

RTFM!  
Les « mailing lists » en tant que nouvelles formes de communication entre scientifiques.

Alexandre Hocquet  
Université de Lorraine & CAK

Communicating Science and Technology II:  
From the 15th century to the present

Paris/Oxford, 10 Mars 2012

# Plan

## 1. Computational chemistry?

## 2. Computational Chemistry List (CCL)?

## 3. CCL en tant que corpus?

## 4. Quelles tensions?

Re: ...  
kzfz-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: HELPDDate: 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@chemes.tn.cornell.edu>Subject: UHF calc's on diradicals/TSDDate: Mon, 18 Jan 9  
n 93 15:29:22 +0100From: oosten@rulhml.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.EDUSubject: RE: PC SURVIVY REEF...Date: wed, 20 Jan 1993 11:47:55 From: "JOHN W. SEWELL" <JWSEWELL@al.crc.uno.edu>Subject: Re: density problemDate: wed, 20 Jan 93  
ke to test a program at ...Date: wed, 20 Jan 1993 12:01:00 From: "Gerrit Klaerner" <gklaerner@chem.ucsb.edu>Subject: Re: Density problemDate: wed, 20 Jan 93 15:27:12 GMTFrom: D. M. ...  
93 15:27:12 GMTFrom: D. M. ...Date: wed, 20 Jan 1993 15:27:12 GMTFrom: D. M. ...Date: wed, 20 Jan 1993 15:27:12 GMTFrom: D. M. ...Date: wed, 20 Jan 1993 15:27:12 GMTFrom: D. M. ...  
le ...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  
From: ...Date: Sun, 24 Jan 93 15:05:30 -0500From: chm\_ramsay@emunix.emich.eduSubject: CHEMICALC:  
Subject: ...Date: Tue, 26 Jan 93 07:20:59 -0600 (CST)From: AHOLDER@VAX1.UMKC.EDUSubject: semiempirical referencesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanabe@tammy.har  
Date: Wed, 27 Jan 93 14:21:31 -0700From: JON RUSHO <rusho@nitrate.chem.utah.edu>Subject: Re: Periodic Table WidgetDate: wed, 27  
93 20:29:00 GMTFrom: ...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 15:28:39 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@mond1.ccr.c.uga.eduDate: Mon, 1 Feb 1993 12:04:28 +0100From: cfat1019@servus.rus.uni-stuttgart.deSubject: Conference AnnouncementDate: 01 Feb 93 19:26:49-0500From: SBPM  
: youlha@b...Subject: Summary: Internals & Non-bondsDate: Tue, 9 Feb 93 11:12:51 CSTFrom: (baell) baell@syd.dah.csiro.au>Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57  
un.nl Subject: Elect...Date: Tue, 9 Feb 93 11:12:51 CSTFrom: (baell) baell@syd.dah.csiro.au>Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57  
and ...Date: Tue, 9 Feb 93 13:04:57 Subject: 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 (NFT)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71127.1231@compuserve.com>Subject: Call for PapersDate: Fri,  
<bobby\_clark@quickmail.clemson.edu>Subject: E-mail searchDate: 6 Feb 1993 10:08:20 -1812From: "Bobby Clark" <bobby\_clark  
500 (EST)From: spollack@ester.mse.uc.edu (S.K. Pollack)Subject: Phosphazene ModelingDate: Mon, 8 Feb 93 07:58:51 ESTFrom  
Date: Tue, 09 Feb 1993 21:39:59 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu  
S.Fred: Zhou Feng <ng...>Date: Wed, 10 Feb 93 16:23:41 -0600Subject: parallel CHARMM?Date: wed, 10 Feb  
-25...Date: Wed, 10 Feb 93 16:23:41 -0600Subject: parallel CHARMM?Date: wed, 10 Feb  
1/4031@hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program  
t: Re: X Windows for PC ..Date: Sat, 13 Feb 93 12:21:47 +0900From: Katushi  
ell.edu>Subject: MPW Fortran?Date: Tue, 16 Feb 93 13:28:40 ESTFrom: Kennet  
TFFrom: "w. Todd wipke" <wipke@SECS.UCSC.EDU>Subject: Final Call Summer Unde  
thu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A whiteside)Subje  
feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet Del Bene" <FR042  
k Kjemi" <bjerkese@kjemi.unit.no>Subject: Summary. Scaled freq for S and H2  
: Carl JugDate: Tue, 23 Feb 93 15:08:43 PSTFrom: wsonnen@alnitak.usc.edu (J  
(g)Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 17:21 EDTFrom: <POD  
nl.gov>Subject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:1  
d.harvard.edu (jill cheney)Subject: Computer Program to Evaluate wigner 3j  
semiempirical calculations simple oxidesFrom: sender@chemdc1.tau.ac.il (Sen  
n.deSubject: Expert Know-How wanted !!Date: 02 Mar 1993 08:13:18 -0500 (ES  
ate.Edu (Gene Carter)Subject: Co MD parameters.Date: Tue, 2 Mar 93 17:22:  
lling Software: Does anyone have STELLA?Date: 04 Mar 1993 17:08:31 -0500 (E  
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 11:23:12 199  
uplingDate: Thu, 11 Mar 93 18:54 EDTFrom: <PODOSNNA%NYUACF1.BITNET@OHST  
r 1993 02:33:09 -0800 (PST)From: Thomas Nhan <tom@cassandra.chem.washingto  
MA.ACS.OHIO-STATE.EDU>Subject: partial charges for fictive atoms in G92Date  
, 15 Mar 1993 21:55:05 -0600 (CST)From: Chris Parkinson <mbdtscp@hpc.ch.mar  
ar 1993 13:58:36 -0400From: ZSHI@ac.dal.caSubject: Information about IBM Re  
st Girona seminar on Molecular SimilarityDate: Thu, 18 Mar 93 10:4  
:11 -0500Subject: Keep the noise down, pleaseDate: 19 Mar 93 11:37:00 ESTF  
23 -0600 (CST)From: Andy Holder <AHOLDER@VAX1.UMKC.EDU>Subject: Announcing  
.ml>Subject: what about simulated annealing?Date: wed, 24 Mar 93 14:11:32  
t: Subject: SC&A Conference speakers - thanksDate: Thu, 25 Mar 93 10:18:48 -0500  
MO@CHEMNA.DICHI.UNINA.ITSSubject: looking for ACES programFrom: Robert Laird <mbdtsp1@hpb.ch.man.ac.uk>Subject: Fe-O calculationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: ratarap@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: BiosynDate: 01 Apr 1993 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edu

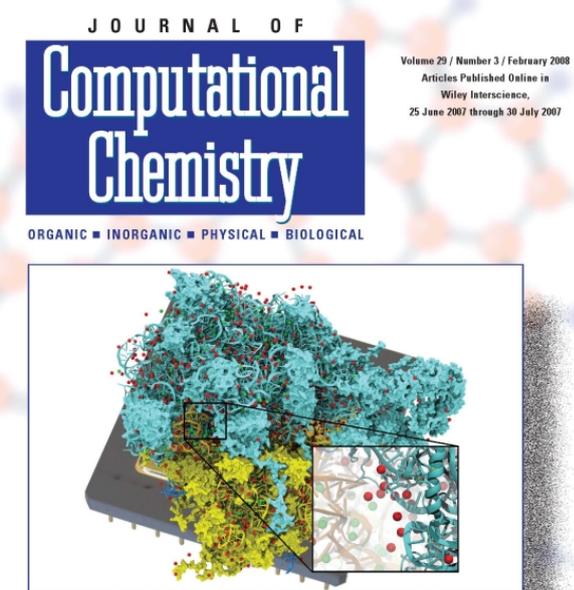
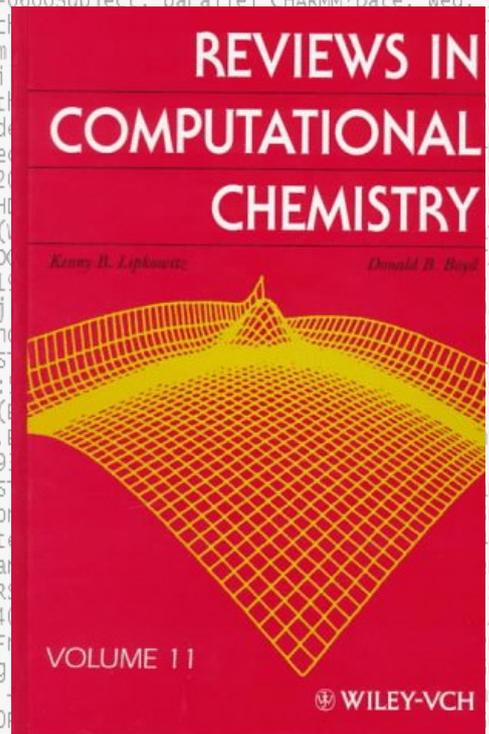
# 1.1 computational chemistry?

