biosym.comSubject: DIBUG ad  
 fi.ameslab.gov (Theresa Windus)S  
 %EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS  
 LOO (WET)From: PREINERT@biolan.u  
 ate: Tue, 16 Feb 93 11:29:01 PS  
 500 (EST)From: "DR. DOUGLAS A. S  
 fisher@scripps.edu (Cindy Fische  
 -0500From: G. Ravishanker <ravi

k kjem1 <bjerkese@kjem1.uio.no>subject: summary. scaled freq for s and hDate: Sun, 21 Feb 1993 20:51:19 +0100 (MET)subject: Long time-scale DynamicsDate: Mon, 22 Feb 93 16:49:  
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 g)Subject: ...drogimband Date: 23 Feb 93 17:31:11 EDTFrom: BOYD\_DONALD\_B@LILLY.COM (BOYD DONALD B. BOYD) <BOYD\_DONALD\_B@LILLY.COM>Subject: X-window terminal emulator for MacDate: Thu,  
 n1.govSubject: ...drogimband Date: 23 Feb 93 17:31:11 EDTFrom: BOYD\_DONALD\_B@LILLY.COM (BOYD DONALD B. BOYD) <BOYD\_DONALD\_B@LILLY.COM>Subject: X-windows Server on MS-windowsDate: Thu, 2  
 d.harvard.edu (jill cheney)subject: Computer Program to Evaluate wigner 3j CoefficientsDate: Fri, 26 Feb 1993 22:08:57 +0100From: ole.swang@kjem1.uio.noSubject: language questi  
 semiempirical calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoch)subject: MOPAC6.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19  
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 r 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu>Subject: PDB source file...Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re  
 MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in g92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq  
 , 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq  
 ar 1993 13:58:56 -0400From: ZSHI@ac.dal.caSubject: Information about IBM R3600Date: 17 Mar 93 16:18:00 EDTFrom: STEPHEN R. HELLER <srheller@astr.arsusda.gov>Subject: Software  
 st Girona Seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01@EBCECAL@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa  
 :11 -0500subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge  
 23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic  
 .milSubject: What about simulated annealing?Date: wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J  
 ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrf10128@aw  
 MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsr1@hpb.ch.man.ac.uk>Subject: Fe-0 calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel  
 uk>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
 ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDRIT@memstvx1.memst.edu

## 2.2. Computational Chemistry List (CCL)

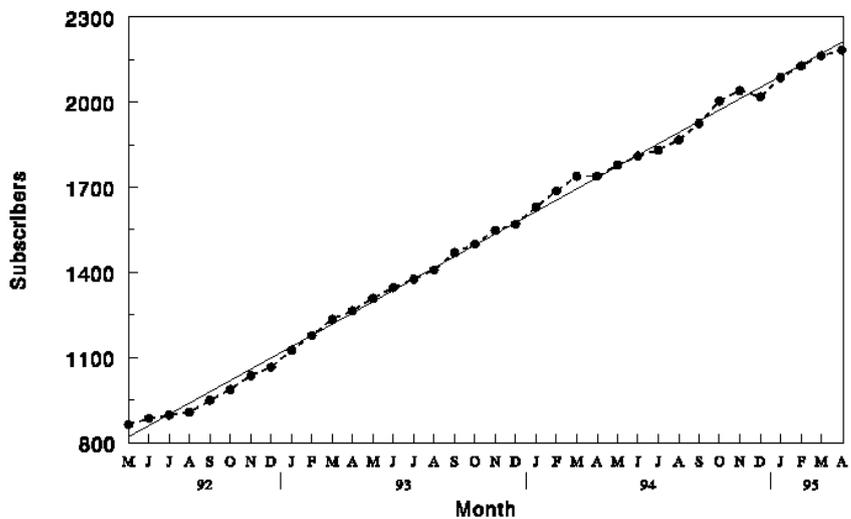
### 1991. Ohio Supercomputing Center.

### Communauté de scientifiques geeks mais pas computer scientists.

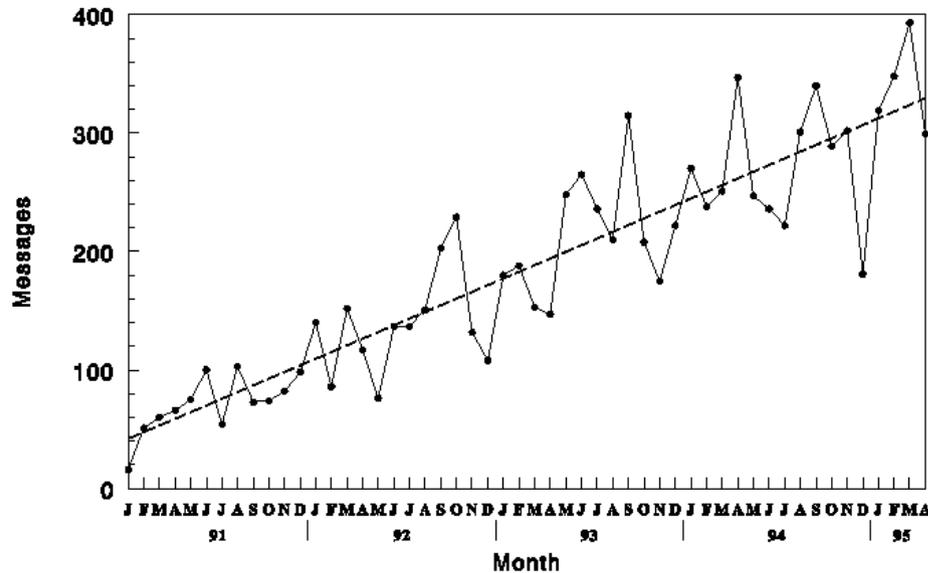
### Discipline émergente (journaux, congrès...) : communauté à

### cimenter.

## Number of subscribers



## Messages per month



## 2.3. Historique

-croissance régulière puis stabilisation (approx. 10 messages par jour)

-academic / for profit

-senior positions / graduate students

-developers / users

-USA / pays émergents

90s: Internet=email; communauté geek et en train de se définir.