## 1.1.1 hardware

## 1.1.2 software

# 1.2. computational chemist?

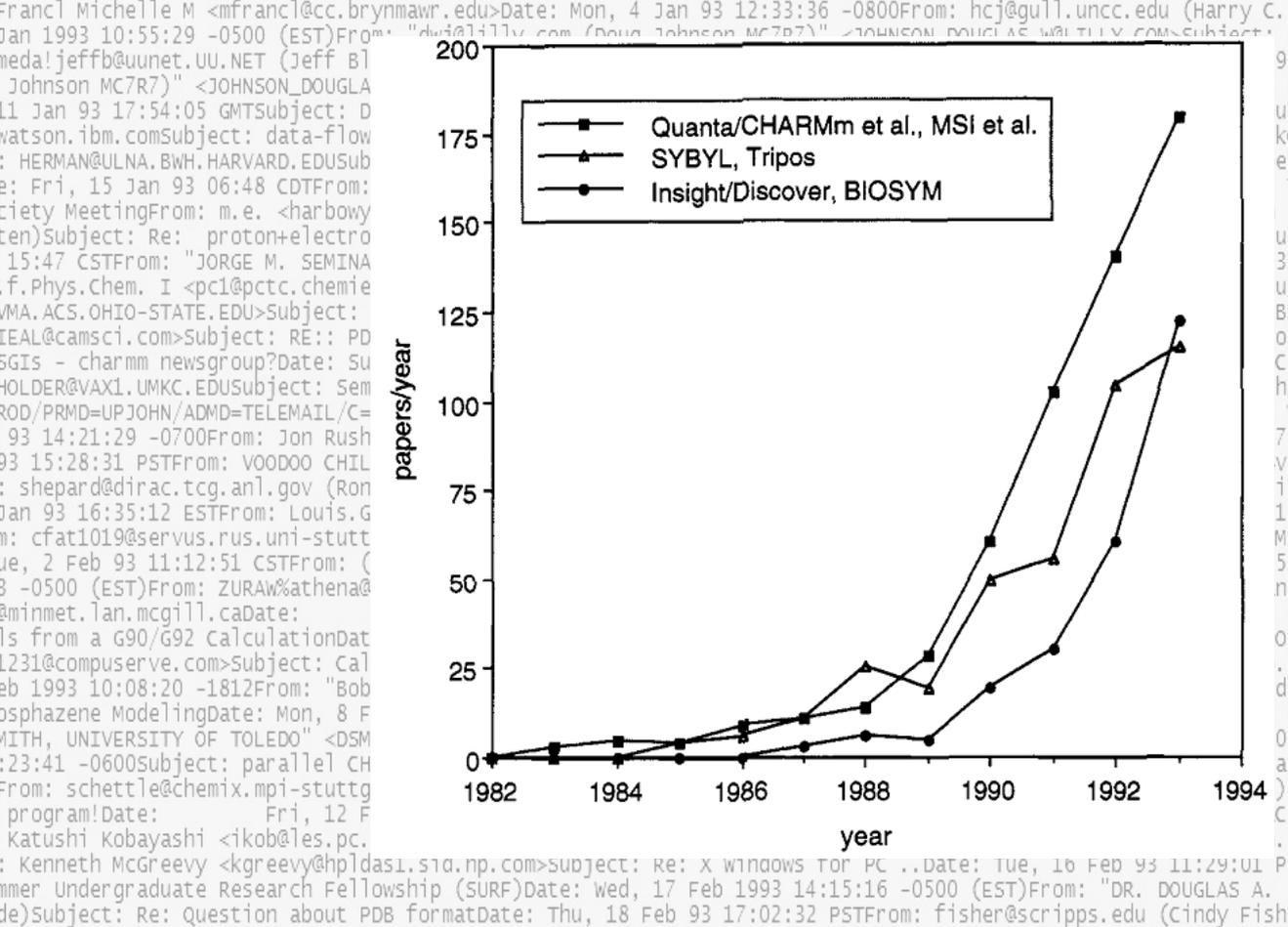
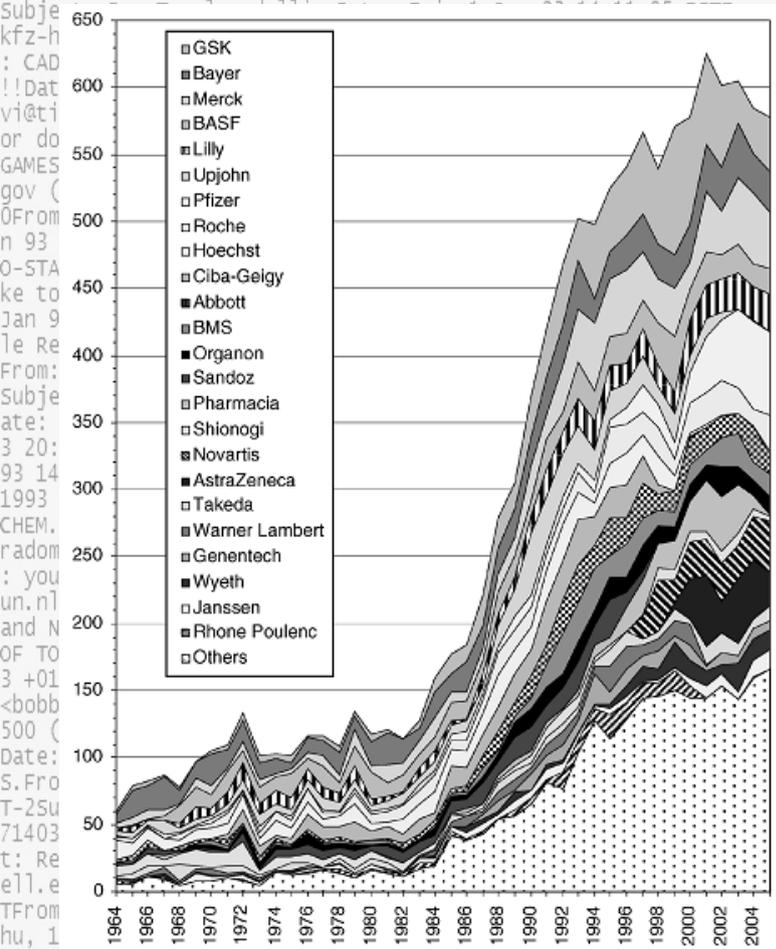
# 1.3. Qu'en dire?



EDITORS: CHARLES L. BROOKS III • GERNOT FRENKING • SHIGEYOSHI SAKAI  
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WILEY  
ISSN 0192-8651







## 1.1.2. Computational Chemistry & Software

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

### Maintenance...

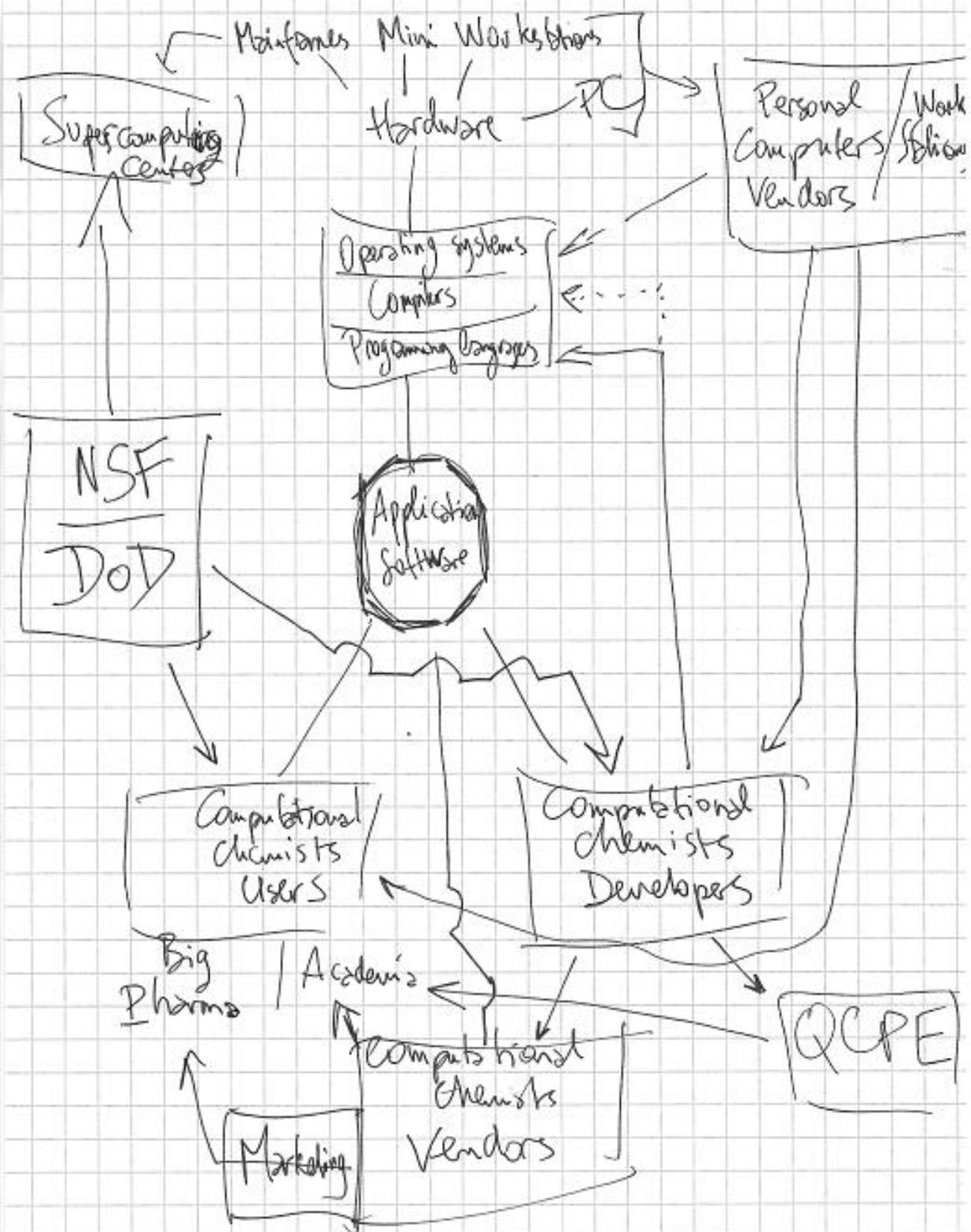
### -80s, 90s : Commercialisation du monde académique + contexte