# 3. CCL en tant que corpus

## 3.1. les acteurs en interaction

## 3.2. informel et barrières abaissées

## 3.3. thèmes abordés

### 3.3.1 learning

### 3.3.2 religious wars

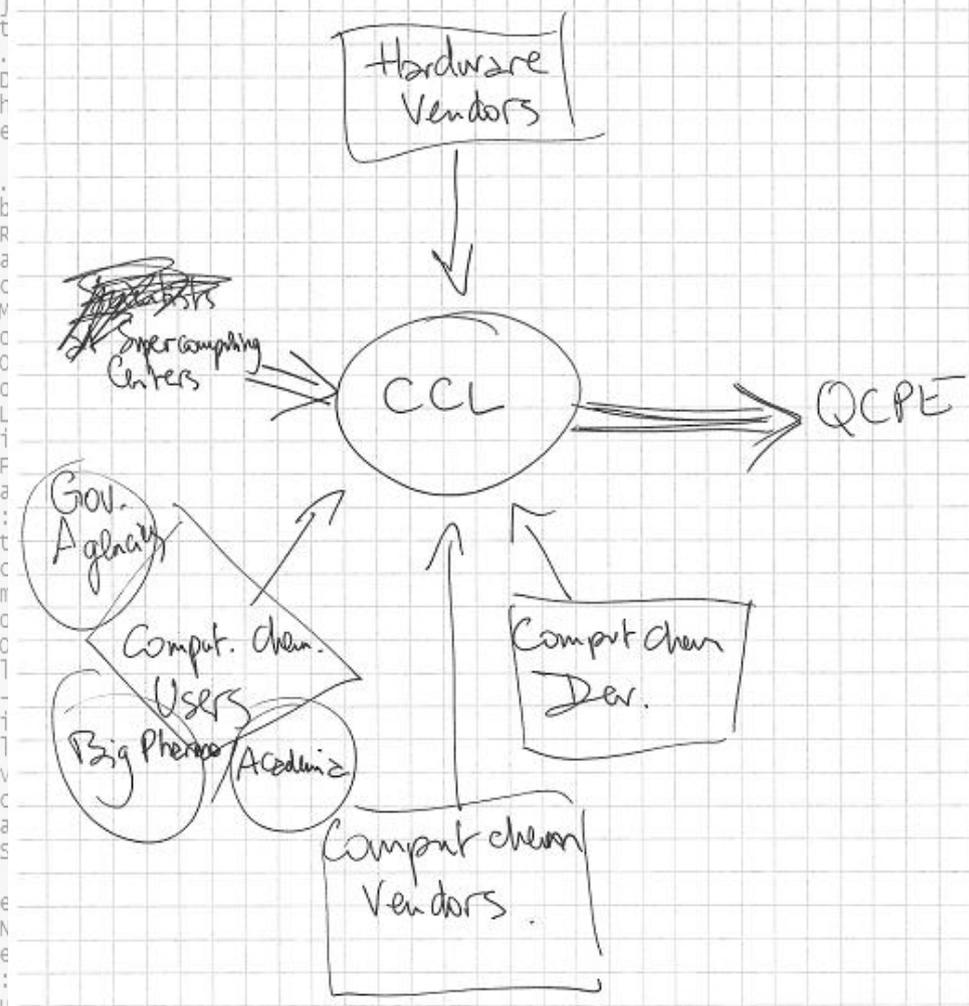
### 3.3.3 help in using software

## 3.4 Mining

# 3.1. Acteurs en interaction

.edu  
.gov  
.com

developers  
users  
vendors



kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500  
CADD videosDate: Wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda.jeffb@uunet.UU.NET (J  
!!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@illy.com (Doug Johnson MC7R7)" <JOHNSON,  
vi@tiberius.cc.cornell.edu>From: ccu@chemreading.ac.ukDate: Mon, 11 Jan 1993 17:54:05 GMTSubj  
or doubledDate: Mon, 11 Jan 1993 17:54:05 GMTSubject: dat  
GAMES and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.  
gov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CD  
0From: dmsch@hpc.monsanto.comSubject: next Molecular Graphics Software WorkshopDate: Fri, 15  
n 93 15:25:25 -0500 (EST)From: oosten@ruihml.LeidenUniv.nl (A.B. van Oosten)Subject: RE: C  
O-STATE.EDU>Subject: RE: PC Survey RESULTSDate: Wed, 20 Jan 1993 15:47 CSTFrom: "JORGE M.  
ke to test a program.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.Phys.Chem. I <pci@pcc.  
Jan 93 13:27:27 -0500 (EST)From: "D. Mathieu" <DEWINDT@FRSAC11.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subj  
le RecurrenceDate: Fri, 22 Jan 1993 13:36:26 +0000From: BDIEAL <BDIEAL@cam.ac.uk>Subject: R  
From: arne@mango.mef.ki.se (Arne Elofsson)Subject: Re: charmm and SGIs - charmm newsgroup?Da  
Subject: This is testDate: 26 Jan 1993 07:20:59 -0600 (CST)From: AHOLDER@VAX1.UMKC.EDUSubjec  
ate: 27 Jan 93 13:32:0500From: /PN=DAVID.W.ELROD/DD.ID=SSW.DW@OHSTVMA.ACS.OHIO-STATE.EDU  
3 20:38:08 GMTSubject: RE: XWD->Mac conversion...Date: Wed, 27 Jan 93 14:21:29 -0700From: Jc  
93 14:47:36 -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 1993 15:28:31 PSTFrom: VOODO  
1993 14:23:55 +22305823 (EST)Date: Fri, 29 Jan 93 15:07:15 CSTFrom: shepard@dirac.tcg.anl.gc  
CHEM.CMU.EDUSubject: RE: Gaussian and excited statesDate: Fri, 29 Jan 93 16:35:12 ESTFrom: L  
radomski@mondli.ccrcc.uga.eduDate: Mon, 1 Feb 1993 12:04:28 +0100From: cfat1019@servus.rus.uni  
: youkha@biosym.comSubject: Summary: Internals & Non-BondsDate: Tue, 2 Feb 93 11:12:51 CSTF  
un.nl>Subject: Electronic Periodic TablesDate: 02 Feb 1993 14:36:03 -0500 (EST)From: ZURAWA  
and NanotechnologiesDate: Wed, 3 Feb 93 10:46:20 MSTFrom: QINGSONG@minmet.lan.mcgill.caDate:  
OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals from a G90/G92 Calculat  
3 +0100 (NFT)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71127.1231@compuserve.com>Subjec  
<bobby\_clark@quickmail.clemson.edu>Subject: E-mail searchDate: 6 Feb 1993 10:08:20 -1812From  
500 (EST)From: spollack@ester.mse.uc.EDU (S.K. Pollack)Subject: Phosphazene ModelingDate: Mo  
Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO  
S.From: Zhou Feng <feng@lisboa.ks.uiuc.edu>Date: Wed, 10 Feb 93 16:23:41 -0600Subject: paral  
T-2Subject: Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100From: schettl@chemix.mpi-  
14031%hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program!Date: Fri  
t: Re: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katushi Kobayashi <ikob@  
ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenneth McGreevy <kgreev  
TFFrom: "w. Todd wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Summer Undergraduate Researc  
hu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A whiteside)Subject: Re: Question a  
feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet DeL Bene" <FR042008@YSUB.YSU.EDU>S  
k kjemi" <bjerkese@kjemi.unit.no>Subject: Summary. Scaled freq for S and HDate: Sun, 21 Feb  
: Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.usc.edu (Wayne Sonnen)Subje  
g)Subject: Re: Hydrogen bond.Date: Wed, 24 Feb 93 17:21 EDTFrom: <PODOSNNA%NYUACF1.BITN  
nl.govSubject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:09 -0500From: fe  
d.harvard.edu (jill cheney)Subject: Computer Program to Evaluate wigner 3j CoefficientsDate:  
semiempirical calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoch)SU  
n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (EST)From: "DONALD B.  
ate.Edu (Gene Carter)Subject: Co MD parameters.Date: Tue, 2 Mar 93 17:22:53 CSTFrom: Greg L  
lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (EST)From: MARYJO@hur  
ar 93 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>Subject: Minimum allowable interatomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoch)  
secc.fi.cnr.itSubject: MO Theory Made VisibleDate: Tue Mar 9 11:23:12 1993Date: Tue, 9 Mar 93 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GROW  
upling.Date: Thu, 11 Mar 93 18:54 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy.  
r 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu>Subject: PDB source file...Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re  
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq  
, 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdts@hpc.ch.man.ac.uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN  
ar 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asr.arsusda.gov>Subject: Software  
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MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsr1@hpb.ch.man.ac.uk>Subject: Fe-o calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel  
uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu

Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <franclm1@cc.brynmawr.edu>Date: Mon, 4 Jan 93 12:33:36 -0800From: hcj@gull.uncc.edu (Harry C. kfz-heidelberg.de)Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON\_DOUGLAS\_W@LILLY.COM>Subject: u  
: CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93 11:01:05 AM>Subject: replies to my posting about PDB searching methodsDate: F  
nsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui  
or molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@  
LPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe  
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ate: wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu  
@royal.crc.uno.edu>Subject: Re: density problemDate: wed, 20 Jan 93  
en.de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milsu  
constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFFrom: "BD  
cDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron  
3 15:05:30 -0500From: chm\_ramsay@emunix.emich.eduSubject: CHEMICALC:  
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om: ole.swang@kjemi.uio.noSubject: language questio  
3 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19  
ject: new book on computational chemistryDate: Tue  
.edu>Subject: Re:Cache on the MacDate: Tue, 2 Mar 9  
organization?From: Jan Labanowski <jkl@ccl.net>Dat  
sFrom: sender@chemdcl.tau.ac.il (Senderowitz Hanoc  
iga.rose.brandeis.edu (steve gallion)Subject: PHY  
e: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy.  
3 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re  
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16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN  
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d GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge  
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gen Dufner)Subject: efg in g92From: "Christopher J  
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Date: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel  
: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
11:43:13 -0600 (CST)From: CUNDRIT@memstvx1.memst.edu

# CHARMm & CHARMM

- *From:* "Don Gregory" <[Don\\_Gregory@atms.MSI.COM](mailto:Don_Gregory@atms.MSI.COM)>
- *Subject:* CHARMm & CHARMM
- *Date:* 28 Mar 1994 09:04:11 +0000

## Summary of transferring software to PC

- *From:* <[JKONG{\\*at\\*}@ac.dal.ca](mailto:JKONG{*at*}@ac.dal.ca)>
- *Subject:* Summary of transferring software to PC
- *Date:* Mon, 25 Oct 1993 10:42:16 -0300

My original question is:

- > Can one install a unix system like linux on a 486 and then run
- > quantum chemistry software like G92?
- > I thought so in principle but I am not sure.

It is interesting to see that there are quite a few people trying to do  
the impression that you can run  
d big memory(16MB), big disk  
have to transfer the codes to  
yet(There is a tool for that  
io responded.

- *From:* Serge Gorelsky <[serge%!@yorku.ca](mailto:serge%!@yorku.ca)>
- *Subject:* gaussian98
- *Date:* Wed, 16 Jun 1999 10:33:37 -0400 (EDT)

Dear colleagues.

While running some DTF calculations on ruthenium complexes with  
Gaussian 98, from time to time I get the warning message like this:  
\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.64964185D-02  
This message appears after convergence of SCF iterations. My  
questions are

1. what are alpha delta epsilon here?
2. is this a matter for serious concern?
3. is this problem related to the basis set or is it some convergence problems?

Any help would be deeply appreciated. Thank you.

### OFFICE MEMO

Subject:

CHARMm & CHARMM

On March 27, Ilya Logunov (U.of Illinois) sent me the latest version of CHARMm. First the file was in a zip file and then a brief point of clarification. CHARMm is available from Molecular Simulations, Burlington, Western U.S. academic users can call Adam Logunov (617) 229-9800 for pricing and information. The standard discount to academics is 90% off the list-price.

Just to make sure everyone is clear on the difference, CHARMm (little m) is the commercial version and CHARMM is the academic version distributed by the group at Harvard.

The added capabilities to CHARMm that make it more useful are:

## gaussian98

Thu, 18 Feb 93 14:22:08 PSTFrom: Ilya Logunov <logunov@chem.illinois.edu>Subject: CHARMm & CHARMM  
feld chargesDate: Fri, 19 Feb 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON\_DOUGLAS\_W@LILLY.COM>Subject: u  
: CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93 11:01:05 AM>Subject: replies to my posting about PDB searching methodsDate: F  
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d GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge  
: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic  
gen Dufner)Subject: efg in g92From: "Christopher J  
i)Subject: Batching files in MOPACFrom: zrf10128@aw  
Date: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel  
: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
11:43:13 -0600 (CST)From: CUNDRIT@memstvx1.memst.edu

Re: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfranc1@c...>Subject: u  
kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON\_DOUGLAS\_W@LILLY.COM>Subject: u  
: CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda!jeffbb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93  
!!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON\_DOUGLAS\_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F  
vi@tiberiu...>Date: Mon, 11 Jan 93 17:54:05 GMTSubject: PDB  
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and Nanoti  
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# IEEE Annals

## A Social History of Bitnet and Listserv, 1985-1991

April-June 2000 (vol. 22 no. 2)

pp. 32-41

David Alan Grier  
Mary Campbell

DOI Bookmark: <http://doi.ieeecomputersociety.org/10.1109/85.841135>

### ABSTRACT

After the engineers built the computer networks, users had to build the social networks that made them useful. Listserv, the combined mailing list and file server, was an important tool for those interested in building network-based organizations. It first appeared on Bitnet, an academic network based on IBM computers. The early versions of Listserv became operational in the mid 1980s, and its early archives show how network users learned to use the software and, perhaps more importantly, how to manage network-based organizations.

questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui  
ograms for molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@  
t: RE:HELPPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe  
NDARIT%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T  
emes.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDDate: Mon, 18 Jan 9  
eutron?Date: wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu  
<JSMCM@royal.crc.uno.edu>Subject: Re: density problemDate: wed, 20 Jan 93  
i-erlangen.de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milSU  
force constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFFrom: "BD  
n the MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron  
24 Jan 93 15:05:30 -0500From: chm\_ramsay@emunix.emich.eduSubject: CHEMICALC:  
pirical referencesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanabe@tammy.ha  
@sprint.comSubject: Computer Assisted Chemistry Course Info RequestedDate: 2  
rusho@nitrate.chem.utah.edu>Subject: Re: Periodic Table WidgetDate: wed, 2  
moris@nl2.ucdavis.edu>Subject: Population Analysis in GaussianFrom: mei@ve  
epard)Subject: excited statesDate: Fri, 29 Jan 1993 16:47:38 -0600From: sliu  
e@um.cc.umich.eduSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 15  
t.deSubject: Conference AnnouncementDate: 01 Feb 93 19:26:49-0500From: SBPM  
ll) <baell@syd.dah.csiro.au>Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57  
a.polaroid.comSubject: 3D structure -> 2D drawing?From: QINGSONG@minmet.lan.  
3 Feb 93 13:04:57Subject: software for calculating zeta potential and e  
Thu, 4 Feb 93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL  
or PapersDate: Fri, 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i  
Clark" <bobby\_clark@quickmail.clemson.edu>Subject: Memory and CPU for Starde  
93 07:58:51 ESTFrom: adit@kodak.COM (Adi Treasurywala)Subject: Coordinates o  
Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: wed, 10  
S.From: Zhou Feng <feng@lisboa.ks.uiuc.edu>Date: wed, 10 Feb 93 16:23:41 -0600Subject: parallel CHARMM?Date: wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG a  
-2Subject: Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100From: schettler@chemix.mpi-stuttgart.mpg.deSubject: Mac summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus)S  
/14031%hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program!Date: Fri, 12 Feb 93 09:48:41 CETFrom: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS  
t: Re: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katushi Kobayashi <ikob@les.pc.uec.ac.jp>Date: Sat, 13 Feb 1993 14:47:09 +0100 (WET)From: PREINERT@biolan.u  
ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenneth McGreevy <kgreevy@hpldas1.sid.hp.com>Subject: Re: X windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS  
TFFrom: "w. Todd wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S  
thu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A Whiteside)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fische  
feld charo...>Date: Fri, 19 Feb 93 14:49:00 ESTFrom: "J. Del Bene" <EB2008@ysu.edu>Subject: BSSE calculationDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ravi  
k kjemi" <delben@ysu.edu>Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fische  
: Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@nitak.usc.edu (Wayne Sonnen)Subject: dna base chargesDate: 23 Feb 93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba  
g)Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 17:21 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: X-window terminal emulator for MacDate: Thu,  
ni.govSubject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:09 -0500From: feng@sgi.chem.temple.edu (Feng Chen)Subject: X-windows Server on MS-windowsDate: Thu, 2  
d.harvard.eduSubject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fische  
ate.Uio (Gene Carter)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fische  
lling Software: Does any...>Date: Tue, 2 Mar 93 17:08:31 -0500 (EST)From: MARYJO@northeastern.eduSubject: PDB subdir organization?From: Jan Labanowski <jkl@cc1.net>Dat  
ar 93 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>Subject: Minimum allowable interatomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoc  
secc.fi.cnr.itSubject: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 1993Date: Tue, 9 Mar 93 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GROW  
upl.pdfDate: Thu, 11 Mar 93 17:08:31 -0500 (EST)From: NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy.  
r 1993 02:33:09 -0800 (PST)From: Thomas Han <thomas@chem.washington.edu>Subject: PDB source file...Date: sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re  
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq  
, 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtscp@hpc.ch.man.ac.uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN  
ar 1993 13:58:36 -0400 (EST)From: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asr.marsusda.gov>Subject: Software  
st Girona seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01@EBCECSAL@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa  
:11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge  
23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic  
.milSubject: What about...>Date: 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J  
ject: 5C&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrf10128@w  
MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtssl@hpb.ch.man.ac.uk>Subject: Fe-o calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel  
uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNARIT@memstvx1.memst.edus

## 3.2. Communication informelle (Erving Goffman backstage)

### Abaisse les barrières :

#### -Hiérarchiques

#### -Géographiques

#### -Culturelles

#### -Disciplinaires

Re: ...  
kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON\_DOUGLAS\_W@LILLY.COM>Subject: u  
: CADD videosDate: Wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda.jeffbb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93  
!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON\_DOUGLAS\_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F  
vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui  
or doubled messagesDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: data-flow programs for molecular modelingDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@  
GAMESS and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSubject: RE:HELPPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe  
Gove (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDTFrom: CUNDARIT%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T  
0From: dmschn@bbbit.monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harbowy@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDate: Mon, 18 Jan 9  
n 93 15:29:22 +0100From: oosten@ruihlml.LeidenUniv.nl (A.B. van Oosten)Subject: Re: proton+electron=neutron?Date: Wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu  
O-STATE.EDU>Subject: RE: PC Survey RESULTSDate: Wed, 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problemDate: Wed, 20 Jan 1993  
ke to test a program.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.P  
Jan 93 13:27:12 GMTFrom: "D. Mathieu" <DEWINDT%FRSAC11.BITNET@OHSTVMA.  
le RecurrenceDate: Fri, 22 Jan 1993 13:36:26 +0000From: BDIEAL <BDIEAL  
From: arne@mango.mef.ki.se (Arne Elofsson)Subject: Re: charmm and SGIs  
Subject: This is testDate: 26 Jan 1993 07:20:59 -0600 (CST)From: AHOLD  
ate: 27 Jan 93 08:59:32-0500From: /PN=DAVID.W.ELROD/DD.ID=SSW.DWELROD/  
3 20:38:08 GMTSubject: Re: XWD->Mac conversion...Date: Wed, 27 Jan 93  
93 14:47:36 -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 1993 1  
1993 14:23:55 +22305823 (EST)Date: Fri, 29 Jan 93 15:07:15 CSTFrom: sh  
CHEM.CMU.EDUSubject: RE: Gaussian and excited statesDate: Fri, 29 Jan  
radomski@mond1.crc.uga.eduDate: Mon, 1 Feb 1993 12:04:28 +0100From: c  
: youkha@biosym.comSubject: Summary: Internals & Non-BondsDate: Tue,  
un.nl>Subject: Electronic Periodic TablesDate: 02 Feb 1993 14:36:03 -0  
and NanotechnologiesDate: Wed, 3 Feb 93 10:46:20 MSTFrom: QINGSONG@min  
OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals f  
3 +0100 (NFT)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71127.1231  
<bobby\_clark@quickmail.clemson.edu>Subject: E-mail searchDate: 6 Feb 1  
500 (EST)From: spollack@ester.mse.uc.EDU (S.K. Pollack)Subject: Phosph  
Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH  
S.From: Zhou Feng <feng@lisboa.ks.uiuc.edu>Date: Wed, 10 Feb 93 16:23:  
T-2Subject: Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100From  
/14031%hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting pro  
t. Re: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Kat  
ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenneth McGreevy <kgreevy@hpldas1.sid.hp.com>Subject: Re: X Windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS  
TFFrom: "w. Todd wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: Wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S  
hu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A whiteside)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fische  
feld char  
k kjemi"  
: Carl Juc  
g)Subject:  
nl.govSub:  
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semiempir  
n.desubjec  
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ar 1993 1:  
st Girona  
:11 -0500:  
23 -0600  
.milsubjec  
ject: SC&J  
MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk>Subject: Fe-0  
uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edus

## USENET News Group ... NO!

- From: "R.G.A. Bone" <[rgab@atapurisima.molres.org](mailto:rgab@atapurisima.molres.org)>
- Subject: USENET News Group ... NO!
- Date: Wed, 27 Apr 94 11:24:39 -0700

Why not start CCL as a USENET NewsGroup ... ?  
... because, even in 1994, there are still some of us who cannot access  
"USENET" (or, WWW, etc.) and for whom, therefore, a listserver like  
CCL  
is the only lifeline.  
Many people in companies are behind so-called "firewalls" in which  
full  
internet-access (except e-mail) is denied.