### économique (Big Pharma + Hardware Vendors) :

### -Business models



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.unc.edu>From: [unclear] Graphics Society N  
 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 13:17:00 (CST)From: [unclear] Mathieu" <DEWINDT@FRSAC11.BITNET@OHSTVMA.AC  
 le RecurrenceDate: Fri, 22 Jan 1993 13:36:26 +0000From: BDIEAL <BDIEAL@c  
 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 +0500 (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 (NST)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71117.1231@cc  
 <bobby\_c1@kku.edu>Date: 05 Feb 93 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 93 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]>Subject: [unclear] Date: 19 Feb 93 14:49:00 ESTFrom: [unclear] and  
 : Carl JugDate: 19 Feb 93 15:18:43 PSTFrom: wsonnen@nitak.usc.edu  
 g)Subject: Re: Hydrogen bond.Date: wed, 24 Feb 93 17:21 EDTFrom: <PC  
 nl.gov>Subject: X-window terminal emulator for MacDate: Thu, 25 Feb 93 17:  
 d.harvard.edu>Subject: [unclear] Date: 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: 2 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: 9 Mar 93 11:23:12 ESTFrom: [unclear] NYUACF1.BITNET@OF  
 r 1993 02:11:23 +0000 (EST)From: [unclear] and  
 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

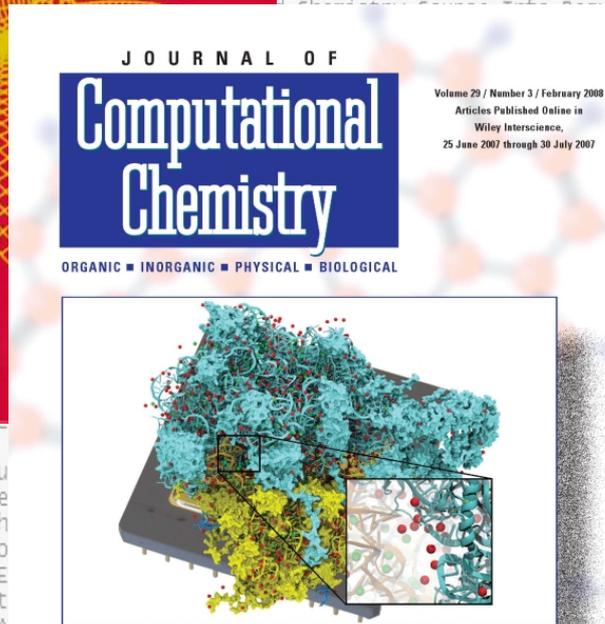
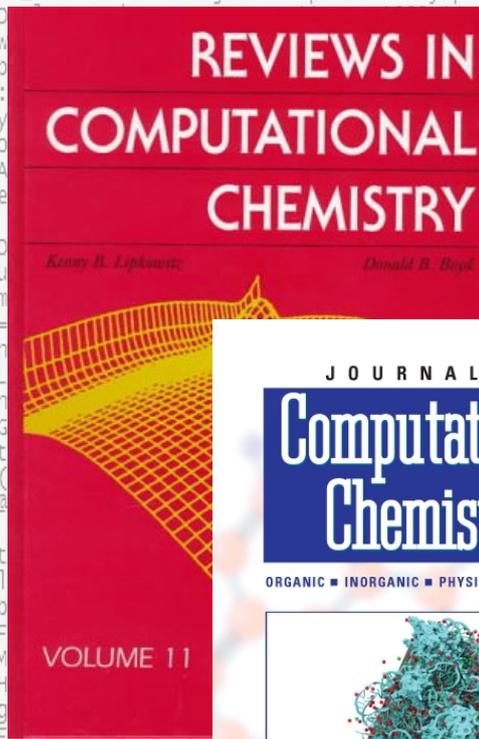


- 1.2 Computational Chemist
- Developers : écrivent le code puis le diffusent
- Users : utilisent le code
- Vendors : vendent le code
- NSF, DoD : financent des projets
- Supercomputers : allouent des ressources de calcul
- Hardware vendors + Operating systems : vendent l'infrastructure

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

- science/technologie
- formes d'innovation
- software en société
- objet technologique qui influence l'activité scientifique.

## Software as a boundary object.



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.

[Wombat Bioactivity Database:](#)



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

**CCL Home**

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

Page supported by:



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... a laboratory without walls for scientific computing

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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.

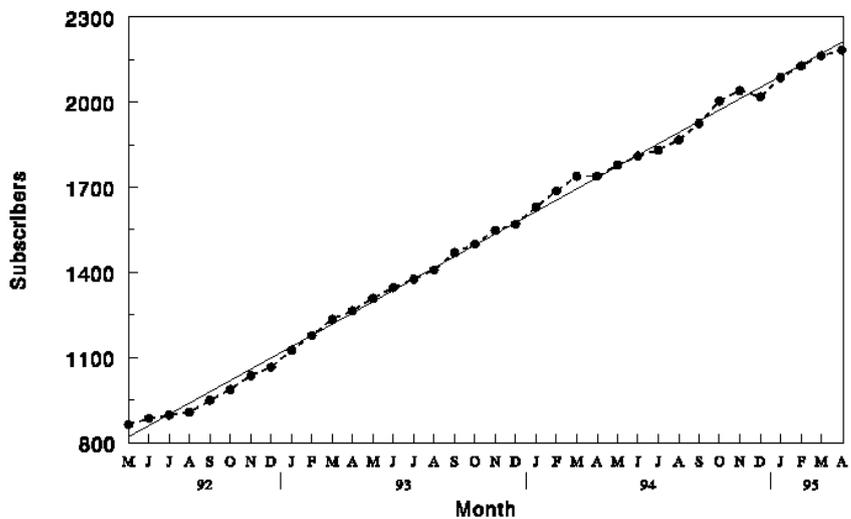
m: hcj@gull.uncc.edu (Harry C. ...  
 \DOUGLAS\_W@LILLY.COM>Subject: u  
 ble surfacesDate: Thu, 7 Jan 93  
 out PDB searching methodsDate: F  
 m: WILLIAMS%XRAY2@ulkyvx02.loui  
 an 93 13:38:09 ESTFrom: rsefeck@  
 500From: jle@world.std.com (Joe  
 E.EDUSubject: Steric strain at T  
 diradicals/TSDate: 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:  
 : 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: ...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  
 n.deSubject: ...Knows Date: 27 Mar 1993 09:18:50 ESTFrom: BOYD\_DONALD\_B@LILLY.COM (BOYD DONALD B. BOYD) <BOYD\_DONALD\_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue  
 ate.Edu (Senderowitz Hanoch)subject: MOPAC6.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19  
 eg 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@ccl.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.crc (Senderowitz Hanoch)subject: MOPAC6.0Date: Sun, 28 Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19  
 uplingDate: Thu, 11 Mar 93 16:35 ESTFrom: <PODOLSKA@LILLY.COM>Subject: ...Knows Date: 27 Mar 1993 09:18:50 ESTFrom: BOYD\_DONALD\_B@LILLY.COM (BOYD DONALD B. BOYD) <BOYD\_DONALD\_B@LILLY.COM>Subject: new book on computational chemistryDate: Tue  
 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  
 oject: 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