## RE:Nobel Prizers

- From: (Andrew Fant) <[fant\(+at+\)umbc3.umbc.edu](mailto:fant(+at+)umbc3.umbc.edu)> (+ at +) umbc3.umbc.edu
- Subject: RE:Nobel Prizers
- Date: Thu, 26 Sep 91 12:36:46 EDT

How about a joint Nobel to John Pople and Michael Dewar for their success  
in making computational tools available to the experimentalist and for  
their efforts to bring theoretical methods to bear on problems that non-  
physical chemists are interested (i.e. organic mechanisms).  
I would not, however, want to be in the same room as the two of them as they  
wait to receive the award, or before they give their lectures.  
Just another uninvolved opinion

MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsrl@hpb.ch.man.ac.uk>Subject: Fe-0  
uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edus

# Rules

By posting to the list, you [agree](#) to adhere to the rules outlined in this document.

These rules, regarding what topics are [acceptable/unacceptable](#) and [commercial announcements](#) discussions. Do not reopen Pandora's box -- please.

## Acceptable Topics

Topics which may appear on the list include:

- **software/hardware-related** issues
  - bugs: Reporting bugs in chemistry software and possible work-arounds
  - programs and utilities
  - availability: Information on the availability of particular software, data, etc.
  - hardware-related issues relevant to the computational chemistry community
- **announcements** of
  - new chemistry software
  - computational chemistry-related workshops and symposia
- **methods**
  - new methods and techniques in computational chemistry
  - Q&A: questions and answers about solving computational chemistry problems
- **opinions** about services and products

## 3.3. Topics

### -Help in using software

### -Learning

### -Religious wars (Flaming, Trolling : Gabriella Coleman trickster)

## Commercial Announcements

**Commercial software: software sold to anyone for** to the *list*, please respect the following rules:

- **Be brief** -- Short (25 lines or less) commercial announcements
- **Be straightforward** -- The subject line should be clear
- **No reposting** -- Reposts of software announcements
- **No "vaporware"** -- Announcements of "vaporware" are not allowed.

# gaussian98

- From: Serge Gorelsky <[serge%20at%20yorku.ca](mailto:serge%20at%20yorku.ca)>
- Subject: gaussian98
- Date: Wed, 16 Jun 1999 10:33:37 -0400 (EDT)

Dear colleagues.

While running some DTF calculations on ruthenium complexes with Gaussian 98, from time to time I get the warning message like this:

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.64964185D-02

This message appears after convergence of SCF iterations. My questions are

1. what are alpha delta epsilon here?
2. is this a matter for serious concern?
3. is this problem related to the basis set or is it some convergence problems?

Any help would be deeply appreciated. Thank you.

500 (EST)From: spoilack@ester.mse.uc.edu (S.K. Poilack)Subject: Phosphazene ModelingDate: Mon, 8 Feb 93 07:58:51 ESTFrom: adit@kodak.com (Adi Treasurywala)Subject: Coordinates of  
Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: wed, 10  
S.From: Zhou Feng <feng@lisboa.ks.uiuc.edu>Date: wed, 10 Feb 93 16:23:41 -0600Subject: parallel CHARMM?Date: wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG ad  
T-2Subject: Re: ZINDO programDate: 11 Feb 1993 13:06:18 +0100From: schettler@chemix.mpi-stuttgart.mpg.deSubject: Mac summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus)S  
/14031%hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program!Date: Fri, 12 Feb 93 09:48:41 CETFrom: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS  
t: Re: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katsushi Kobayashi <ikob@les.pc.uec.ac.jp>Date: Sat, 13 Feb 1993 14:47:09 +0100 (WET)From: PREINERT@biolan.u  
ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: 1 PS  
TFFrom: "w. Todd wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Su A. S  
hu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A Whitesi ishe  
feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet DeJ Bene ravi  
k Kjemi" <bjerkese@kjemi.unit.no>Subject: Summary. Scaled freq for :49:  
: Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.u x@ba  
g)Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 17:21 EDTFri Thu,  
nl.govSubject: X-window terminal emulator for MacDate: Thu, 25 Feb Th,  
d.harvard.edu (jill cheney)Subject: Computer Program to Evaluate w  
semiempirical calculations simple oxidesFrom: sender@chemdc1.tau.ac  
n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -  
tate.Edu (Gene Carter)Subject: Co MD parameters.Date: Tue, 2 Mar 9  
lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31  
ar 93 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PS  
secc.fi.cnr.it>Subject: MO Theory Made VisibleDate: Tue Mar 09 11:2  
uplingDate: Thu, 11 Mar 93 18:54 EDTFrom: <Podosnna%NYUACF1.BT  
r 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.w  
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in  
, 15 Mar 1993 13:58:50 -0400From: Chris Parkinson <mbdtscp@h  
ar 1993 13:58:50 -0400From: 25SH@AC.dal.caSubject: Information abou  
st Girona seminar on Molecular SimilarityDate: Thu, 18 Mar  
:11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37  
23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Ani  
.milSubject: what about simulated annealing?Date: wed, 24 Mar 93 1  
ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:  
MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Rob  
uk>Subject: Polyrate QueryDate: Tue, 30 Mar 1993 19:31:32 +0200Fro  
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200

# -Learning

# -Help in using software

# Macromolecular modeling review

- From: <[rswenson { \\*at \\* } magnus.acs.ohio-state.edu](mailto:rswenson%20at%20magnus.acs.ohio-state.edu)>
- Subject: Macromolecular modeling review
- Date: Mon, 01 Aug 1994 17:45:06 -0400

I am involved in the organization of a special topics course for graduate students (principally in Biochemistry and the biological sciences) covering various aspects of "protein engineering". We would like to include a component this year covering the use of computational methods for the modelling of mutated protein structures, particularly with respect to predicting the structural consequences of amino acid substitutions. Another aspect that could be included is the application of such methods in the de novo design of novel protein structures. I would greatly appreciate input from the group as to any good, general review articles, books, etc. that would introduce the basics to students with general biochemical training and varied expertise in the subject area. Thank you.