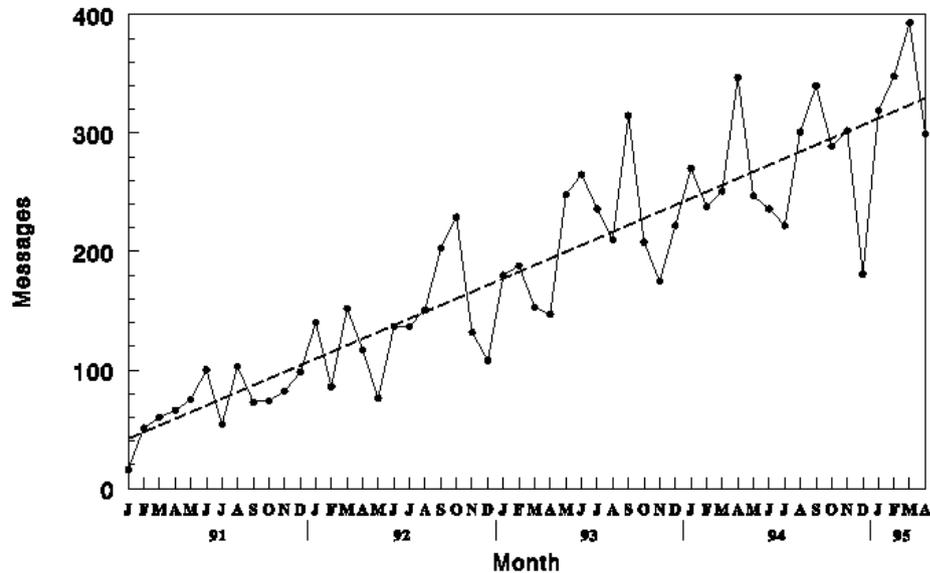
## 2.2. Computational Chemistry List (CCL)

**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 help in using software

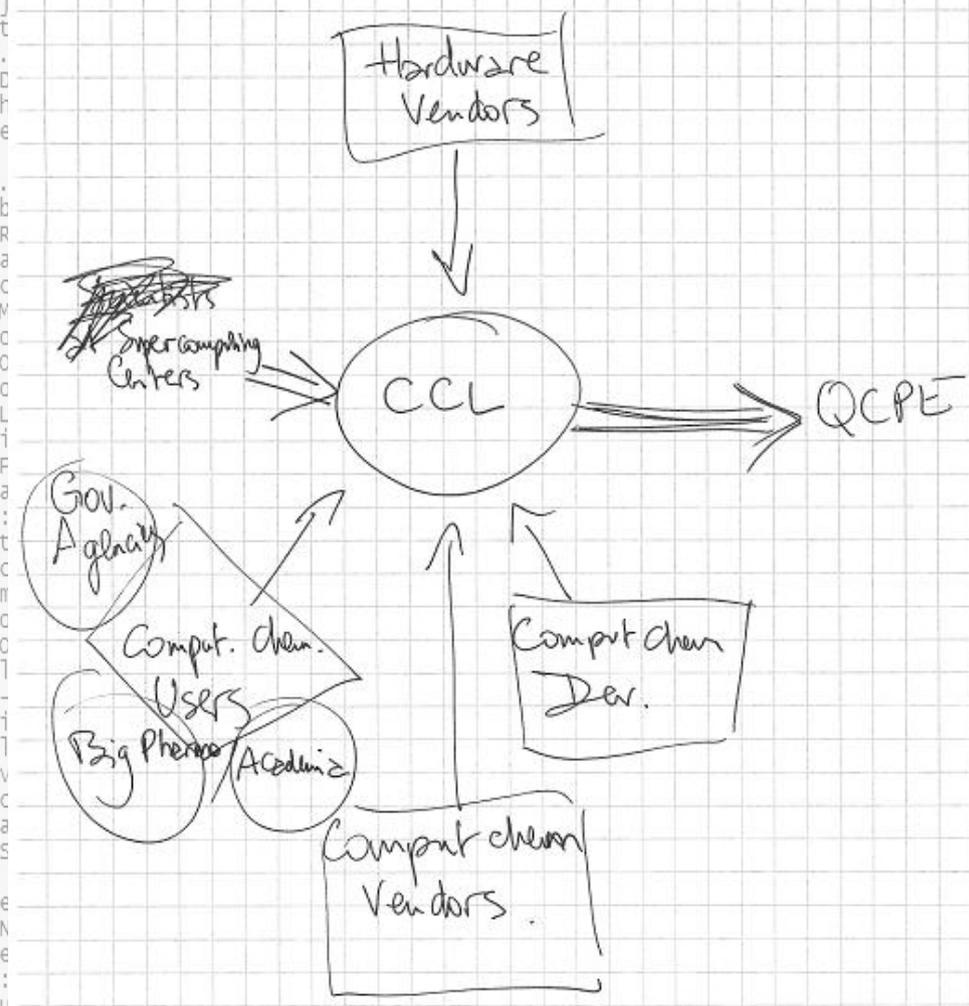
### 3.3.2 learning

### 3.3.3 religious wars, flame wars

# 3.1. Acteurs en interaction

- .edu
- .gov
- .com
- developers
- users
- vendors

Is the CCL a public sphere?



The Structural Transformation of the Public Sphere  
An Inquiry into a Category of Bourgeois Society  
Jürgen Habermas  
translated by Thomas Burger  
with the assistance of Frederick Lawrence

Re: [mailto:francj@cc.brynmawr.edu] Date: Fri, 14:11:05 EST From: francj@cc.brynmawr.edu Date: Mon, 4 Jan 93 12:33:36 -0800 From: hcj@gull.uncc.edu (Harry C. kfz-heidelberg.de) Subject: Energy contribution of hbonds? Date: 06 Jan 1993 10:55:29 -0500 From: "dwj@illy.com (Doug Johnson MC7R7)" <JOHNSON, vi@tiberius.cc.cornell.edu> From: ccuph@reading.ac.uk Date: Mon, 11 Jan 1993 17:54:05 GMT Subject: or doubled Date: 11 Jan 1993 13:36:26 +0000 From: BDIEAL <BDIEAL@cam.ac.uk> Subject: dat GAMESS and MOPAC Date: Thu, 14 Jan 1993 10:42:35 -0500 (EST) From: HERMAN@ULNA.BWH.HARVARD. gov (Ron Shepard) Subject: Re: Cartesian vs Internal coordinates Date: Fri, 15 Jan 93 06:48 CD 0 From: dmsch@monsanto.com Subject: next Molecular Graphics Software From: oosten@ruihml.LeidenUniv.nl (A.B. van Oosten) Date: 15 Jan 93 15:25:00 -0500 (EST) Subject: RE: PC Survey RESULTS Date: Wed, 20 Jan 1993 15:47 CST From: "JORGE M. ke to test a program. Date: Thu, 21 Jan 93 12:19:42 +0100 From: Inst.f.Phys.Chem. I <pci@pctc. le Recurrence Date: Fri, 22 Jan 1993 13:36:26 +0000 From: 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 test Date: 26 Jan 1993 07:20:59 -0600 (CST) From: AHOLDER@VAX1.UMKC.EDU Subjec Date: 27 Jan 93 13:32:05 From: /PN=DAVID.W.ELROD/DD.ID=SSW.DW@ELROD.COM Subject: DMD=TELEM 3 20:38:08 GMT Subject: RE: XWD->Mac conversion... Date: Wed, 27 Jan 93 14:21:29 -0700 From: Jc 93 14:47:36 -0500 From: caves@tammy.harvard.edu Date: Thu, 28 Jan 1993 15:28:31 PST From: VOODO 1993 14:23:55 +22305823 (EST) Date: Fri, 29 Jan 93 15:07:15 CST From: shepard@dirac.tcg.anl.gc CHEM.CMU.EDU Subject: RE: Gaussian and excited states Date: Fri, 29 Jan 93 16:35:12 EST From: L radomski@mond1.ccrs.uga.edu Date: Mon, 1 Feb 1993 12:04:28 +0100 From: cfat1019@servus.rus.uni : youkha@biosym.com Subject: Summary: Internals & Non-Bonds Date: Tue, 2 Feb 93 11:12:51 CST un.nl> Subject: Electronic Periodic Tables Date: 02 Feb 1993 14:36:03 -0500 (EST) From: ZURAW@a and Nanotechnologies Date: Wed, 3 Feb 93 10:46:20 MST From: QINGSONG@minmet.lan.mcgill.ca Date: OF TOLEDO" <ikob@univ.toledo.edu> Subject: RE: Orbitals from a G90/G92 Calculat 3 +0100 (NF) Date: 15 Feb 1993 11:12:12 From: E.Prof@univ.toledo.edu Subject: <bobby\_clark@quickmail.clemson.edu> Subject: E-mail search Date: 6 Feb 1993 10:08:20 -1812 From 500 (EST) From: spollack@ester.mse.uc.edu (S.K. Pollack) Subject: Phosphazene Modeling Date: Mo Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST) From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO S.From: Zhong@chem.siu.edu Date: Wed, 10 Feb 93 16:23:41 -0600 Subject: paral T-2 Subject: Re: ZINDO program Date: 11 Feb 1993 11:12:12 From: mix.mpi- 1/4031%hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STAT <ikob@univ.toledo.edu> Subject: X Windows for PC .. Date: Sat, 13 Feb 1993 11:12:12 From: ell.edu Subject: MPW Fortran? Date: Tue, 16 Feb 1993 11:12:12 From: "w. Todd wipke" <wipke@secs.ucsc.edu> Date: Thu, 18 Feb 93 14:22:08 PST From: raw@autod feld charges Date: Fri, 19 Feb 93 14:49:00 k Kjemi" <bjerkese@kjemi.unit.no> Subject: : Carl Jug Date: Tue, 23 Feb 93 15:08:43 PST g) Subject: Re: Hydrogen bond. Date: w n1.gov Subject: X-window terminal emulator d.harvard.edu (jill cheney) Subject: Compu semiempirical calculations simple oxides Fr n.de Subject: Expert Know-How wanted !! Dat ate.Edu (Gene Carter) Subject: Co MD para lling Software: Does anyone have STELLA? D ar 93 17:30:16 GMT Date: Sun, 7 Mar 93 secc.fi.cnr.it Subject: MO Theory Made Vis upling Date: Thu, 11 Mar 93 18:54 EDT r 1993 02:33:09 -0800 (PST) From: Thomas N MA.ACS.OHIO-STATE.EDU Subject: partial ch , 15 Mar 1993 21:55:05 -0600 (CST) From: C ar 1993 13:58:36 -0400 From: ZSHI@ac.dal.c st Girona seminar on Molecular Similarity :11 -0500 Subject: Keep the noise down, pl 23 -0600 (CST) From: Andy Holder <AHOLDER@ .mil Subject: what about simulated anneal ict: 5C&A Conference speakers - thanks Da MO@CHEMNA.DICHI.UNINA.IT Subject: looking uk> Subject: Polyrate query Date: Tue, 30 M ulz) Subject: Stephen R. Wilson Date: Thu, MARYJO@northwestern.edu Subject: PUB subdit organization From: Jan Labanowski <jlab@cc1.net> Dat e: Minimum allowable interatomic separations From: sender@chemd1.tau.ac.il (Senderowitz Hanoc 9 Mar 93 10:52:25 -0500 From: gallion@auriga.rose.brandeis.edu Subject: GROW. OHIO-STATE.EDU Subject: Software for PC Date: Fri, 12 Mar 93 04:51:15 GMT From: jim@quanta.phy. ect: PDB source file... Date: Sun, 14 Mar 93 11:06:13 +0100 From: doelz@comp.bioz.unibas.ch (Re 14 Mar 1993 12:55 EST From: HSUS@chemv2.mps.ohio-state.edu Subject: Problem with vibrational freq ict: MM2 code for UNIX systems Date: Tue, 16 Mar 93 11:49:33 GMT Subject: Re: MM2 code for UN 17 Mar 93 16:18:00 EDT From: "STEPHEN R. HELLER" <srheller@asr.marsusda.gov> Subject: Software om: ZSYAMP01%EBCECAL@OHSTVMA.ACS.OHIO-STATE.EDU Subject: First Congress of the ISTD (pa @wrair-emh1.army.mil Subject: Program called GRID Date: Fri, 19 Mar 93 14:33:18 EST From: Ge Date: 21 Mar 1993 17:36:57 -0600 (CST) From: Andy Holder <AHOLDER@VAX1.UMKC.EDU> Subject: Semic dufner@ws01.pc.chemie.th-darmstadt.de (Hagen Dufner) Subject: efg in g92 From: "Christopher J 5@cleveland.freenet.edu (Dr. Gene A. Nelson) Subject: Batching files in MOPAC From: zrfl0128@aw @hpb.ch.man.ac.uk Subject: Fe-0 calculation Date: Mon, 29 Mar 93 15:49:03 BST From: rafapa@obel 2.uni-heidelberg.de (Andreas Schulz) Subject: NBO analyses Date: Tue, 30 Mar 1993 16:04:42 - io.no Subject: Biosym Date: 01 Apr 1993 11:43:13 -0600 (CST) From: CUNDARIT@memstvx1.memst.edu









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.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  
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@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@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:  
d.harvard  
semiempir  
n.desubjec  
tate.Edu  
lling Soft  
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secc.fi.c  
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MA.ACS.OHI  
, 15 Mar 1  
ar 1993 1  
st Girona  
:11 -0500:  
23 -0600  
.milsubjec  
ject: SC&A  
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.edu

## 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.edu





# full disclosure of methods?

- *From:* "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <[DSMITH-AatT-uoft02.utoledo.edu](mailto:DSMITH-AatT-uoft02.utoledo.edu)>
- *Subject:* full disclosure of methods?
- *Date:* Sat, 26 Jun 1993 11:21:56 -0500 (EST)

Mark Thompson recently wrote, regarding the SAM1 topic currently under discussion:

>Let me address the more fundamental issue that this topic  
>brings forth. I share Graham Hurst's concerns. One of the  
>basic tenets of good science is that of reproducibility,  
>and independant verification.

This is, I think, universally true and accepted. However, it is rarely

# commercialization

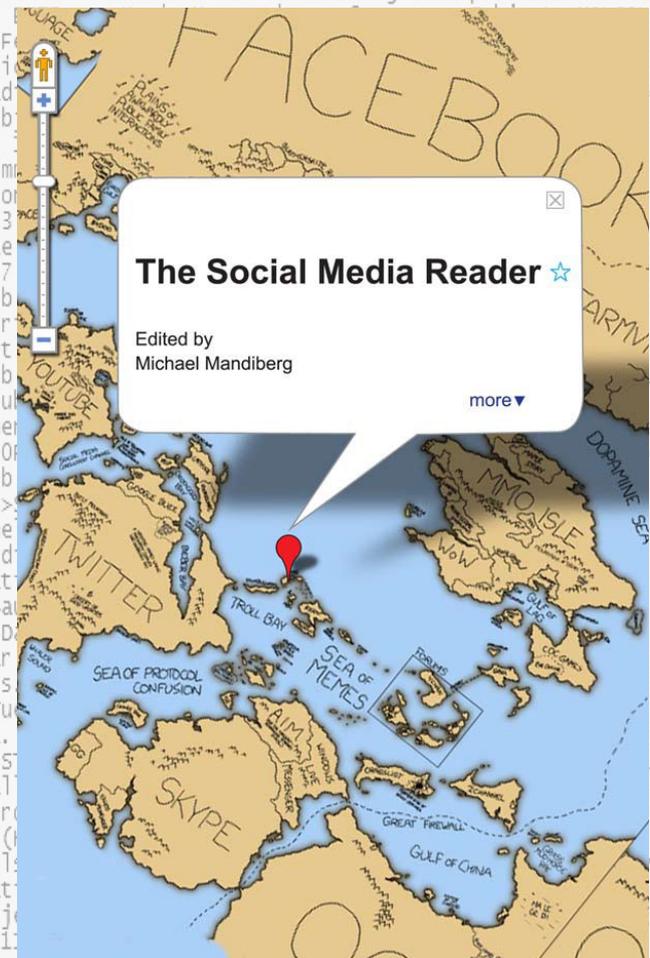
- *From:* [ross\\_AT\\_zeno.mmwb.ucsf.EDU](mailto:ross_AT_zeno.mmwb.ucsf.EDU) (Bill Ross)
- *Subject:* commercialization
- *Date:* Tue, 10 Mar 92 10:43:13 -0800

I think that codes developed under govt funding should be made available for distribution/maintenance costs. I haven't devoted much thought to the ideal legal permissions to grant. If subsequent commercialization adds value, the precommercial version should remain available on the same terms. This "nothing for anyone" policy is the closest I can imagine to fair for myriad unsung contributors as well as being the appropriate consequence of public funding (assigning credit is another side of the coin). Once a transition to commercial code has occurred, further developments transpire under known ground rules and participants can negotiate a slice of the pie. Hopefully funding agencies factor in the degree of commercialization in allocating funds.