Re: Taxol: molfile Date: Fri, 1 Jan 93 14:11:05 EST From: Franci Michelle M <mbm@bryn.mawr.edu> Subject: Taxol  
kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON,DOUGLAS\_W@LILLY.COM>Subject: u  
: CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda!jeffbb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93  
!!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON,DOUGLAS\_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F  
vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui  
or doubled messagesDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: data-flow programs for molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@  
GAMESS and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSubject: RE:HELPPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe  
Gaw (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDTFrom: CUNDARIT@MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T  
0From: dmschn@bbt.monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harbowy@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDate: Mon, 18 Jan 9  
n 93 15:29:22 +0100From: oosten@ruihml.LeidenUniv.nl (A.B. van Oosten)Subject: Re: proton+electron+neutron?Date: wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu  
O-STATE.EDU>Subject: RE: PC Survey RESULTSDate: wed, 20 Jan 1993 15:47 CSTFrom: "JORGE M. SEMINARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problemDate: wed, 20 Jan 93  
ke to test Date: Fri, 22 Jan 1993 13:36:26 +0000From: BDIEAL <BDIEAL@camsci.com>Subject: Re: PDB on the MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron  
le RecurrenceDate: Fri, 22 Jan 1993 13:36:26 +0000From: BDIEAL <BDIEAL@camsci.com>Subject: Re: PDB on the MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron  
From: arne@mango.mef.ki.se (Arne Elofsson)Subject: Re: charmm and SGIs - charmm newsgroup?Date: Sun, 24 Jan 93 15:05:30 -0500From: chm\_ramsay@emunix.emich.eduSubject: CHEMICALC:  
Subject: "w. Todd Wipke" <wipke@secs.ucsc.edu>Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S  
Date: 27 Jan 93 08:39:32 -0500From: PN-DAY,ED.W.ELKROD,ED.D.SSW.DWELROD/PRND=UPJOHN/ADM=TELEMAIL/C=US/@sprint.comSubject: Computer Assisted Chemistry Course Info RequestedDate: 27  
3 20:38:08 GMTSubject: Re: XWD->Mac conversion...Date: wed, 27 Jan 93 14:21:31 -0700From: Jon Rusho <rusho@nitrate.chem.utah.edu>Subject: Re: Periodic Table WidgetDate: wed, 27  
93 14:47:36 -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 1993 15:28:29 PSTFrom: VOODOO CHILE <morris@gn12.ucdavis.edu>Subject: Population Analysis in GaussianFrom: mei@ve  
1993 14:23:55 +22305823 (EST)Date: Fri, 29 Jan 93 15:07:15 CSTFrom: shepard@dirac.tcg.anl.gov (Ron Shepard)Subject: excited statesDate: Fri, 29 Jan 1993 16:47:38 -0600From: sliu  
CHEM.CMU.EDUSubject: RE: Gaussian and excited statesDate: Fri, 29 Jan 93 16:35:12 ESTFrom: Louis.Grace@um.cc.umich.eduSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 15  
radomski@bondl.ccr.c.uga.eduDate: Mon, 1 Feb 1993 12:04:28 +0100From: cfat101@servus.uni-stuttgart.deSubject: Conference AnnouncementDate: 01 Feb 93 19:26:49-0500From: SBPM  
: youkha@bioml.comSubject: Summary: Internals & Non-BndsDate: Tue, 2 Feb 93 11:12:51 CSTFrom: (bael) <bael@svd.dabessing.aus>Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57  
un.nl>Subject: Summary: Internals & Non-BndsDate: Tue, 2 Feb 93 11:12:51 CSTFrom: (bael) <bael@svd.dabessing.aus>Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57  
and NanotechnologiesDate: wed, 3 Feb 93 10:48:20 MSTFrom: QINGSONG@minmet.lan.lcgill.caDate: 3 Feb 93 13:04:57Subject: software for calculating zeta potential and e  
OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals from a G90/G92 CalculationDate: Thu, 4 Feb 93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL  
3 +0100 (CST)From: ELLIOTT,KEVIN Date: Thu, 4 Feb 93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL  
<bobby\_c...@...>Subject: Memory and CPU for Starde  
500 (EST)From: spollack@ester.mse.uc.EDU (S.K. Pollack)Subject: Phosphazene ModelingDate: Mon, 8 Feb 93 07:58:51 ESTFrom: adit@kodak.com (Adi Treasurywala)Subject: Coordinates o  
Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: wed, 10  
S.From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: wed, 10  
-2Subject: Re: XWD->Mac conversion...Date: wed, 10 Feb 93 15:46:43 -0800From: rickl@biosym.comSubject: DIBUG  
/14031@hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program!Date: Fri, 12 Feb 93 09:48:41 CETFrom: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS.T  
ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kenneth McGreevy <kgreevy@hpldas1.sid.hp.com>Subject: Re: X windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS  
TFFrom: "w. Todd wipke" <wipke@secs.ucsc.edu>Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S  
thu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A Whiteside)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fishe  
feld chargeDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "FR042008@YSUB.YSU.EDU" <FR042008@YSUB.YSU.EDU>Subject: BSSE calculationDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ravi  
k kjemi@uio.uio.no>Subject: Summary: Scaled freq for S and HDate: Sun, 21 Feb 1993 20:51:19 +0100 (MET)Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49:  
: Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.usc.edu (Wayne Sonnen)Subject: dna base chargesDate: 23 Feb 93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba  
g)Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 17:21 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: X-window terminal emulator for MacDate: Thu,  
nl.govSubject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:00 -0500From: feng@sgi.chem.temple.edu (Feng Chen)Subject: X-windows Server on MS-windowsDate: Thu, 2  
d.harvard.eduSubject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:00 -0500From: feng@sgi.chem.temple.edu (Feng Chen)Subject: X-windows Server on MS-windowsDate: Thu, 2  
semiempirical calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoch)Subject: MOPAC6.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19  
n. Subject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (EST)From: "DONALD B. BOYD" <BOYD\_DONALD\_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue  
ate.Edu>Subject: Re:Cache on the MacDate: Tue, 2 Mar 9  
lling software. Does anyone have STELLA?Date: 04 Mar 1993 17:00:51 (EST)From: MARK JORDAN@CHESTER.EDUSubject: PDB subdir organization?From: Jan Labanowski <jkl@cc1.net>Dat  
ar 93 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>Subject: Minimum allowable interatomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoc  
succ.fai.cnr.it>Subject: MO theory Made visibleDate: Tue Mar 09 11:23:12 1993Date: Tue, 9 Mar 93 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GRO  
uplingDate: 09 Mar 1993 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GRO  
r 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tomcassandra.chem.washington.edu>Subject: PDB source file...Date: Sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re  
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq  
r 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asr.usda.gov>Subject: Software  
st Girona seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01@EBCECS@AL@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa  
:11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge  
23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic  
.ml>Subject: what about simulated annealing?Date: wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J  
Subject: 5C&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrf10128@w  
MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsr1@hpb.ch.man.ac.uk>Subject: Fe-o calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel  
uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu

# -Tensions : flame war du 25 juin 1993.

## 1. Reproductibilité

## -question éthique, question pratique

## 2. Publication : reconnaissance du code

## -question de statut de la computational science,

## (voir computing science)

## 3. Ouverture du code

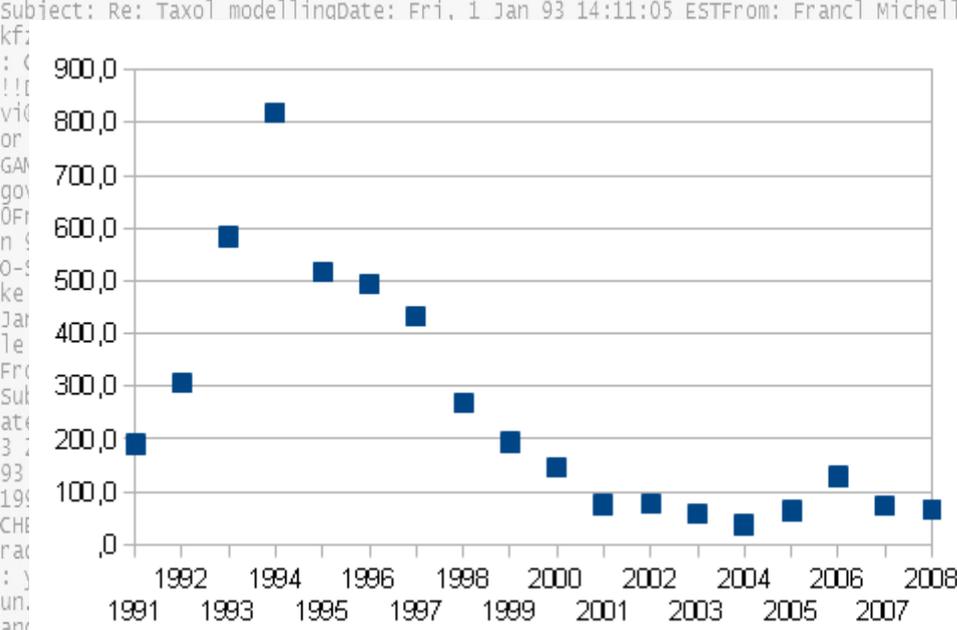
## -question technique, question idéologique

## 4. Commercialisation éventuelle

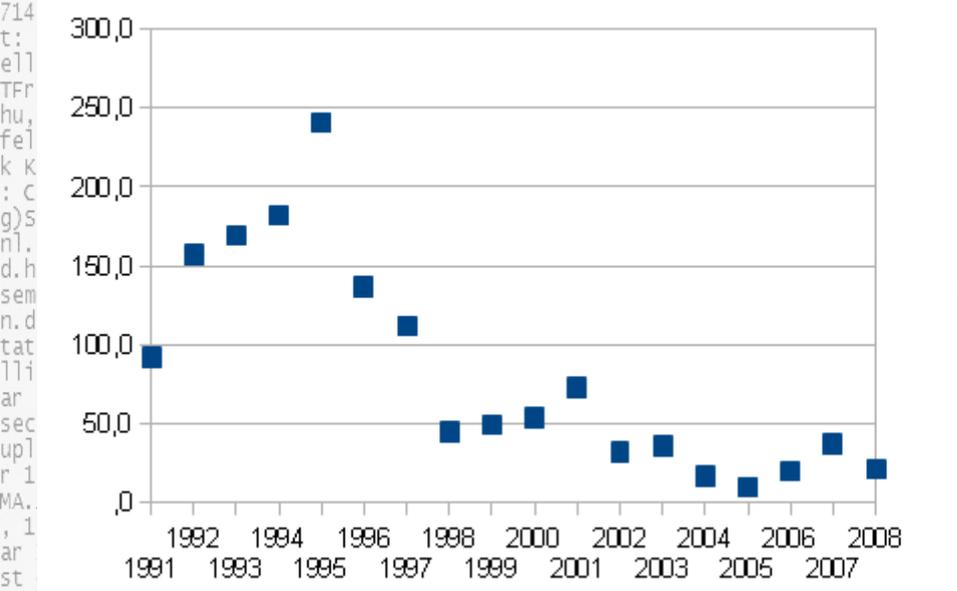
## -question éthique, question pratique (licensing)