Bill Ross

**Gabriella Coleman : Hacker  
and Troller as Trickster**

# -Religious wars (Flaming, Trolling)



Re: ...  
kfz-heidelberg.de>Subject: energy contribution of hbonds?Date: 06 Jan 1993 10:55:29 -0500 (EST)From: "dwj@lilly.com (Doug Johnson...<JOHNSON,DOUGLAS\_W@LILLY.COM>Subject: replie  
CADD videosDate: wed, 6 Jan 93 13:03:33 -0800From: chiremvl@andromeda!jeffb@uunet.UU.NET (Jeff Blaney)Subject: Re: Polygon-ba  
!!Date: 08 Jan 1993 09:19:39 -0500 (EST)From: "dwj@lilly.com (Doug Johnson MC7R7)" <JOHNSON,DOUGLAS\_W@LILLY.COM>Subject: replie  
vi@tiberius.tc.cornell.edu>From: scsupham@reading.ac.ukDate: Mon, 11 Jan 93 17:54:05 GMTSubject: DMol questionsDate: Mon, 11 Ja  
or doubled messagesDate: wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.comSubject: data-flow programs for molecular model  
GAMES and MOPACDate: Thu, 14 Jan 1993 10:42:35 -0500 (EST)From: HERMAN@ULNA.BWH.HARVARD.EDUSubject: RE:HELPPDate: Thu, 14 Ja  
gov (Ron Shepard)Subject: Re: Cartesian vs Internal coordinatesDate: Fri, 15 Jan 93 06:48 CDTFrom: CUNDARIT@MEMSTVX1.BITNET@OHS  
OFrom: dmschn@bbbit.monsanto.comSubject: next Molecular Graphics Society MeetingFrom: m.e. <harbowy@chemres.tn.cornell.edu>Subje  
n 93 15:29:22 +0100From: oosten@ruihml.LeidenUniv.nl (A.B. van Oosten)Subject: Re: proton+electron=neutron?Date: wed, 20 Jan 9  
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Jan 93 15:12:17 GMTSubject: "DEWINDT@FRSAC11.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>Subject: force constant symmetry  
le RecurrenceDate: Fri, 22 Jan 1993 13:36:26 +0000From: BDIEAL <BDIEAL@camsci.com>Subject: RE:: PDB on the MacDate: Thu, 21 Jan  
From: arne@mango.mef.ki.se (Arne Elofsson)Subject: Re: charmm and SGIs - charmm newsgroup?Date: Sun, 24 Jan 93 15:05:30 -0500Fr  
Subject: This is testDate: 26 Jan 1993 07:20:59 -0600 (CST)From: AHOLDER@VAX1.UMKC.EDUSubject: semiempirical referencesDate: Tu  
ate: 27 Jan 93 08:59:32-0500From: /PN=DAVID.W.ELROD/DD.ID=SSW.DWELROD/PRND=UPJOHN/ADMN=TELEMAIL/C=US/@sprint.comSubject: Comput  
3 20:38:08 GMTSubject: Re: XWD->Mac conversion...Date: wed, 27 Jan 93 14:21:29 -0700From: Jon Rusho <rusho@ntrate.chem.utah.edu>  
93 14:47:36 -0500From: caves@tammy.harvard.eduDate: Thu, 28 Jan 1993 15:28:31 PSTFrom: VOODOO CHILE <morris@gn12.ucdavis.edu>Su  
1993 14:23:56 GMTSubject: Re: excited statesDate: Thu, 28 Jan 1993 15:28:31 PSTFrom: VOODOO CHILE <morris@gn12.ucdavis.edu>Su  
1993 14:23:56 GMTSubject: Re: excited statesDate: Thu, 28 Jan 1993 15:28:31 PSTFrom: VOODOO CHILE <morris@gn12.ucdavis.edu>Su  
CHEM.CMU.EDUSubject: RE: Gaussian and excited statesDate: Fri, 29 Jan 93 16:55:12 ESTFrom: Louis.Grace@um.cc.umich.eduSubject: r  
radomski@ondl.ccr.c.uga.eduDate: Mon, 1 Feb 1993 12:04:28 +0100From: cfat1019@servus.rus.uni-stuttgart.deSubject: Conference Ar  
: youkha@hawaii.crc.su.seSubject: Summary: The Journals & Non-BondsDate: Tue, 2 Feb 93 11:12:51 CSEFrom: baell@syd.dah.csiro.a  
un.nl>Subject: Re: Gaussian and excited statesDate: Fri, 29 Jan 93 16:55:12 ESTFrom: Louis.Grace@um.cc.umich.eduSubject: r  
and NanotechnologiesDate: wed, 3 Feb 93 10:46:20 MSTFrom: QINGSONG@minmet.lan.mcgill.caDate: 3 Feb 93 13:04:57Subject:   
OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subject: Re: Plotting Orbitals from a G90/G92 calculationDate: Thu, 4 Feb 93 11:27:53 EST  
3 +0100 (NFT)Date: 05 Feb 93 09:28:33 ESTFrom: Elliot King <71127.1231@compuserve.com>Subject: Call for PapersDate: Fri, 5 Feb  
<bobby\_clark@quickmail.clemson.edu>Subject: E-mail searchDate: 6 Feb 1993 10:08:20 -1812From: "Bobby Clark" <bobby\_clark@quic  
500 (EST)From: spollack@ester.mse.uc.edu (S.K. Pollack)Subject: Phosphazene ModelingDate: Mon, 8 Feb 93 07:58:51 ESTFrom: adit@  
Date: Tue, 09 Feb 1993 21:39:58 -0500 (EST)From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <DSMITH@uoft02.utoledo.edu>Subjec  
S.From: zhong@uiowa.edu (Zhong Chen)Date: Wed, 10 Feb 93 15:  
2Subject: Re: Gaussian and excited statesDate: Fri, 29 Jan 93 16:55:12 ESTFrom: Louis.Grace@um.cc.umich.eduSubject: r  
/14031@hkuxa.hku.hk@OHSTVMA.ACS.OHIO-STATE.EDUSubject: MO Plotting program!Date: Fri, 12 Feb 93 09:48:41 CETFrom: Norbe  
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 Fe  
ell.edu>Subject: Re: Gaussian and excited statesDate: Fri, 29 Jan 93 16:55:12 ESTFrom: Louis.Grace@um.cc.umich.eduSubject: r  
TFFrom: "W. Todd Wipke" <wipke@secs.UCSC.EDU>Subject: Final Call Summer Undergraduate Research Fellowship (SURF)Date: wed, 17 Fe  
Thu, 18 Feb 93 14:22:08 PSTFrom: raw@autodesk.com (Robert A Whiteside)Subject: Re: Question about PDB formatDate: Thu, 18 Feb 93  
feld chargesDate: Fri, 19 Feb 93 14:49:00 ESTFrom: "Janet Del Bene" <FR042008@YSU.EDU>Subject: ESSE calculationDate: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ravi  
k kjemi" <swang@kjemi.uio.no>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.hariamp@chemie.uni-erlangen.deSubject: 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  
upliff.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 <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@asr.ususda.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  
.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 <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: CUNDARIT@memstvx1.memst.edu

STEVEN SHAPIN AND SIMON SCHAFER

# LEVIATHAN

AND THE

# AIR-PUMP

HOBBS, BOYLE, AND THE EXPERIMENTAL LIFE



## 4. Tensions

## - Controverse scientifique : utile pour

## l'historien, oblige les acteurs à se dévoiler.

## - Sociologie pragmatique des épreuves : la

## situation de crise (tensions) permet d'observer

## des changements de structure...et rend les

## acteurs bavards.

# -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,

## (voire computing science)

## 3. Ouverture du code

## -question technique, question idéologique

## 4. Commercialisation éventuelle

## -question éthique, question pratique (licensing)

## Le cas de Gaussian.

Re: Taxol: Re: Taxol: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michel M <francl@cc.jhu.edu> 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  
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  
!!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.com Subject: data-flow programs for molecular modelingDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@  
GAMES and the...Date: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@watson.ibm.com Subject: data-flow programs for molecular modelingDate: Wed, 13 Jan 93 13:38:09 ESTFrom: rsefeck@  
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  
OFrom: dmschn@bbt.monsanto.com Subject: next Molecular Graphics Society MeetingFrom: m.e. <harbowy@chemes.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.EDUSubject: 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 a program.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.f.Phys.Chem. I <pci@pcc.chemie.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.EDUSubject: force constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFFrom: "BD  
le Recurrence" <le@math.berkeley.edu> Date: Wed, 27 Jan 1993 11:46:30 PSTFrom: BDIEAL <BDIEAL@camsci.com> Subject: RE: PDB on the MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron  
From: ar@cam.ac.uk <ar@cam.ac.uk> Subject: Re: charmm and SGIs - charmm newsgroup?Date: Sun, 24 Jan 93 15:05:30 -0500From: chm\_ramsay@emunix.emich.edu Subject: CHEMICALC:  
Subject: This is testDate: 26 Jan 1993 07:20:59 -0600 (CST)From: AHOLDER@VAX1.UMKC.EDUSubject: Semiempirical referencesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanabe@tammy.ha  
ate: 27 Jan 93 08:59:32-0500From: /PN=DAVID.W.ELROD/DD.ID=SSW.DWELROD/PRMD=UPJOHN/ADM=TELEMAIL/C=US/@sprint.com Subject: Computer Assisted Chemistry Course Info RequestedDate: 27  
3 20:38:08 GMTSubject: YWP <YWP@cam.ac.uk> Date: Wed, 27 Jan 93 14:21:30 -0500From: Jan Rusho <rusho@nitrate.chem.utah.edu> Subject: Re: Periodic Table WidgetDate: wed, 27  
93 14:47:36 GMTSubject: YWP <YWP@cam.ac.uk> Date: Wed, 27 Jan 93 14:21:30 -0500From: CHILE <morris@gn12.ucdavis.edu> Subject: Population Analysis in GaussianFrom: mei@ve  
1993 14:2: <mei@vega.chem.uconn.edu> Date: Wed, 27 Jan 1993 14:21:30 -0500From: CHILE <morris@gn12.ucdavis.edu> Subject: Population Analysis in GaussianFrom: mei@ve  
ted statesDate: Fri, 29 Jan 1993 16:47:38 -0600From: sliu  
bje: Gaussian and excited statesDate: Fri, 29 Jan 93 15  
ence AnnouncementDate: 01 Feb 93 19:26:49-0500From: SBPM  
csiro.au>Subject: DMF dielectricDate: Mon, 1 Feb 93 17:57  
ct: 3D structure -> 2D drawing?From: QINGSONG@minmet.lan  
bje: software for calculating zeta potential and e  
:53 ESTFrom: Kevin Moore <kmoore@ncsc.org> Subject: MOLSOL  
5 Feb 1993 16:17:32 +0100From: ivan@gandalf.ciam.unibo.i  
quickmail.clemson.edu> Subject: Memory and CPU for Starde  
: adit@kodak.COM (Adi Treasurywala) Subject: Coordinates o  
>Subject: parallel workstations and serversDate: Wed, 10  
>93 15:46:43 -0800From: rickl@biosym.com Subject: DIBUG ad  
>summeryFrom: theresa@si.fi.ameslab.gov (Theresa Windus)S  
>: Norbert Mueller <K360171%EDVZ.UNI-Linz.AC.%@OHSTVMA.ACS  
>: 13 Feb 1993 14:47:09 +0100 (WET)From: PREINERT@biolan.u  
>: Re: X Windows for PC ..Date: Tue, 16 Feb 93 11:29:01 PS  
>: 17 Feb 1993 14:15:16 -0500 (EST)From: "DR. DOUGLAS A. S  
>: Feb 93 17:02:32 PSTFrom: fisher@scripps.edu (Cindy Fishe  
>: Fri, 19 Feb 93 11:53:05 -0500From: G. Ravishanker <ravi  
>: Subject: Long Time-scale DynamicsDate: Mon, 22 Feb 93 16:49:  
>: Feb 93 15:38:36-2300From: "Alexandre MICU P16A" <alex@ba  
>U>Subject: X-window terminal emulator for MacDate: Thu,  
>: (Chen)Subject: X-windows Server on MS-windowsDate: Thu, 7  
>: 0100From: ole.swang@kjemi.uio.no Subject: language questi  
>: Feb 93 13:44:41 GMT-2:00Date: Mon, 1 Mar 1993 15:25:19  
>COM>Subject: new book on computational chemistryDate: Tue  
>: ornell.edu>Subject: Re:Cache on the MacDate: Tue, 2 Mar 9  
>: subdir organization?From: Jan Labanowski <jkl@cc1.net>Dat  
>: arationsFrom: sender@chemdcl.tau.ac.il (Senderowitz Hanoc  
>: on@auriga.rose.brandeis.edu (steve gallion)Subject: GROW  
>: PCDate: Fri, 12 Mar 93 04:51:15 GMTFrom: jim@quanta.phy.  
>: Mar 93 11:06:13 +0100From: doelz@comp.bioz.unibas.ch (Re  
>: .mps.ohio-state.edu Subject: Problem with vibrational freq  
>: : Tue, 16 Mar 93 11:49:33 GMTSubject: Re: MM2 code for UN  
>: N R. HELLER" <srheller@asrr.ususda.gov> Subject: Software  
>: IO-STATE.EDUSubject: First Congress of the ISTCP (pa  
>: called GRIDDate: Fri, 19 Mar 93 14:33:18 ESTFrom: Ge  
>: T)From: Andy Holder <AHOLDER@VAX1.UMKC.EDUSubject: Semic  
>: de (Hagen Dufner)Subject: efg in g92From: "Christopher J  
>: Nelson)Subject: Batching files in MOPACFrom: zrf10128@aw  
>: ulationDate: Mon, 29 Mar 93 15:49:03 BSTFrom: rafapa@obel  
>: Subject: NBO analysesDate: Tue, 30 Mar 1993 16:04:42 -  
>: 93 11:43:13 -0600 (CST)From: CUNDARIT@memstvx1.memst.edus

# Tensions : flame war du 25 juin 1993.

## 1. Reproductibilité

## - question éthique, question pratique

# full disclosure of methods?

- From: "DR. DOUGLAS A. SMITH, UNIVERSITY OF TOLEDO" <[DSMITH-A@quickmail.clemson.edu](mailto:DSMITH-A@quickmail.clemson.edu)>
- Subject: full disclosure of methods?
- Date: Sat, 26 Jun 1993 11:21:56 -0500 (EST)

Mark Thompson recently wrote, regarding the SAM1 topic currently under discussion:

>Let me address the more fundamental issue that this topic  
>brings forth. I share Graham Hurst's concerns. One of the  
>basic tenets of good science is that of reproducibility,  
>and independant verification.

This is, I think, universally true and accepted. However, it is rarely followed. For example, there has been talk over the years that people who use molecular mechanics for their research should publish the parameters used for each study as part of the paper (or at least they should publish the differences between their parameters and the "standard" parameters in the set used, e.g. MM2, AMBER, etc.). I think that this issue was raised in a paper by Peter Kollman a few years ago. This is a particular problem when people use MM2, which has been parameterized by many, many people in addition to Lou Allinger for special situations and molecules. Another place this occurs is in programs such as MacroModel, where parameters of all types and qualities are available through user set switches. Similarly, in other commercial codes such as Hyperchem (with which I have experience) many parameters other than the "standard" Allinger MM2 parameters exist.

## Tensions : flame war du 25 juin 1993.

## 2. Publication : reconnaissance du code

## Problème de la propriété intellectuelle

## Re: full disclosure of methods?

- **From:** [st-amant { \\*at \\* } cgl.ucsf.edu](mailto:st-amant@at.cgl.ucsf.edu) (Alain St-Amant)
- **Subject:** Re: full disclosure of methods?
- **Date:** Sat, 26 Jun 93 12:21:56 -0700

Douglas Smith recently wrote in the current discussion on the disclosure of parameters:

> Besides, who ever said we had to reveal all our secrets and make them  
> readily available and accessible? When software copyrights and patents  
> really provide adequate protection, maybe I will agree with that attitude.  
I'll assume that Dr. Smith is referring to the specific algorithms that are implemented that make the program more efficient but do not affect the final results. In which case, I might agree.

Of course, I couldn't disagree more if he is referring to some development in the methodology that actually affects the final results in any way. The point that interests me however, is the question of software copyrights and patents to which Dr. Smith alludes. I have been trying to get a feel for what can be copyrighted and patented and I get a different answer from everyone. Can only specific code be copyrighted or can the structure and algorithms be copyrighted as well? How 'modified' should code be before it can be called legally (and ethically if anyone is interested in expressing an opinion) a new program? Or is it simply forbidden for code to "evolve" into a new program?

I will summarize to the net any e-mail sent to me, but I think that this would make for an interesting discussion and it would be as interesting to hear how

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

From: Taxol modellingDate: Fri, 1 Jan 93 14:11:05 ESTFrom: Francl Michelle M <mfran1@cc.brynmawr.edu>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@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 the...Date: Fri, 15 Jan 93 06:48 CDTFrom: CUNDARIT@MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDUSubject: Steric strain at T  
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@chemes.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.EDUSubject: 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 a program.Date: Thu, 21 Jan 93 12:19:42 +0100From: Inst.fv.Phys.Chem. I <pci@pctc.chemie.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.EDUSubject: force constant symmetry and Gaussian90Date: 22 Jan 93 13:06:32 UTFFrom: "BD  
le Recur...Date: Fri, 22 Jan 1993 13:30:26 +0000From: BDIEAL <BDIEAL@camsci.com>Subject: RE: PDB on the MacDate: Thu, 21 Jan 93 17:31:46 -0500From: system@alchemy.chem.utoron  
From: ar...Date: Sun, 24 Jan 1993 15:05:30 -0500From: chm\_ramsay@emunix.emich.eduSubject: CHEMICALC:  
Subject: This is testDate: 26 Jan 1993 07:20:59 -0600 (CST)From: AHOLDER@VAX1.UMKC.EDUSubject: semiempirical referencesDate: Tue, 26 Jan 93 12:57:08 -0500From: watanabe@tammy.ha  
ate: 27 Jan 93 08:59:32-0500From: /PN=DAVID.W.ELROD/DD.ID=SSW.DWELROD/PRMD=UPJOHN/ADMD=TELEMAIL/C=US/@sprint.comSubject: Computer Assisted Chemistry Course Info RequestedDate: 27  
3 20:38:08 GMTSubject: YWB>Re: compsci...Date: Wed, 27 Jan 93 11:21:29 -0700From: Bibo\_rusho@nitrate.chem.utah.eduSubject: Re: Periodic Table WidgetDate: wed, 27  
93 14:47:36 GMTFrom: ...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  
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  
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## - Tensions : flame war du 25 juin 1993.

## 3. Ouverture du code

## - question technique, question idéologique

# SAM1 and AM1 references

- From: [ADAMO # - at - # CHEMNA.DICHI.UNINA.IT](mailto:ADAMO#-at-#CHEMNA.DICHI.UNINA.IT)
- Subject: SAM1 and AM1 references
- Date: Mon, 28 Jun 1993 16:27:52 +0100 (CET)

Dear netters,

we want add some comments on the debats entitled "SAM1 reference".

1. It is about 1 year that AMPAC realese 4.0 with SAM1 parametrization is commercially available. This means about 1 year before any clafiricatory (?) paper appeared.
2. Contrary to MOPAC and earlier version of AMAPC (up to 2.1), AMPAC version 4.x is in a "black box" format. That is, only executable files are available to the user. So no check is possible on the parametrization.
3. It seems to us, that the policy of prof. Holder is (and perhaps will be) to distribute only binary code of the program. In this connection we had an e-mail talk with prof. Holder that we add (see below).