## Le cas de Gaussian.





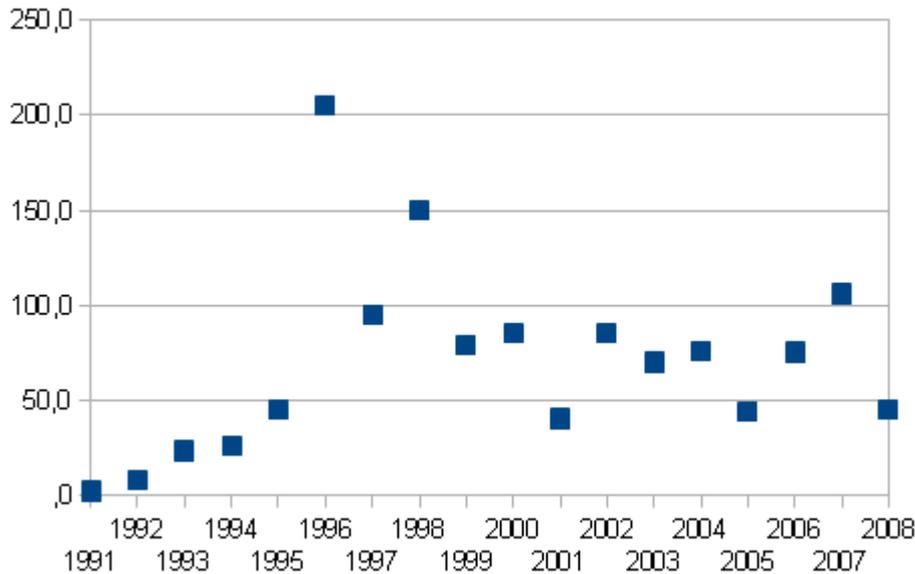
■ graphics



■ supercomputer

From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON\_DOUGLAS\_W@LILLY.COM>Subject: u  
 (Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93  
 GLAS\_W@LILLY.COM>Subject: replies to my posting about PDB searching methodsDate: F  
 : DMol questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui  
 low programs for molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@  
 Subject: RE:HELPPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe  
 om: CUNDARIT%MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T  
 owy@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDDate: Mon, 18 Jan 9  
 tron=neutron?Date: wed, 20 Jan 93 10:11:36 ESTFrom: landman@hal.physics.wayne.edu  
 INARIO" <JSMCM@royal.crc.uno.edu>Subject: Re: density problemDate: wed, 20 Jan 93  
 mie.uni-erlangen.de>Date: 21 Jan 93 07:50:00 ESTFrom: nauss@wrair-emh1.army.milSU  
 t: force constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFFrom: "BD  
 PDB on the MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron  
 Sun, 24 Jan 93 15:05:30 -0500From: chm\_ramsay@emunix.emich.eduSubject: CHEMICALC:  
 Semiempirical referencesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanabe@tammy.ha  
 /C=US/@sprint.comSubject: Computer Assisted Chemistry Course Info RequestedDate: W  
 usho <rusho@nitrate.chem.utah.edu>Subject: Re: Periodic Table WidgetDate: wed, 27  
 HILE <morris@gn12.ucdavis.edu>Subject: Population Analysis in GaussianFrom: mei@ve  
 Ron Shepard)Subject: excited statesDate: Fri, 29 Jan 1993 16:47:38 -0600From: sliu  
 s.Grace@um.cc.umich.eduSubject: Gaussian and excited statesDate: Fri, 29 Jan 93 15  
 uttgart.de>Subject: Conference AnnouncementDate: 01 Feb 93 19:26:49-0500From: SBPM  
 i: (baell) <baell@syd.dah.csiro.au>Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57  
 na@leia.polaroid.com>Subject: 3D structure -> 2D drawing?From: QINGSONG@minmet.lan.  
 3 Feb 93 13:04:57Subject: software for calculating zeta potential and e  
 Date: Thu, 4 Feb 93 11:27:53 ESTFrom: Kevin Moore <kmoore@ncsc.org>Subject: MOLSOL  
 3 +0100 (NFT)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71127.1231@compuserve.com>Subject: Call for PapersDate: Fri, 5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i  
 <bobby\_clark@quickmail.clemson.edu>Subject: E-mail searchDate: 6 Feb 1993 10:08:20 -1812From: "Bobby Clark" <bobby\_clark@quickmail.clemson.edu>Subject: Memory and CPU for Starde  
 500 (EST)From: spollack@ester.mse.uc.EDU (S.K. Pollack)Subject: Phosphazene ModelingDate: Mon, 8 Feb 93 07:58:51 ESTFrom: adit@kodak.COM (Adi Treasurywala)Subject: Coordinates o  
 Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: parallel workstations and serversDate: wed, 10  
 S,From: Zhou Feng <feng@lisha.ks.uiuc.edu>Date: wed, 10 Feb 93 16:23:41 -0600Subject: parallel  
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 23 -ubuu (CSI)FROM: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: ANNOUNCING AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic  
 .mil>Subject: what about simulated annealing?Date: wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g2fFrom: "Christopher J  
 ject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrf10128@aw  
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 ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu

...: Re: Taxol: Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON\_DOUGLAS\_W@LILLY.COM>Subject: u  
: CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-based solvent accessible surfacesDate: Thu, 7 Jan 93  
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vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, 11 Jan 1993 14:33 ESTFrom: WILLIAMS%XRAY2@ulkyvxo2.loui  
or doubled messagesDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: data-flow programs for molecular modelingDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@  
GAMES and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSubject: RE:HELPPDate: Thu, 14 Jan 1993 11:18:26 -0500From: jle@world.std.com (Joe  
gov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDTFrom: CUNDARIT@MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T  
0From: dmschn@bbt.monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harbowy@chemres.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDDate: Mon, 18 Jan 9  
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S.From: Zhou F  
T-2Subject:  
/14031%hkuxa.f  
t: Re: X Wind  
ell.edu>Subject: mw fortranDate: Tue, 10 Feb 93 15:28:40 ESTFrom: kenneth mcgreevy <kgreevy@np1da1.stg.np.com>Subject: Re: X windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS  
TFrom: "w. Todd wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: wed, 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S  
thu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A whiteside)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fishe  
feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet Del Bene" <FR042008@YSUB.YSU.EDU>Subject: BSSE calculationDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ravi  
k kjemi" <bjerkese@kjemi.uio.no>Subject: Summary. Scaled freq for s and HDate: Sun, 21 Feb 1993 20:51:19 +0100 (MET)Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49:  
: Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.usc.edu (wayne sonnen)Subject: dna base chargesDate: 23 Feb 93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba  
g)Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 17:21 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: X-window terminal emulator for MacDate: Thu,  
nl.govSubject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:19:09 -0500From: feng@sgi.chem.temple.edu (Feng Chen)Subject: X-windows Server on MS-windowsDate: Thu, 2  
d.harvard.edu (jill cheney)Subject: Computer program to Evaluate wigner 3j CoefficientsDate: Fri, 26 Feb 1993 22:08:57 +0100From: ole.swang@kjemi.uio.noSubject: language questi  
semiempirical calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoch)Subject: MOPAC6.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19  
n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (EST)From: "DONALD B. BOYD" <BOYD\_DONALD\_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue  
ate.Edu (Gene Carter)Subject: Co MD parameters.Date: Tue, 2 Mar 93 17:22:53 CSTFrom: Greg Landrum <landrum@chemres.tn.cornell.edu>Subject: Re:Cache on the MacDate: Tue, 2 Mar 9  
lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (EST)From: MARYJO@northeastern.eduSubject: PDB subdir organization?From: Jan Labanowski <jkl@cc1.net>Dat  
ar 93 17:30:16 GMTDate: Sun, 7 Mar 93 12:36 ESTFrom: <SML108@PSUVM.PSU.EDU>Subject: Minimum allowable interatomic separationsFrom: sender@chemdc1.tau.ac.il (Senderowitz Hanoc  
secc.fi.cnr.itSubject: MO Theory Made VisibleDate: Tue Mar 09 11:23:12 1993Date: Tue, 9 Mar 93 10:52:25 -0500From: gallion@auriga.rose.brandeis.edu (steve gallion)Subject: GROW  
upliffDate: Thu, 11 Mar 93 18:54 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: Software for PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy.  
r 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washington.edu>Subject: PDB source file...Date: sun, 14 Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re  
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date: Mon, 15 Mar 1993 12:55 ESTFrom: HSUS@chemv2.mps.ohio-state.eduSubject: Problem with vibrational freq  
, 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtscp@hpc.ch.man.ac.uk>Subject: MM2 code for UNIX systemsDate: Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN  
ar 1993 13:58:26 -0400From: ZSHI@ac.dal.caSubject: Information about IBM RS6000Date: 17 Mar 93 16:18:00 EDTFrom: "STEPHEN R. HELLER" <srheller@asrr.arsusda.gov>Subject: Software  
st Girona seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:40:05 CETFrom: ZSYAMP01@EBCESCAL@OHSTVMA.ACS.OHIO-STATE.EDUSubject: First Congress of the ISTCP (pa  
:11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTFrom: nauss@wrair-emh1.army.milSubject: Program called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge  
23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing AMPAC 4.5Date: 21 Mar 1993 17:36:57 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Semic  
.milSubject: what about simulated annealing?Date: wed, 24 Mar 93 14:11:32 +0100From: dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner)Subject: efg in g92From: "Christopher J  
ject: 5C&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500From: au195@cleveland.freenet.edu (Dr. Gene A. Nelson)Subject: Batching files in MOPACFrom: zrf10128@w  
MO@CHEMNA.DICHI.UNINA.ITSubject: looking for ACES programFrom: Robert Laird <mbdtsr1@hpb.ch.man.ac.uk>Subject: Fe-o calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel  
uk>Subject: Polyrate queryDate: Tue, 30 Mar 1993 19:31:32 +0200From: c62@aixfile1.urz.uni-heidelberg.de (Andreas Schulz)Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
ulz)Subject: Stephen R. WilsonDate: Thu, 1 Apr 1993 16:33:29 +0200From: oles@gollum.uio.noSubject: BiosymDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu



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