Moreover, we should like to know your opinion on the actual trend in commercializing computational packages without source code. Does this trend encourage the development of science? And also: up to what limit a computational package can be considered as a product of a single research group?

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.

# Diversités d'acteurs, diversités de stratégies scientifiques (vendre, partager...), de stratégies économiques (code source, licenses, copyright,...), évolution au cours du temps...

## - Kelty : Free software

### 1. part of a movement

### 2. sharing source code

### 3. concerns about definition of openness

### 4. concerns about licensing

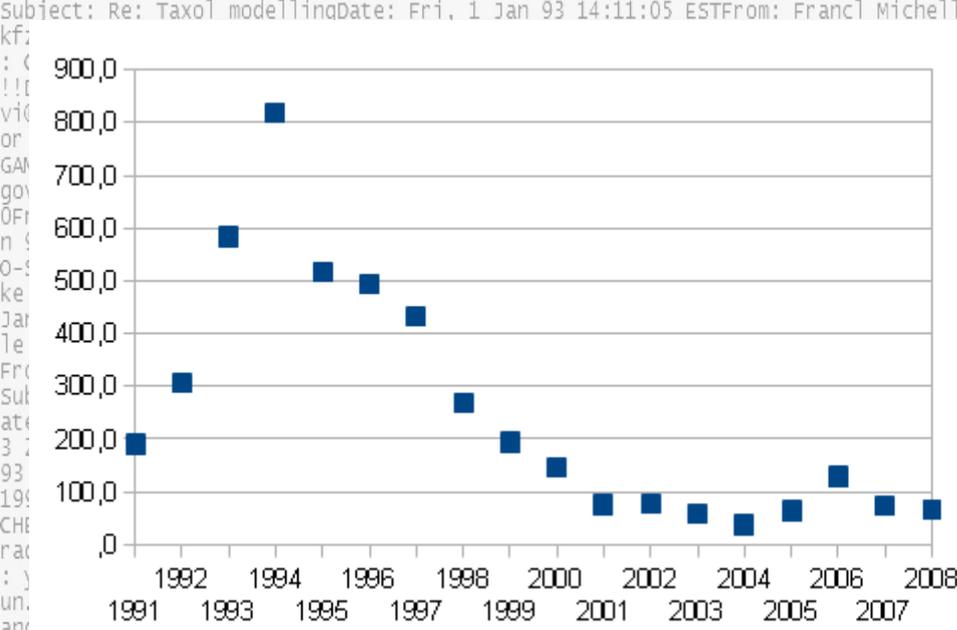
### 5. cooperation

# Free Software, à la marge du monde académique.

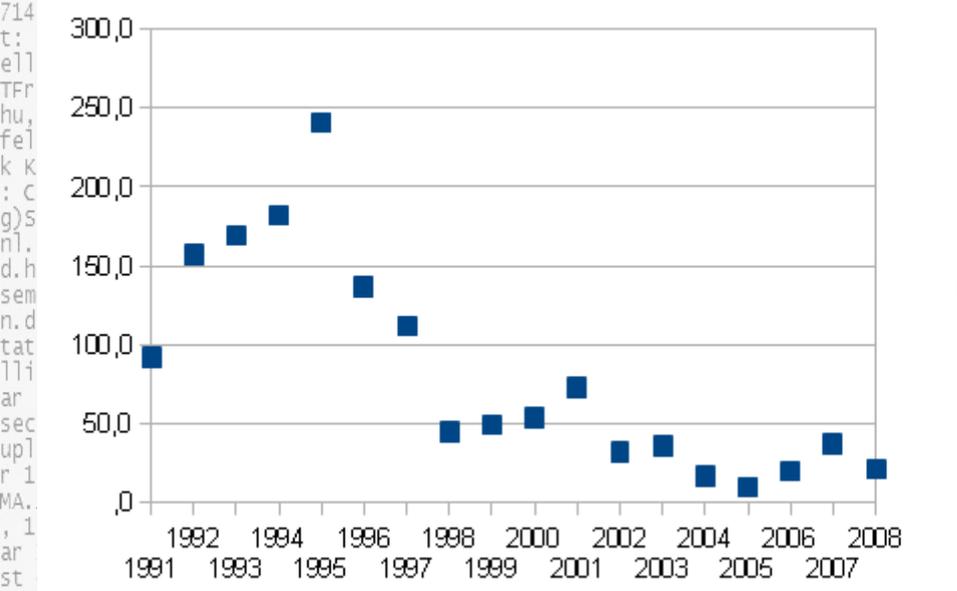


THE CULTURAL SIGNIFICANCE OF FREE SOFTWARE





■ 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  
 M@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.edus

...: Re: Taxol... Date: Fri, 1 Jan 1993 14:11:05 EST... From: Francl Michelle M <mfranl@cc.brynmawr.edu>... Subject: u...  
...: CADD videos... Date: wed, 6 Jan 93 13:03:33 -0800... From: chiremvl@andromeda!jeffb@uunet.UU.NET (Jeff Blaney)... Subject: Re: Polygon-based solvent accessible surfaces... Date: 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 methods... Date: F...  
...: vi@tiberius.tc.cornell.edu>... From: scsupham@reading.ac.uk... Date: Mon, 11 Jan 93 17:54:05 GMT... Subject: DMol questions... Date: Mon, 11 Jan 1993 14:33 EST... From: WILLIAMS%XRAY2@ulkyvxo2.loui...  
...: or doubled messages... Date: wed, 13 Jan 93 13:38:09 EST... From: rsefeck@watson.ibm.com... Subject: data-flow programs for molecular modeling... Date: wed, 13 Jan 93 13:38:09 EST... From: rsefeck@...  
...: GAMESS and MOPAC... Date: Thu, 14 Jan 1993 10:42:35 -0500 (EST)... From: HERMAN@ULNA.BWH.HARVARD.EDU... Subject: RE:HELPP... Date: Thu, 14 Jan 1993 11:18:26 -0500... From: jle@world.std.com (Joe...  
...: gov (Ron Shepard)... Subject: Re: Cartesian vs Internal coordinates... Date: Fri, 15 Jan 93 06:48 CDT... From: CUNDARIT@MEMSTVX1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU... Subject: Steric strain at T...  
...: 0From: dmschn@bbt.monsanto.com... Subject: next Molecular Graphics Society Meeting... From: m.e. <harbowy@chemres.tn.cornell.edu>... Subject: UHF calc's on diradicals/TSD... Date: Mon, 18 Jan 9...  
...: n 93 15:29:22...  
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...: CHEM.CMU.EDU...  
...: radomski@mond...  
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...: T-2... Subject: ...  
...: /14031%hkuxa...  
...: t: Re: X Wind...  
...: ell.edu>... Subject: ...  
...: 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 PST... From: raw@autodesk.com (Robert A whiteside)... Subject: Re: Question about PDB format... Date: Thu, 18 Feb 93 17:02:32 PST... From: fisher@scripps.edu (Cindy Fishe...  
...: feld charges... Date: Fri, 19 Feb 93 14:49:00 EST... From: "Janet Del Bene" <FR042008@YSUB.YSU.EDU>... Subject: BSSE calculation... Date: Fri, 19 Feb 93 11:53:05 -0500... From: 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 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: Re: Hydrogen bond... Date: wed, 24 Feb 93 17:21 EDT... From: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>... Subject: X-window terminal emulator for Mac... Date: Thu...  
...: nl.gov... Subject: X-window terminal emulator for Mac... Date: Thu, 25 Feb 93 17:19:09 -0500... From: feng@sgi.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 Hanoch)... Subject: MOPAC6.0... Date: Sun, 28 Feb 93 13:44:41 GMT-2:00... Date: Mon, 1 Mar 1993 15:25:19...  
...: n.de... 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 chemistry... Date: Tue...  
...: 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@PSUVM.PSU.EDU>... Subject: Minimum allowable interatomic separations... From: sender@chemdc1.tau.ac.il (Senderowitz Hanoc...  
...: scc.fdnr.it... Subject: MO Theory Made Visible... Date: Tue Mar 09 11:23:12 1993... Date: Tue, 9 Mar 93 10:52:25 -0500... From: gallion@auriga.rose.brandeis.edu (steve gallion)... Subject: GROW...  
...: upling.fdnr. Thu, 11 Mar 93 18:54 EDT... From: <PODOSNNA%NYUACF1.BITNET@OHSTVMA.ACS.OHIO-STATE.EDU>... Subject: Software for PCDate: 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 13:58:26 -0400... From: ZSHI@ac.dal.ca... Subject: Information about IBM RS6000... Date: 17 Mar 93 16:18:00 EDT... From: "STEPHEN R. HELLER" <srheller@asrr.arsusda.gov>... Subject: Software...  
...: st Girona seminar on Molecular Similarity... Date: Thu, 18 Mar 93 10:40:05 CET... From: ZSYAMP01@EBCESCAL@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...  
...: Subject: 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.ITS... Subject: looking for ACES program... From: Robert Laird <mbdtsrl@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: CUNDARIT@memstvx1.memst.edu

